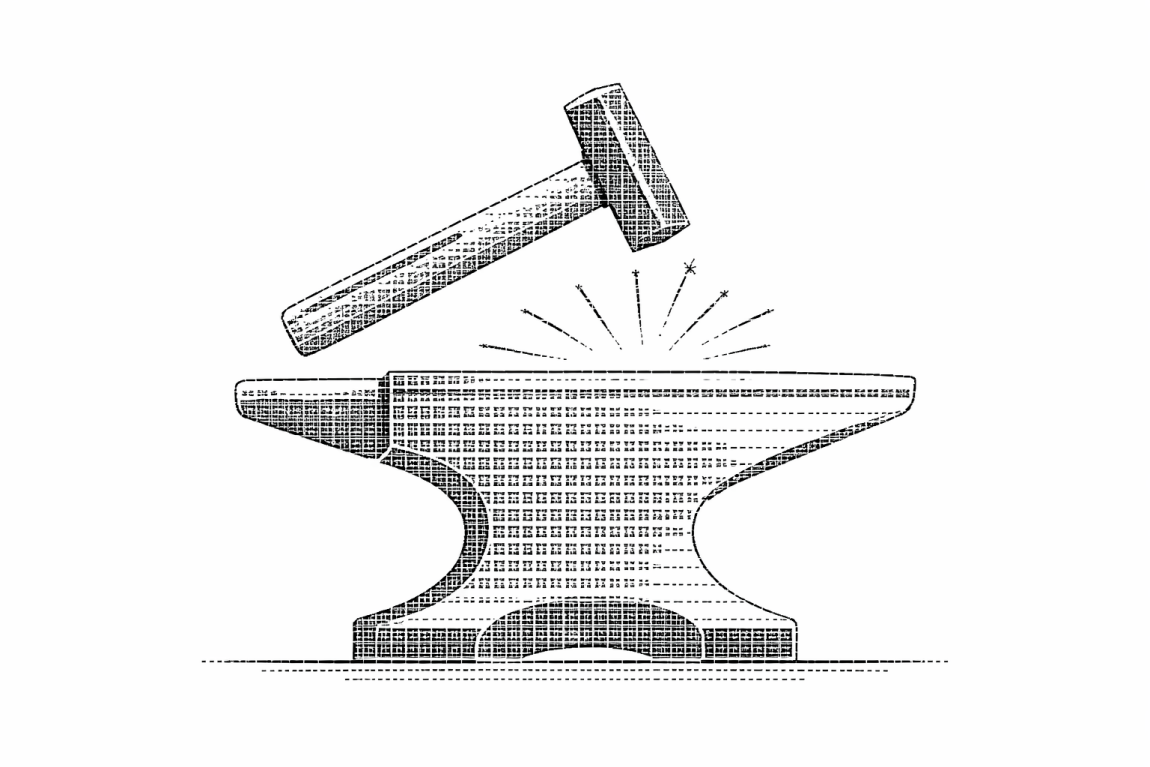
Crystals, Green-Functions, Thermal Quantum Field Theory and Applications in Quasi-Equilibrium Materials Science



by

Sebastian Kalhöfer

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James Gleick about Isaac Newton in [20]:

> "*Newton formed his argument in classic greek geometrical style. Axioms, Lemmas, Corollaries, QED. As the best model available for perfection in knowledge, it gave his physical program the stamp of certainty. He proved facts about triangles and tangents, chords and parallelograms and from there, by a long chain of arguments, proved facts about the moon and the tides.*"

David Hilbert in a lecture[1] given at the International Congress of Mathematicians in Paris 1900 [25]:

> *"Zudem ist es ein Irrtum zu glauben, dass die Strenge in der Beweisführung die Feindin der Einfachheit wäre."*

Galileo Galilei (not verbatim translated) in [11]:

> *The book of nature is written in the language of mathematics.*

Lucius Annaeus Seneca in his Hercules Furens, see also [50]:

> *"Non est ad astra mollis e terris via."*

If you find any mistakes, please contact[2] me so that I can correct them.

[1] The explicit sentence can be found on page 257.

[2] `sebastian.kalhoefer@gmail.com`

This still needs to be done or digitalized or double-checked

Legend:

- colorless = Not important for the doctoral thesis.
- |———————| = Important for the doctoral thesis but very (too?) difficult / tedious to do cleanly.
- Proofs that were generated by AI (Claude Opus 5.5 with /effort xhigh) and need to be checked.

References (used in the text but not yet in the bibliography):

- **Nolting, statistical physics volume**, p. 73, 74, 88 f., 106–113, 151, 157: Chapter 9.
- **"Nolting 2"**, p. 277: Subsection 29.1.1.
- **Fließbach**, Statistische Physik, Eq. (6.20): Theorem 9.20.
- **Tong**, lecture notes on statistical physics, below Eq. (1.11): Lemma 9.54.
- **"Some book, page 314"** (Ehrenfest classification of phase transitions): Section 9.5.
- **Further reading list** (Callen; Texier, Roux; Diu, Guthmann, Lederer, Roulet; Jancovici; Landau, Lifschitz; Huang; Barrat, Hansen): end of Subsection 9.8.3.
- **Schwabl, volume unclear** ([47] or [48]?), p. 24, 25, 35, 46: Section 29.8; p. 186: Appendix, Section on the specific heat in the Sommerfeld-approximation.
- **Zirnbauer, lecture notes unclear**, p. 67, 68: Theorem 7.48; **Zirnbauer, SS 2020, Sheet 6, Exercise 3 a)**: Appendix, Proofs for Part II.
- **Gross, AQM 2013**, Sheet 5, Exercise 1 a), c): Lemma 7.42.
- **Mariño, QFT lecture notes**, p. 46 f. ([33] are his path-integral notes): Section 29.8, Section 30.2.
- **GW01**: Section 29.8.
- **Henk**, p. 145, 275: Section 29.8, Corollary 30.8.
- **Bulla**, lecture notes: Theorem 29.63, Section 30.2.
- **Rickayzen**, p. 209: Section 30.2.
- **Cuevas**, p. 233: Chapter 12 (phononic displacement Green-functions).
- **Ashcroft, Mermin**: Chapter "Crystals" (quote).
- **Demtröder**, Experimentalphysik 3: figures in Chapter "Crystals" and in the appendix.
- **"Supermathematics"**, p. 64, Eq. (3.31): Chapter 16, Appendix, Proofs for Part V.
- **Wilson**, Graph Theory, and **arXiv:1301.6918**: Theorem 38.25.
- **Polyak**, notes on Feynman diagrams, Eq. (18): Chapter 38.
- **Metsch 2020**, Exercise Sheet 5: Section 30.2.
- **von Neumann**, Mathematical Foundations of Quantum Mechanics: Chapter 3 (separability of $L^2(\mathbb{R})$).
- **GPAW documentation** (electron-phonon coupling, URL): Chapter 40.
- **Giustino**, derivation of the electron-phonon coupling (maybe [19]?): Section 5.2.

- **Internal notes** (not citable): Draft Summary, Waste-Folders 1, 3, 6, Pinboard, PP3, "06 Superhydrides / Success of Eliashberg", Lab-Sheet, own notes 02 and 03.

Chapter 3:

- Filling in the missing reference ("as in TBD") in Remark 3.19.1. *[Ref.: none given]*
- Updating the proof of Corollary 3.13 (appendix) such that the details are fine, and adding the one- and two-dimensional cases. *[Ref.: the weblink in the proof; Waste-Folder 1; [85] in Waste-Folder 3]*

Chapter 5:

- section 5.2: the derivation of the electron-phonon-coupling, as in Felicianos article. *[Ref.: Feliciano Giustino; cf. Waste-Folder 6, topic 10]*

Chapter 6: The derivation of the Bloch-Theorem and the reference to Slater-determinants solving the non-interacting problem. *[Ref.: none given]*

Chapter 7:

- Proof of Corollary 7.33. *[Ref.: none given]*
- Proof of Corollary 7.37. *[Ref.: none given]*
- Looking up what a derivation is in mathematics and adding a remark on that, as in Remark 7.37.1. *[Ref.: none given]*
- Proof of Corollary 7.41. *[Ref.: none given]*
- Proof of Lemma 7.42 (only needs to be digitalized). *[Ref.: Gross, AQM2013, Sheet 5, Exercise 1 a), c)]*
- Looking up what a derivation is in mathematics and adding a remark on that in Corollary 7.45. *[Ref.: none given]*
- Elaborating on Definition 7.47. *[Ref.: none given]*
- Proof of Corollary 7.49. *[Ref.: clean derivation of the Landauer-formula; Zirnbauer p. 67, 68]*
- Filling in the "TBD" at Equation 7.34. *[Ref.: none given]*
- Proof of Theorem 7.23 (continuing it). *[Ref.: none given]*
- Proof of Corollary 7.26 (with computation rules of determinants / permanents). *[Ref.: none given]*
- Proof of Corollary 7.29 (including the definition of the hermitian adjoint). *[Ref.: none given]*
- Proof of Lemma 7.31. *[Ref.: none given]*
- Proof of Theorem 7.34 (orthonormality). *[Ref.: none given]*
- Proof of Lemma 7.38. *[Ref.: none given]*
- Proof of Lemma 7.39. *[Ref.: none given]*
- Proof of Lemma 7.46. *[Ref.: none given]*
- Updating Theorem 7.48 and its proof for n-body operators ("one step needs to be filled"). *[Ref.: clean derivation of the Landauer-formula; Zirnbauer p. 67, 68]*

Chapter 8:

- Updating Definition 8.14 (is important for Eliashberg-theory from the Operator-formalism) *[Ref.: none given]*
- Proof of Lemma 8.38 (only needs to be digitalized). *[Ref.: [19]; Waste-Folder 1, Topic 6]*
- Proving the identity $[c(\tau)]^\dagger = c^\dagger(-\tau)$, etc. (is important for Eliashberg-theory from the Operator-formalism) *[Ref.: none given]*
- Updating Definition 8.13 (inside the same "To Be Updated" block). *[Ref.: none given]*
- Clarifying "XXZ-Model + Jordan-Wigner-Transformation (???)" in Notation 8.1. *[Ref.: none given]*
- Updating the proofs of 8.10 and 8.25 w.r.t. the ensemble Hamiltonian. *[Ref.: none given]*
- Elaborating the proof of Equation 8.27 with the BCH-series. *[Ref.: [32, Eq. (3.44), (3.67)]; [62, Sheet 10, Exercise 1b)]]*
- Filling in the missing Lemma reference (basis change) after Lemma 8.28. *[Ref.: none given]*
- Filling in the missing reference for the "GW-system" near Equation 8.36. *[Ref.: none given]*
- Filling in the "TBD" in Definition 8.41. *[Ref.: none given]*

Chapter 9:

- Proof of Lemma 9.6. *[Ref.: Nolting p. 106 f.]*
- Proof of Theorem 9.7. *[Ref.: Nolting p. 108]*
- Proof of Theorem 9.10. *[Ref.: Nolting p. 109]*
- Elaborating on Remark 9.11.1. *[Ref.: Nolting p. 151]*
- Proof of Corollary 9.17. *[Ref.: Nolting p. 113]*
- Definition 9.19 (Thermal equilibrium of two systems). *[Ref.: none given]*
- Proof of Theorem 9.20. *[Ref.: Fließbach, Eq. (6.20)]*
- Elaborating on Hypothesis 9.25. *[Ref.: none given]*
- Proof of Theorem 9.27. *[Ref.: none given]*
- Proof of Theorem 9.29. *[Ref.: own notes 03, p. 28]*
- Introduction to the grand canonical ensemble in section 9.5. *[Ref.: Nolting p. 157 (minimality of the grand canonical potential)]*
- Proof of the equivalence of ensembles in section 9.6. *[Ref.: Nolting p. 74; Nolting p. 88 f. (partly)]*
- Elaborating on Legendre-transformations in thermodynamics in section 9.7. *[Ref.: [47] (?, your own note: "Was it Schwabl . . . ?)]*
- Elaborating on the transition from microcanonical to canonical ensemble in section 9.8.2. *[Ref.: none given]*
- Proof of Lemma 9.54. *[Ref.: [47] (first two identities), Nolting p. 73 (third); Tong lecture notes, below Eq. (1.11)]*
- Elaborating on Theorem 9.60. *[Ref.: own notes 03, p. 41, 42; 02, p. 129; 03, p. 22]*
- Elaborating on the transition from canonical to grand canonical ensemble in section 9.8.3. *[Ref.: none given]*

- Filling in the missing references (density matrix definition, stationary von Neumann equation) in Corollary 9.17 and Theorem 9.27. *[Ref.: none given]*
- Ehrenfest classification of phase transitions in section 9.5. *[Ref.: "some book, page 314"]*
- Proof of the third identity in Lemma 9.65. *[Ref.: none given]*

Chapter 10:

- Thermodynamic relations for mixed-systems as in Remark 10.7.3. *[Ref.: none given]*

Chapter 12:

- Elaborating the proof of 12.3 (cyclicity of the trace and BCH-formula). *[Ref.: none given]*
- Filling in the missing Definition / Lemma references (statistical commutator, Heisenberg equation of motion) in the proof of Lemma 12.6. *[Ref.: none given]*

Chapter 13:

- Filling in the missing Lemma references and the equation-of-motion technique for hybridized systems in the proof of Theorem 13.7. *[Ref.: [17, p. 25]]*

Chapter 16:

- Going through the proof of Lemma 16.33. *[Ref.: none given]*
- Proof of the trace-log-identity in Corollary 16.19; *[Ref.: [4] Ch. 3.2 (bosons), Ch. 4.1 (fermions); [63]]*
- Elaborating on Remark 16.33.2. *[Ref.: none given]*
- Updating section 16.2. *[Ref.: [60]]*
- Implementing and Updating Section **??** from my Master-thesis *[Ref.: [27]]*
- Updating the proofs in subsections 16.1.7 and 16.1.8. *[Ref.: none given]*
- Filling in the missing reference (symmetries of the effective action) at Equation 16.60. *[Ref.: none given]*
- Finishing Lemma 16.51 and adding the literature reference. *[Ref.: none given]*

Chapter "More Algebraic Concepts in Quantum Field Theory" (no label):

- Fixing the order of logic at Equation 17.2. *[Ref.: none given]*
- Non-hermitian case at Equation 17.6. *[Ref.: none given]*
- Revising the HST proofs in the appendix (page 593 ff.) for the new prefactor convention of the functional derivative. *[Ref.: none given]*

Chapter 21:

- Calculating the polarization in Theorem 21.4. *[Ref.: none given]*

Chapter 18:

- Just fixing the things from my master-thesis and then referencing the Thomale-paper for the rest of the details. *[Ref.: [27], [43]]*

- Implementing the implications of the symmetries in section 18.1.2 (only needs to be copied from the Thomale-paper). *[Ref.: [27], [43]]*

Chapter 20:

- Elaborating on Theorem 20.26. *[Ref.: none given]*
- Elaborating on subsection 20.2.3. *[Ref.: none given]*
- Adding the value in Remark 20.14.1. *[Ref.: none given]*
- Figuring out which identity I was referring to in Remark 20.14.3. *[Ref.: none given]*
- Proofs for the coherent states in Equation 20.4 (only need to be digitalized). *[Ref.: [38, p. 29]; [4, p. 163 (fermions), p. 159 (bosons)]]*
- Proof of Lemma 20.6 (only needs to be digitalized). *[Ref.: [38, p. 30] or [4, p. 181] (fermions); [38, p. 21] or [4, p. 159] (bosons)]*
- Proof of Theorem 20.7. *[Ref.: none given]*
- Proof of Lemma 20.11 (only needs to be digitalized). *[Ref.: [38, p. 24 f.]]*
- Proof of Lemma 20.12 (only needs to be digitalized). *[Ref.: none given]*
- Finite set of Matsubara-frequencies in the proof related to Equation 20.19. *[Ref.: none given]*
- Lemma 20.24. *[Ref.: none given]*

Chapter 22:

- Checking if the details are really compatible with the definition of the Green-functions introduced earlier. *[Ref.: none given]*
- Adding references to earlier identities (?). *[Ref.: none given]*

Chapter 23:

- Stating Corollary 23.20 in general ("should hold IN GENERAL") and proving it. *[Ref.: none given]*

Chapter 24:

- Adding the equations also in the interacting case. *[Ref.: [31] (for the plot)]*
- Fact 24.10. *[Ref.: none given]*
- The "TBD"s around the phononic free energy, Equation 24.21. *[Ref.: none given]*
- Theorem 24.15 (only needs to be digitalized) and updating its proof, since one of the terms does not necessarily vanish. *[Ref.: Pinboard, Topic 17; Waste-Folder 1, topic 18; [32, Sec. 3.6.1]]*

Chapter 25:

- Proof of Corollary 25.13 (TBD and missing reference). *[Ref.: none given]*
- Proof of Corollary 25.15 (to be continued). *[Ref.: none given]*
- Interaction contribution in Equation 25.20 (only needs to be digitalized) and the corresponding Theorem. *[Ref.: PP3]*

- Bethe-Salpeter reference and going beyond the approximation in the proofs of Theorems 25.11 and 25.10. *[Ref.: Waste-Folder 1]*

Chapter 26:

- Cleaning the whole thing up. *[Ref.: none given]*
- Doing the calculation for the equation of motion for the last Green-function. *[Ref.: none given]*
- The "TBD"s in the Gorkov equations of motion, Equations 26.25 – 26.28 (possibly the same as the previous item). *[Ref.: none given]*
- Missing Lemma / Corollary references in Theorem 26.25 and its preparations, and "term II (still?)" in its proof. *[Ref.: none given]*
- Double-checking everything from Equation 26.143 to Lemma 26.51 (is ϕ real?; N_F; incorrect unit in Equation 26.153). *[Ref.: none given]*
- Proof of Theorem 26.50: fixing the momentum indices and writing down the Pauli-matrix identities. *[Ref.: none given]*
- Proof of Lemma 26.51. *[Ref.: 06 Superhydrides Success of Eliashberg]*
- "Derivative of the temperature" at Equation 26.170. *[Ref.: none given]*

Chapter "Material Analysis with Quantum Espresso & …" (no label):

- The "TBD" at Equation 27.1. *[Ref.: none given]*
- Continuing after Figure 27.4. *[Ref.: none given]*
- Space groups for V3, H2S, YH6 and LaH10. *[Ref.: none given]*

Appendix:

- Section 30.2 and the free electron gas: Fermi-energy and DOS as a function of density, Sommerfeld-approximation, band-structure and reduced zone-scheme. *[Ref.: none given]*
- Notation conflict and missing references in Corollary 30.8 and its proof. *[Ref.: Henk p. 275]*
- Proofs of Lemma 30.18, Theorem 30.30 (including the coefficients TBD_1, TBD_2) and Corollary 30.22. *[Ref.: none given]*
- Missing Lemma references in the proof on page 388. *[Ref.: none given]*
- Second quantization in the operator formalism, subsection 29.1.1 ff.: overlaps of quasi-occupation-number-states, basis change etc. *[Ref.: [38, p. 10, 14, 15, 17, 18, 19, 22]; [4, p. 44]; Nolting 2 p. 277; [48, p. 1 ff.]]*
- Theorem 29.63 (formulating cleanly and digitalizing), Equations 29.92 and 29.94. *[Ref.: Bulla script]*
- Section 29.6, Theorem 29.80 (missing references, elaboration) and Corollary 29.83. *[Ref.: none given]*
- Section 29.8. *[Ref.: [38, Problem 1.6 and p. 18]; Schwabl p. 24, 25, 35; [48, Eq. (2.1.6)]; GW01; [6]; Mariño QFT-notes p. 46 f.]*
- Missing references and "TBD"s in the section on the trinity of electronic basis sets (before section 29.11). *[Ref.: none given]*
- Redoing the proof on page 646 with graph theory. *[Ref.: [46]]*

- Adding pictures to the proof on page 640. *[Ref.: none given]*
- Experimental chapter on the internal energy with the Bethe-Salpeter-equation: missing references and the interacting contribution. *[Ref.: none given]*

Chapter 38: Getting a clean setup of Feynman-diagrams in condensed matter theory and drawing their pictures. *[Ref.: none given]*

- Drawing the pre-graph examples in Definition 38.1. *[Ref.: none given]*
- Re-creating the pictures for Corollary 38.7 and Definition 38.35 as tikzpictures. *[Ref.: none given]*
- The "TBD"s in Theorem 38.30 and after Definition 38.35. *[Ref.: none given]*
- Implementing the potential sign-factor in Equation 38.92. *[Ref.: none given]*

Chapter 41:

- Theorem 41.1. *[Ref.: none given]*
- Continuing after Equation 41.15. *[Ref.: none given]*

Chapter "Experimental: My Road to Reality …" (no label):

- Fixing the inconsistent notation in the figure after Equation 44.7. *[Ref.: none given]*

Part I.

Fundamentals on Quantum Mechanics and Crystals

Motivation and Overview

After this part of the notes you will understand ...

- what donuts in Figure 1 have to do with materials theory,
- how and why one determines the band-structure of a crystal, and how and why it is usually represented by pictures like in Figure 2,

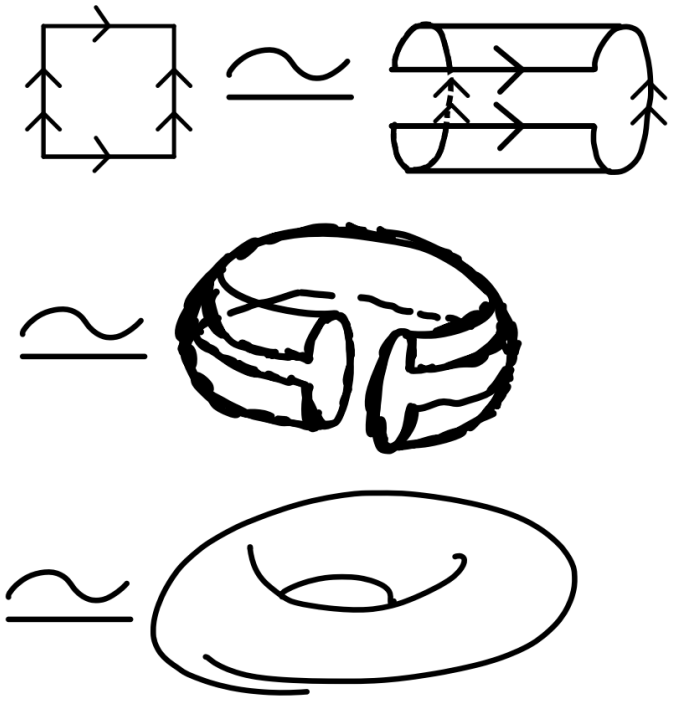


Figure 1.: Identifying the boundaries of a square yields a torus („donut“). One also says that the two objects are „homeomorphic“ to each other.

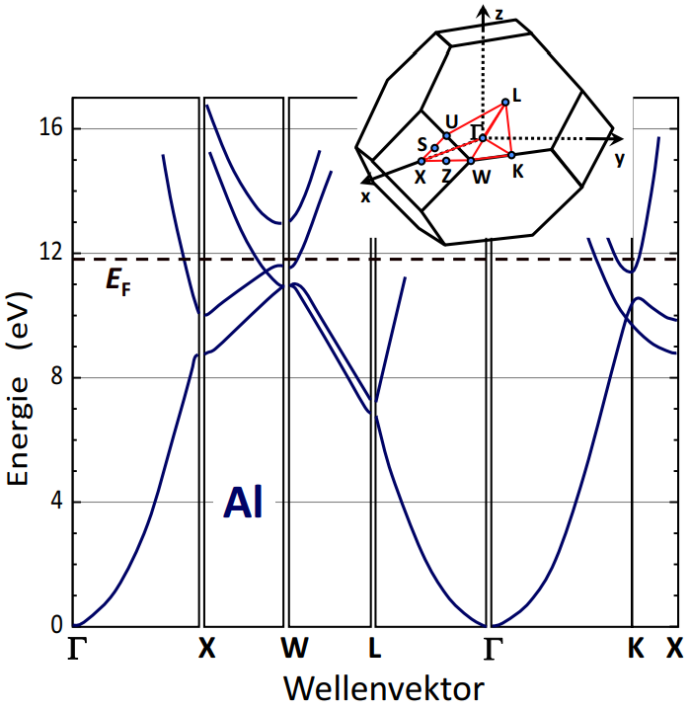


Figure 2.: The Band-Structure of Aluminium along the high-symmetry **k**-points. Taken from [GM].

1. Fourier-Expansions

Fact 1.1 The Fourier-transformation exists in all kinds of shapes and colours. One can expand

- finite sequences of numbers in the complex plane [1]
- periodic functions on a finite interval $(0, L)$[2],
- antiperiodic functions on a finite interval $(0, \hbar\beta)$ leading to the so-called Matsubara-frequencies[3].
- sufficiently fast decaying functions[4] on $\mathbb{R}$,

Here we will get to know the different versions that are most important for materials theory.

Remark 1.1.1 We wish to warn the reader, that in various different situations various *different* standard-conventions have established throughout the scientific literature. This makes it particular difficult for newcomers. For example the Forier-transformed dynamical matrices have a different prefactor conventions than the fourier-transformed ionic elongations although both of them are just discrete Fourier-transformations on the underlying lattice [9].

1.1. Fourier for a Discrete Function on a Finite Set of Points

Definition 1.2 For a sequence of N (complex or real-valued) numbers $\left\{\xi_1, \ldots, \xi_N\right\} \subset \mathbb{C}^{d_{\mathrm{x}}}$, one introduces their *discrete Fourier-transformated sequence* as another sequence of numbers $\left\{\hat{\xi}_1, \ldots, \hat{\xi}_N\right\} \subset \mathbb{C}^{d_{\mathrm{x}}}$ as

$$\hat{\xi}_j = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \xi_n \, \mathrm{e}^{+\mathrm{i}2\pi \frac{n}{N} j} \tag{1.1}$$

Remark 1.2.1 There are many prefactor-conventions in this definition, which can be quite annoying when one looks at literature, and the corresponding authors don't state which one they used. The sign in the exponent could have been chosen the other way around in Equations (1.1) and (1.2). The sign-convention chosen above refers usually to j representing a „space-like"-coordinate, whereas the other sign-convention refers to „time-like"-coordinates. The prefactor $\frac{1}{\sqrt{N}}$ in Equation (1.1) can also be exchanged for 1, or $\frac{1}{N}$, or sometimes $\frac{1}{\sqrt{Na}} \equiv 1/\sqrt{L}$ or $\frac{1}{Na} \equiv 1/L$ with corresponding changes in the Equation (1.2) accordingly, whereas a represents a so-called "lattice constant" (will be introduced later). If one chooses the last prefactor convention, one also sometimes encounters

[1] Cf. Definition 1.2
[2] Cf. Theorem 1.7
[3] Cf. Lemma 1.11
[4] Notice that these functions coincide at $x = \pm\infty$, such that they are "periodic to zero at infinity", which is the main idea behind the derivation of the underlying formulae. Cf. also Notation 1.17.

integral notations, although one is strictly speaking working with discrete variables. This trend is particularly present in thermal quantum field theory (cf. Equation (20.19) in Chapter 20), when one introduces Graßmann-variables in integral notation for their temporal argument, although they actually refer to discrete variables. Notice further that one of the prefactor-conventions here corresponds to the usual Fourier-transformation for periodic functions (with slightly changed notation).

Remark 1.2.2 As we will see below, one introduces the same notation for position-*operators* of ions that are centered around a crystal-site. Consequently, one finds Fourier-transforms of operators and the inverse transformations.

Lemma 1.3 The inverse transformation reads

$$\xi_j = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \hat{\xi}_n \, \mathrm{e}^{-\mathrm{i}2\pi \frac{n}{N} j} \tag{1.2}$$

Proof 1.3 See Appendix, Proofs, page 491.

1.2. Fourier for a Continuous, Periodic Function on a Finite Interval

This section briefly lists basic terms and concepts that are mostly assumed to be known to clarify the notation.

Notation 1.4 We consider the set of periodic, square-integrable functions on (a, b) as

$$L^2_{\mathrm{per}}(a,b) = \left\{ f : (a,b) \longrightarrow \mathbb{C} \quad \middle| \quad f(a) = f(b) \right\} \tag{1.3}$$

Lemma 1.5 The set $L^2_{\mathrm{per}}(a, b)$ is, equipped with point-wise addition and scalar-multiplication a complex vector space.

Proof 1.5 One easily verifies the different properties.

Lemma 1.6 The mapping

$$\begin{aligned} \langle \, , \, \rangle : L^2_{\mathrm{per}}(a,b) \times L^2_{\mathrm{per}}(a,b) &\longrightarrow \mathbb{C} \\ (f,g) &\mapsto \langle f, g \rangle \equiv \langle f | g \rangle \end{aligned} \tag{1.4}$$

with

$$\langle f, g\rangle := \int_a^b \overline{f(x)} g(x)\, dx.$$

defines a hermitian scalar-product on $L^2_{\text{per}}(a, b)$.

Proof 1.6 See Kaul, Fischer, Band 2.

Theorem 1.7 For $f \in L^2_{\text{per}}(a, b)$ one finds the *Fourier-expansion* in terms of complex exponentials as

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{\pm i \frac{2\pi n x}{b-a}}, \tag{1.5}$$

where the Fourier coefficients c_n are given by

$$c_n = \frac{1}{b-a} \int_a^b f(x) e^{\mp i \frac{2\pi n x}{b-a}}\, dx. \tag{1.6}$$

which converges in the L^2-sense[5].

Proof 1.7 A proof, that periodic functions can be expanded in this way, is given in the literature[6].

Remark 1.7.1 The sign is convention; In analogy to electromagnetic waves one usually agrees to use the one sign-convention "$\pm \equiv +$" if ξ represents a space-like-argument, and the other sign-convention "$\pm \equiv -$" if it is a time-like-argument. Notice that just as in the discrete case, one oftentimes shifts around prefactors into / out of the Fourier-coefficients.

Remark 1.7.2 One immediately finds for the functions defined on a three-torus (i.e. periodic in three arguments[7]) similar expansions.

Notation 1.8 For $f \in L^2_{\text{per}}([a, b])$ we denote its periodic standard-continuation on $\mathbb{R}$ with the same symbol for notational simplicity.

Fact 1.9 The plane-waves provide a basis for $L^2_{\text{per}}([a, b])$. Together with the scalar-product, this turns the space into a Hilbert-space.

[5] This means that

$$\lim_{N\to\infty} \int_a^b \left| f(x) - \sum_{n=-N}^{N} c_n e^{\pm i \frac{2\pi n x}{b-a}} \right|^2 dx = 0. \tag{1.7}$$

[6] In the book [14], one finds the expansion and the identities for the coefficients for periodic functions that are defined on the interval $[0, 2\pi]$. So one will not circumvent a little bit of effort with the substitution rule, in order to reproduce the results above.

[7] Notice that wave-functions in a crystal (after applying of Born-von-Karman-boundary-conditions fall into this category.

1.3. Fourier for a Continuous, Statistical Function on a Finite Interval

Notation 1.10 For reasons, that are difficult to motivate several chapters in advance, we consider functions

$$\mathscr{G}_\zeta \in L^2_{\mathrm{per}}(-\hbar\beta, +\hbar\beta) \tag{1.8}$$

with time-like argument

$$\begin{aligned} \mathscr{G}_\zeta : (-\hbar\beta, +\hbar\beta) &\longrightarrow \mathbb{C} \\ \tau &\longmapsto \mathscr{G}_\zeta(\tau) \end{aligned}$$

and which carry a *statistical index* $\zeta \in \{-1, +1\}$ such that the *statistics-condition* is fulfilled

$$\forall \tau \in (-\hbar\beta, 0) : \quad \mathscr{G}_\zeta(\tau + \hbar\beta) = \zeta \mathscr{G}_\zeta(\tau). \tag{1.9}$$

Remark 1.10.1 We call a function that obeys this condition to be *ζ-periodic.*

Remark 1.10.2 The statistical index ζ represents *bosonic* ($\zeta = +1$) and *fermionic* ($\zeta = -1$) functions.

Remark 1.10.3 Denoting it's analytic standard-continuation on $\mathbb{R}$ with the same symbol, we obtain the property

$$\forall \tau \in \mathbb{R} : \quad \mathscr{G}_\zeta(\tau + \hbar\beta) = \zeta \mathscr{G}_\zeta(\tau). \tag{1.10}$$

Lemma 1.11 By a Fourier-expansion one finds the expansion for the periodic standard-continuation as

$$\mathscr{G}_\zeta(\tau) = \frac{1}{\hbar\beta} \sum_{\omega_n \in \Omega_\zeta} \mathscr{G}_\zeta(\mathrm{i}\omega_n)\, \mathrm{e}^{-\mathrm{i}\omega_n \tau} \tag{1.11}$$

with coefficients

$$\mathscr{G}_\zeta(\mathrm{i}\omega_n) = \int_0^{\hbar\beta} \mathrm{d}\tau\, \mathscr{G}_\zeta(\tau)\, \mathrm{e}^{\mathrm{i}\omega_n \tau}. \tag{1.12}$$

and *Matsubara-frequencies* that depend on the statistics

$$\Omega_\zeta = \frac{2\mathbb{Z} + 1 - \theta(\zeta)}{\hbar\beta}\pi. \tag{1.13}$$

Proof 1.11 See Appendix, Proofs, page 491.

Corollary 1.12 For future reference we note the identity

$$\forall \omega_m \in \Omega_{+1} \,:\, \int_0^{\hbar\beta} \mathrm{d}\tau \, \mathrm{e}^{\mathrm{i}\tau\omega_m} = \delta_{\omega_m,0}\hbar\beta \tag{1.14}$$

Proof 1.12 See Appendix, Proofs, page 493.

Remark 1.12.1 Notice that the difference of two fermionic Matsubara-frequencies is again a bosonic Matsubara-frequency.

For reasons that are difficult to motivate several chapters in advance, we introduce the following Lemma.

Lemma 1.13 For a Matsubara-frequency $\omega_n \in \Omega_{\mathrm{S}_{X,X'}}$ with $\mathrm{S}_{X,X'} \in \{-1,+1\}$ it holds

$$\frac{1}{\hbar}\int_0^{\hbar\beta} \mathrm{d}\tau \, \mathrm{e}^{\mathrm{i}\omega_n\tau}\mathrm{e}^{\tau(\xi_n-\xi_m)/\hbar} = \frac{1}{\hbar}\frac{\mathrm{S}_{X,X'}\,\mathrm{e}^{\beta(\xi_n-\xi_m)}-1}{\mathrm{i}\omega_n+\left(\xi_n-\xi_m\right)/\hbar} \tag{1.15}$$

Proof 1.13 With the definition of the Matsubara-frequencies in Equation (1.13), we remark the trivial identity

$$\mathrm{e}^{\mathrm{i}\hbar\omega_n\beta} = \mathrm{S}_{X,X'} \tag{1.16}$$

and then we compute straightforwardly

$$\begin{aligned}
\frac{1}{\hbar}\int_0^{\hbar\beta} \mathrm{d}\tau \, \mathrm{e}^{\mathrm{i}\omega_n\tau}\mathrm{e}^{\tau(\xi_n-\xi_m)/\hbar} &= \frac{1}{\hbar}\int_0^{\hbar\beta} \mathrm{d}\tau \, \mathrm{e}^{\tau\left[\mathrm{i}\omega_n+(\xi_n-\xi_m)/\hbar\right]} \\
&= \frac{1}{\hbar}\frac{1}{\mathrm{i}\omega_n+\left(\xi_n-\xi_m\right)/\hbar}\left[\mathrm{e}^{\tau\left[\mathrm{i}\omega_n+(\xi_n-\xi_m)/\hbar\right]}\right]_0^{\hbar\beta} \\
&= \frac{1}{\hbar}\frac{1}{\mathrm{i}\omega_n+\left(\xi_n-\xi_m\right)/\hbar}\left[\mathrm{S}_{X,X'}\,\mathrm{e}^{\beta(\xi_n-\xi_m)}-1\right] \\
&= \frac{1}{\hbar}\frac{\mathrm{S}_{X,X'}\,\mathrm{e}^{\beta(\xi_n-\xi_m)}-1}{\mathrm{i}\omega_n+\left(\xi_n-\xi_m\right)/\hbar}
\end{aligned}$$

Definition 1.14 For each $\zeta \in \{-1,+1\}$ we denote the corresponding subspace of $L^2_{\mathrm{per}}(-\hbar\beta,+\hbar\beta)$ for which Equation (1.9) is fulfilled with $L_{\mathrm{B}} \equiv L_1$ and $L_{\mathrm{F}} \equiv L_{-1}$ respectively.

Lemma 1.15 The space of periodic functions can be decomposed into the direct sum of bosonic and fermionic functions as

$$L^2_{\mathrm{per}}(-\hbar\beta, +\hbar\beta) = L_{\mathrm{B}} \oplus L_{\mathrm{F}} \equiv \bigoplus_{\zeta\in\{-1,+1\}} L_\zeta \tag{1.17}$$

Proof 1.15 The plane-waves can be divided into bosonic and fermionic parts by considering the corresponding Matsubara-frequencies. The bosonic and fermionic plane-waves are linearly independent, and they span the whole space of periodic functions.

Lemma 1.16 On L_ζ we obtain the resolution of identity

$$\mathbb{1}_{L_\zeta} \equiv \sum_{\omega_n \in \Omega_\zeta} |\, \mathrm{i}\omega_n \,\rangle\langle\, \mathrm{i}\omega_n \,| \tag{1.18}$$

with plane waves

$$\langle\, \tau \,|\, \mathrm{i}\omega_n \,\rangle \equiv \mathrm{e}^{-\mathrm{i}\omega_n\tau}, \qquad \langle\, \mathrm{i}\omega_n \,|\, \tau \,\rangle \equiv \mathrm{e}^{+\mathrm{i}\omega_n\tau} \tag{1.19}$$

and the delta-function

$$\delta(\tau) = \frac{1}{\hbar\beta} \sum_{\omega_n \in \Omega_\zeta} \mathrm{e}^{-\mathrm{i}\omega_n\tau} \tag{1.20}$$

Proof 1.16 See Appendix, Proofs, page 493.

1.4. Fourier for a Continuous, Decaying Function on an Infinite Interval

Notation 1.17 For „sufficiently smooth“ complex-valued functions and distributions that decay „sufficiently fast“ at space-time-infinity

$$\begin{aligned} f :\ & \mathbb{R}^3 \times \mathbb{R} \to \mathbb{C} \\ & (\vec{x}, t) \ \mapsto f(\vec{x}, t) \equiv \int \frac{\mathrm{d}^3k}{(2\pi)^3} \int \frac{\mathrm{d}\omega}{2\pi}\, \mathrm{e}^{\,\mathrm{i}\left(+\vec{k}\cdot\vec{x}-\omega t\right)} f(\vec{k}, \omega) \end{aligned}$$

we write for the ("physical") *Fourier-transformation*

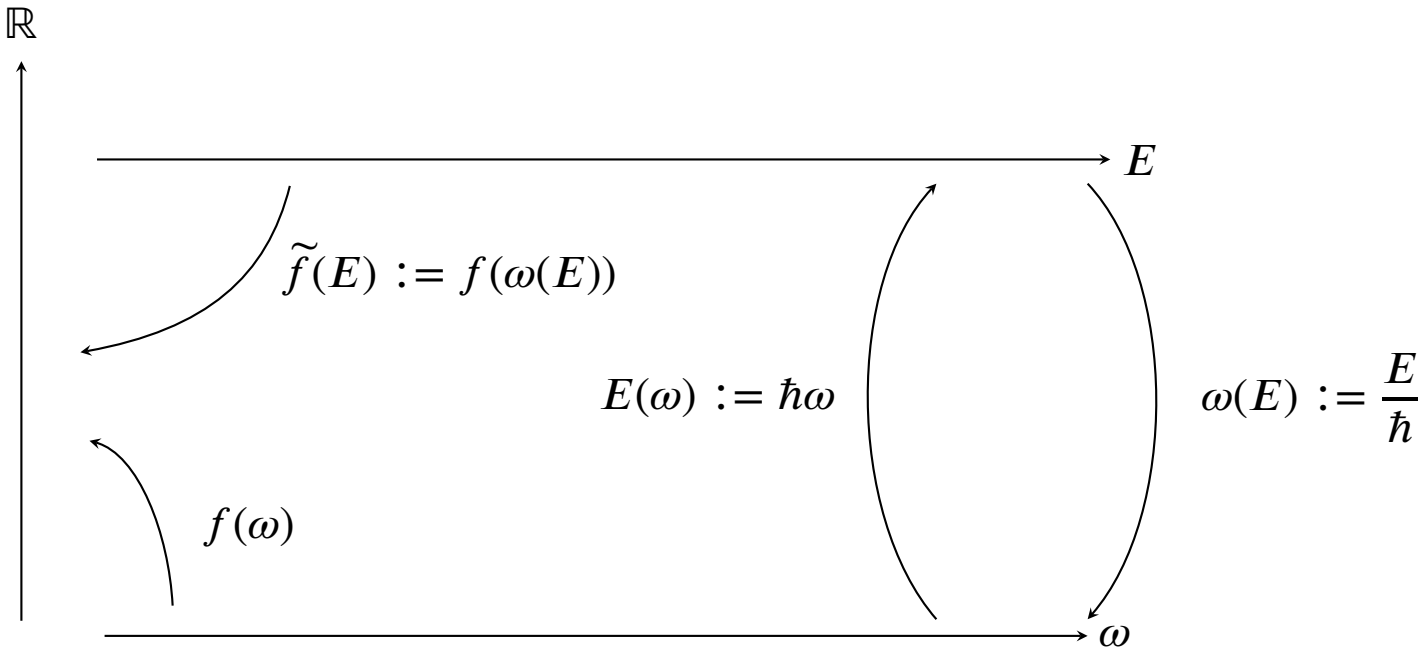
$$
\begin{aligned}
(\mathscr{F}f) &: \mathbb{R}^3 \times \mathbb{R} \to \mathbb{C} \\
(\vec{k},\omega) &\mapsto (\mathscr{F}f)(\vec{k},\omega) \equiv f(\vec{k},\omega) \equiv \int \mathrm{d}^3x \int \mathrm{d}t\, \mathrm{e}^{-\mathrm{i}\left(+\vec{k}\cdot\vec{x}-\omega t\right)} f(\vec{x},t)
\end{aligned}
$$

Proof 1.17 A proof for this expansion, can be found in [14].

Fact 1.18 Transitioning from frequency to energy integrals happens so often, that we consider it to be reasonable to add the transition-formula here

$$
\int_{\mathbb{R}} d\omega\, f(\omega) \overset{\text{SR.}}{=} \int_{\mathbb{R}} dE\, f\big(\omega(E)\big)\, \omega'(E) = \int_{\mathbb{R}} dE\, f\Big(\frac{E}{\hbar}\Big)\, \frac{1}{\hbar} \equiv \frac{1}{\hbar} \int_{\mathbb{R}} dE\, \widetilde{f}(E). \tag{1.21}
$$

The figure illustrates the transition.



For reasons that are impossible to understand several chapters in advance, we compute the following integrals.

Lemma 1.19 Let $\xi_\bullet \in \mathbb{R}$ and $\epsilon > 0$. Then we obtain

$$
\frac{\mathrm{i}}{\hbar} \int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t}\, \mathrm{e}^{-\epsilon|t|}\, \mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar}\, \theta(t) = \frac{-1}{\hbar} \frac{1}{\omega + \mathrm{i}\epsilon + (\xi_n - \xi_m)/\hbar} \tag{1.22}
$$

Proof 1.19 We compute straightforwardly

$$\begin{aligned}\frac{\mathrm{i}}{\hbar}\int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t}\, \mathrm{e}^{-\epsilon|t|}\, \mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar}\, \theta(t) &= \frac{\mathrm{i}}{\hbar}\int_0^\infty \mathrm{d}t\, \mathrm{e}^{t\left(-\epsilon+\mathrm{i}\left[\omega+(\xi_n-\xi_m)/\hbar\right]\right)} \\ &= \frac{\mathrm{i}}{\hbar}\frac{-1}{-\epsilon+\mathrm{i}\left[\omega+(\xi_n-\xi_m)/\hbar\right]} \\ &= \frac{-1}{\hbar}\frac{1}{\omega+\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar}\end{aligned}$$

Lemma 1.20 Let $\xi_\bullet \in \mathbb{R}$. Then we obtain

$$\frac{\mathrm{i}}{\hbar}\int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t}\, \mathrm{e}^{-\epsilon|t|}\, \mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar}\, \theta(-t) = \frac{1}{\hbar}\frac{1}{\omega-\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar} \tag{1.23}$$

Proof 1.20 We compute straightforwardly

$$\begin{aligned}\frac{\mathrm{i}}{\hbar}\int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t}\, \mathrm{e}^{-\epsilon|t|}\, \mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar}\, \theta(-t) &= \frac{\mathrm{i}}{\hbar}\int_{-\infty}^0 \mathrm{d}t\, \mathrm{e}^{t\left(+\epsilon+\mathrm{i}\left[\omega+(\xi_n-\xi_m)/\hbar\right]\right)} \\ &= \frac{\mathrm{i}}{\hbar}\frac{1}{+\epsilon+\mathrm{i}\left[\omega+(\xi_n-\xi_m)/\hbar\right]} \\ &= \frac{1}{\hbar}\frac{1}{\omega-\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar}\end{aligned}$$

Fact 1.21 Notice that these results can be summarized by the identity

$$\frac{\mathrm{i}}{\hbar}\int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t}\, \mathrm{e}^{-\epsilon|t|}\, \mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar}\, \theta(\pm t) = \frac{\mp 1}{\hbar}\frac{1}{\omega\pm\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar} \tag{1.24}$$

Notice further the standard-identity

Theorem 1.22 We therefore note the standard-identities for test-functions that decay sufficiently fast at infinity

$$\delta(\omega) = \frac{1}{2\pi}\int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t} \tag{1.25}$$

Proof 1.22 See, for example, [14], page 324.

2. Quantum Mechanics

There is at least three formalisms with which one can describe quantum-mechanical systems:

1. The „wavefunction-formalism“,
2. The „density-matrix-formalism“,
3. The „path-integral-formalism“.

In this chapter we will focus on the wavefunction-formalism, the other formalisms build upon it.

2.1. Fundamentals about Hilbert-Spaces

Definition 2.1 A Hilbert-space $\mathcal{H}$ is a complex vector space, with a hermitian[1] scalar-product

$$\begin{aligned} \langle\ ,\ \rangle : \mathcal{H} \times \mathcal{H} &\to \mathbb{C} \\ (\psi, \chi) &\mapsto \langle \psi, \chi \rangle \equiv \langle \psi | \chi \rangle \end{aligned}$$

which is complete and has a countable orthonormal basis[2].

Notation 2.2 The countable orthonormal basis from the definition above is usually denoted as $\{|1\rangle, |2\rangle, \dots, |d_{\mathcal{H}}\rangle\}$ such that

$$\mathcal{H} = \mathrm{span}_{\mathbb{C}}\{|1\rangle, |2\rangle, \dots, |d_{\mathcal{H}}\rangle\} \tag{2.1}$$

and most oftentimes the basis is specified further, depending on the context of the problem.

Fact 2.3 Some common single-particle Hilbert-spaces[3] to work with are in $d_{\mathbf{x}} \in \{1, 2, 3\}$ spatial-dimensions ...

- $\mathcal{H} = L^2(\mathbb{R}^{d_{\mathbf{x}}})$ with $\langle \psi | \chi \rangle = \int \mathrm{d}^{d_{\mathbf{x}}}\mathbf{x}\, \overline{\psi}(\mathbf{x})\chi(\mathbf{x})$ for a Schrödinger-particle in space,
- $\mathcal{H} = L^2(\mathbb{T}^{d_{\mathbf{x}}})$ with $\langle \psi | \chi \rangle = \int_{\mathrm{vol}} \mathrm{d}^{d_{\mathbf{x}}}\mathbf{x}\, \overline{\psi}(\mathbf{x})\chi(\mathbf{x})$ for a Schrödinger-particle in a $d_{\mathbf{x}}$-dimensionsional „crystal“[4],

[1] Recall that a hermitian scalar-product is linear w.r.t. the second argument, obeys $\langle \psi_1, \psi_2 \rangle = \langle \psi_2, \psi_1 \rangle^*$ and is positive semidefinite.

[2] Note that the latter condition is equivalent to the Hilbert-space being „separable“. The precise meaning of this can be looked up. Usually (in almost all situations) one is however doing quite well with the abovementioned definition.

[3] Proving that these spaces fall into the definition above is far from trivial. For example the separability of $L^2(\mathbb{R})$ takes (according to "folklore") about 6 pages in J. von Neumanns book.

[4] The precise meaning of the word „crystal“ will be introduced later. At this point we note, that one can identify coordinates $\mathbf{x}$ in a „crystal“ (with periodic boundary conditions) with angles on a torus.

- $\mathcal{H} = \mathbb{C}^2$ with complex standard-scalarproduct for a two-level-system,
- $\mathcal{H} = L^2(\mathbb{R}^{d_x}) \otimes \mathbb{C}^2$ with scalar-product $\langle \psi | \chi \rangle = \sum_{\sigma \in \{\uparrow,\downarrow\}} \int \mathrm{d}^{d_x}\mathbf{x}\, \overline{\psi}_\sigma(\mathbf{x}) \chi_\sigma(\mathbf{x}) \equiv \sum\!\!\!\!\!\!\int_{\sigma,\mathbf{x}} \overline{\psi}_\sigma(\mathbf{x}) \chi_\sigma(\mathbf{x})$ for a Pauli-particle in space,
- $\mathcal{H} = L^2(\mathbb{T}^{d_x}) \otimes \mathbb{C}^2$ with scalar-product $\langle \psi | \chi \rangle = \sum_{\sigma \in \{\uparrow,\downarrow\}} \int_{\mathrm{vol}} \mathrm{d}^{d_x}\mathbf{x}\, \overline{\psi}_\sigma(\mathbf{x}) \chi_\sigma(\mathbf{x}) \equiv \sum\!\!\!\!\!\!\int_{\sigma,\mathbf{x}} \overline{\psi}_\sigma(\mathbf{x}) \chi_\sigma(\mathbf{x})$ for a Pauli-particle in a „crystal“,

Remark 2.3.1 For the Hilbert space in physics, it is common practice to consider those elements as equivalent / equal, that differ only on sets of measure zero, thereby working with equivalence classes. However, since these distinctions have no effect on the observables considered in this work, we shall not concern ourselves with them here.

Remark 2.3.2 When there is more than one particle present, new structures and phenomena related to permutation symmetry appear. It turns out that the generalization to n-particle quantum mechanics depends on whether the particles under consideration are distinguishable or indistinguishable. In the former case the Hilbert space $\mathcal{H}$ of the many-particle system is simply the tensor product

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_n. \tag{2.2}$$

Remark 2.3.3 The Hilbert-spaces for indistiguishable many-particle-systems are a little bit tedious to introduce (approximately 20 pages in the book from Negele and Orland). We will consider them in a later chapter. Apart from the single-particle-examples however, everything in this chapter also applies for many-particle-systems.

Notation 2.4 For vectors $\psi \in \mathcal{H}$ one agrees on the notation $|\psi\rangle \equiv \psi$. One calls these kind of vectors „ket“-vectors. Through the canonical isomorphism[5] to the dual-space

$$\begin{aligned} \mathrm{J}_{\mathcal{H}} &: \mathcal{H} \to \mathcal{H}^* \\ &\psi \mapsto \mathrm{J}_{\mathcal{H}}(\psi) \equiv \langle \psi, \bullet \rangle \equiv \langle \psi | \bullet \rangle \end{aligned}$$

one introduces so-called „bra“-vectors. Taking a bra- and a ket-vector $\langle \chi |$ and $|\psi\rangle$ and „calculating their bra-c-ket“ $\langle \chi | \psi \rangle$ is therefore equivalent to calculating the scalar-product between two vectors.

Notation 2.5 An *operator* A is a linear mapping defined on the Hilbert-space

$$\begin{aligned} A &: \mathcal{H} \mapsto \mathcal{H} \\ &|\psi\rangle \mapsto A|\psi\rangle \end{aligned}$$

[5] Isomorph, as a *real* vector space, not as a complex vector-space, since the mapping $\mathrm{J}_{\mathcal{H}}$ is anti-linear. (Cf. Zirnbauer-Lecture-Notes.)

Remark 2.5.1 In the case that $\mathcal{H}$ represents a single-particle Hilbert-space, one also speaks of a *single-particle-operator*. In the case that $\mathcal{H}$ represents a many-particle Hilbert-space, and the action of A is not trivial on the different sectors, one also speaks of a *many-particle-operator*.

Remark 2.5.2 Sometimes one also encounters notations as $|A\psi\rangle \equiv A|\psi\rangle$. For the corresponding bra-vector one writes $\mathrm{J}_{\mathcal{H}}(A\psi) \equiv \langle A\psi|\bullet\rangle$.

Notation 2.6 Let $\mathcal{H} = \mathrm{span}_{\mathbb{C}}\{|1\rangle, |2\rangle, \dots\}$ be spanned by an orthonormal basis[6]. Then we have the matrix of mat A w.r.t. this basis defined as

$$(\mathrm{mat}\, A)_{i,j} \equiv \langle i|A|j\rangle. \tag{2.3}$$

Remark 2.6.1 As a special case of an operator, let us introduce the *projector* $\mathrm{P}_\chi \equiv |\chi\rangle\langle\chi|$ of a state $\chi \in \mathcal{H}$ as a linear mapping

$$\begin{aligned} \mathrm{P}_\chi : &\mathcal{H} \to \mathcal{H} \\ &\psi \mapsto \mathrm{P}_\chi(\psi) \equiv |\chi\rangle\langle\chi|\psi\rangle. \end{aligned}$$

Remark 2.6.2 In Section 9.1 we will understand how the matrix-representation of projectors are related to dyadic products in linear algebra.

Remark 2.6.3 Note that

$$\mathbb{1} \equiv \mathrm{Id}_{\mathcal{H}} \equiv \sum_n |n\rangle\langle n|, \tag{2.4}$$

for an orthonormal system of the Hilbert-space, which can serve as a useful mnemonic in the following sense:

- A vector $\psi \equiv |\psi\rangle$ can be expanded w.r.t. the basis as

$$|\psi\rangle = \mathbb{1}|\psi\rangle = \sum_n |n\rangle\langle n|\psi\rangle \tag{2.5}$$

  which is the same expression that one encounters in linear algebra for finite-dimensional vector spaces.

- The quantity $A|\psi\rangle$ represents again a vector that can be expanded w.r.t. the basis as

$$A|\psi\rangle = A\mathbb{1}|\psi\rangle = \sum_n A|n\rangle\langle n|\psi\rangle \tag{2.6}$$

  this yields for the m-th component of the vector $A|\psi\rangle$

[6] Case-dependent: Could be a finite basis, but also infinite.

$$\langle m|A|\psi\rangle = \sum_n \langle m|A|n\rangle\langle n|\psi\rangle \tag{2.7}$$

with matrix-elements $\langle m|A|n\rangle \in \mathbb{C}$.

Notation 2.7 In the case of a single, spinless particle, i.e. for $V \in \left\{\mathbb{T}^{d_{\mathbf{x}}}, \mathbb{R}^{d_{\mathbf{x}}}\right\}$, with $d_{\mathbf{x}} \in \{1,2,3\}$, as a mnemonic, one usually introduces for $\mathcal{H} = L^2(V)$ so-called *position-eigenbasis* $|\mathbf{x}\rangle$ with $\mathbf{x} \in V$, giving a special version of the unity-operator

$$\mathrm{Id}_{\mathcal{H}} \equiv \int_V \mathrm{d}^{d_{\mathbf{x}}}\mathbf{x}\, |\mathbf{x}\rangle\langle\mathbf{x}|. \tag{2.8}$$

By direct comparison of the expressions

$$\int \mathrm{d}^{d_{\mathbf{x}}}\mathbf{x}\, \overline{\chi}(\mathbf{x})\psi(\mathbf{x}) = \langle\chi|\psi\rangle = \langle\chi|\,\mathrm{Id}_{\mathcal{H}}\,|\psi\rangle = \int \mathrm{d}^{d_{\mathbf{x}}}\mathbf{x}\, \langle\chi|\mathbf{x}\rangle\,\langle\mathbf{x}|\psi\rangle, \tag{2.9}$$

one sees that it must hold

$$\langle\chi|\mathbf{x}\rangle = \overline{\chi}(\mathbf{x}), \qquad \langle\mathbf{x}|\psi\rangle = \psi(\mathbf{x}). \tag{2.10}$$

Remark 2.7.1 Although one finds in almost every physics-textbook that one must handle these "functions" with a lot of care, note that a regularization of a delta-function is square-integrable. Within the framework of solid-state-physics, one finds the well-defined, discrete „twins“ of position-eigenstates in so-called „Wannier-states“. Adopting a continuum-notation one finds well defined expressions and justifications for the „state-vectors“ $|\mathbf{x}\rangle$ above.

Notation 2.8 In the case of a single, spin-$\frac{1}{2}$ particle, i.e. for $\mathcal{H} = L^2(V) \otimes \mathbb{C}^2$, with $V \in \left\{\mathbb{T}^{d_{\mathbf{x}}}, \mathbb{R}^{d_{\mathbf{x}}}\right\}$, and $d_{\mathbf{x}} \in \{1,2,3\}$ and some basis for $\mathbb{C}^2 \equiv \mathrm{span}_{\mathbb{C}}\{|\uparrow\rangle, |\downarrow\rangle\}$ (let it be the eigenstates of σ_z here for concreteness), one also finds a resolution of identity w.r.t. to the product-basis

$$\mathrm{Id}_{\mathcal{H}} \equiv \sum\!\!\!\!\!\!\int_{\substack{\mathbf{x}\in V \\ \sigma\in\{\uparrow,\downarrow\}}} |\mathbf{x},\sigma\rangle\langle\mathbf{x},\sigma| \equiv \sum\!\!\!\!\!\!\int |x\rangle\langle x| \tag{2.11}$$

with coordinate-representation of states $|\psi\rangle \in \mathcal{H}$ w.r.t. our chosen basis given by

$$\langle x|\psi\rangle \equiv \psi(x) \equiv \psi_\sigma(\mathbf{x}). \tag{2.12}$$

Remark 2.8.1 In the case of more than one particle (with, or without spin) present, one can also introduce position-eigenstates as a product-basis of single-particle-position-eigenstates. This is elaborated in section 29.1.1.

Notation 2.9 Let A be a linear operator. The hermitian adjoint of A is the unique linear mapping $A^\dagger : \mathcal{H} \to \mathcal{H}$ that fulfills the following condition:

$$\forall \psi, \chi \in \mathcal{H} \times \mathcal{H} : \quad \langle \chi | A^\dagger | \psi \rangle = \langle \psi | A | \chi \rangle^* \equiv \langle \psi | A \chi \rangle^* = \langle A\chi | \psi \rangle \tag{2.13}$$

where we introduce the notations

$$\langle \psi | A^\dagger \equiv \langle A\psi | \equiv \mathrm{J}_{\mathcal{H}} \left(A | \psi \rangle \right). \tag{2.14}$$

Remark 2.9.1 If $A = A^\dagger$, then[7] we call the operator A *self-adjoint* or *hermitian*[8]. For reasons that will become clear in the next chapter, we will call self-adjoing operators *observables*[9]

Remark 2.9.2 Some properties of hermitian operators are:

- Their eigenvalues are real,
- eigenvectors associated to different eigenvalues are orthogonal,
- they can be diagonalized in an orthonormal basis of eigenvectors (spectral-theorem).

2.2. Canonical Quantization (from Classical Physics to Quantum Physics)

Hypothesis 2.10 Let

$$\begin{aligned} H &\equiv H(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N, \mathbf{p}_1, \mathbf{p}_2, \dots, \mathbf{p}_N, t) \\ &\equiv H(x_{1,1}, \dots, x_{1,d_\mathbf{x}}, x_{2,1}, \dots, x_{2,d_\mathbf{x}}, \dots, p_{1,1}, \dots, p_{1,d_\mathbf{x}}, p_{2,1}, \dots, p_{2,d_\mathbf{x}}, \dots, t) \\ &\equiv H(x_1, x_2, \dots, x_{d_\mathbf{x} N}, p_1, p_2, \dots, p_{d_\mathbf{x} N}, t) \\ &\equiv H(x, p, t) \end{aligned} \tag{2.15}$$

be the Hamilton-function of a classical, non-relativistic, N-(Newton-)particle system in $d_\mathbf{x}$ dimensions. Let us further assume, that H is a linear-combination of expressions of the type

1. $p_i p_j$,
2. $p_i f_j(x_1, x_2, \dots, t)$
3. $F(x_1, x_2, \dots, t)$

with functions f_i and F. The *canonically-quantized Hamilton-operator*, which we also denote by H[10], is obtained by replacing the expressions in the following way:

1. $p_i p_j \mapsto \frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial x_i} \frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial x_j} = -\hbar^2 \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j}$,
2. $p_i f_j(x_1, x_2, \dots, t) = \frac{1}{2} \left(p_i f_j(x_1, x_2, \dots, t) + f_j(x_1, x_2, \dots, t) p_i \right) \mapsto \frac{1}{2} \left(\frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial x_i} f_i(x_1, x_2, \dots, t) + f_i(x_1, x_2, \dots, t) \frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial x_i} \right)$

[7] Recall that two operators are considered to be identical if their action on an arbitrary vector of the vector space is the same.
[8] As we are physicist, we throw both of these kinds of operators into the same pot.
[9] Mnemonic: „[observ]able-vari[able]“.
[10] One has to conclude from the context, whether one is speaking about a Hamilton-function or a Hamilton-operator.

3. $F(x_1, x_2, \dots, t) \mapsto F(x_1, x_2, \dots, t)$

Remark 2.10.1 There is no mathematical way of proving that this is the correct technique to quantize a classical system. The only possibility is to compare the results of the quantization scheme with the results of experiments.

Remark 2.10.2 Note that the canonical quantization is a mapping from functions to operators. Sometimes one encounters the notation $x \equiv \hat{x}$ or $p_x \equiv \hat{p_x} \equiv \hbar/\mathrm{i}\partial_x$ to highlight this fact.

Remark 2.10.3 As an example, consider the Hamilton-function of a single, non-relativistic particle in a time-independent potential $V \equiv V(\mathbf{x})$

$$H(\mathbf{x}, \mathbf{p}) = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}). \tag{2.16}$$

Then, the canonically-quantized Hamilton-operator reads

$$H = -\hbar^2 \frac{\Delta}{2m} + V(\mathbf{x}). \tag{2.17}$$

Lemma 2.11 Notice further, that one has on the operator-level the so-called canonical commutation relations (CCR)

$$\left[x_i,\ p_j\right] = \mathrm{i}\hbar\delta_{i,j}. \tag{2.18}$$

Proof 2.11 See Appendix, Proofs, page 493.

Definition 2.12 We consider an N-particle system in $d_{\mathbf{x}} \in \{1, 2, 3\}$ dimensions. The Schrödinger-equation associated to this system reads

$$\mathrm{i}\hbar \left(\partial_t \psi\right)(\mathbf{x}, t) = (H\psi)(\mathbf{x}, t). \tag{2.19}$$

with canonically-quantized (and potentially time-dependent) Hamilton-operator $H(t)$.

Remark 2.12.1 Particles[11] (with mass m etc.), that obey the Schrödinger-equation, are called *Schrödinger-particles*.

Theorem 2.13 The formal solution to equation (2.19) is given by application of *time-evolution operator*

[11] In the broadest sense of the word.

$$\psi(\mathbf{x}, t_\mathrm{f}) = U(t_\mathrm{f}, t_\mathrm{i})\psi(\mathbf{x}, t_\mathrm{i}) \tag{2.20}$$

with

$$U(t_\mathrm{f}, t_\mathrm{i}) = \mathrm{T}_t \exp\left(-\frac{\mathrm{i}}{\hbar}\int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t'\, H(t')\right) = \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{\mathrm{i}}{\hbar}\right)^n \int_{[t_\mathrm{i}, t_\mathrm{f}]^n} \mathrm{d}t_1 \cdots \mathrm{d}t_n\, \mathrm{T}_t \prod_{j=1}^{n} H(t_j). \tag{2.21}$$

Remark 2.13.1 Notice, that the formal solution to this equation is for time-independent potentials given by

$$\psi(\mathbf{x}, t) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H\left(t-t_0\right)}\psi(\mathbf{x}, t_0) \equiv U(t, t_0)\psi(\mathbf{x}, t_0) \tag{2.22}$$

assuming we have $\psi(\mathbf{x}, t_0)$ given (which is most often not the case). The operator U is called *time-evolution-operator* and can be generalized for time-dependent potentials.

Definition 2.14 A time-dependent pure state $t \mapsto \psi(t) \equiv \psi_t \in \mathcal{H}$ is called *stationary*, if it satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\, \psi_t \mid A \mid \psi_t \,\rangle \equiv \frac{\mathrm{d}}{\mathrm{d}t}\langle\, A \,\rangle_{\psi_t} = 0 \quad \text{for all hermitian operators } A. \tag{2.23}$$

Remark 2.14.1 As examples:

- An electron moving through free space is not in stationary state (the expectation-value of the position operator changes with time).
- The ground state of the electronic system of a solid is (in the wavefunction-formalism (and as we shall see later, in the "density-matrix" formalism as well), and in absence of interactions) a stationary state (in the non-interacting case: a product of a so-called „Slater-determinant“ (to be introduced later) and plane wave for the spatial and temporal part respectively; the expectation-value of all observables are then constant in time, if there is no external perturbation).

Theorem 2.15 For a time-independent potential-function $V \equiv V(\mathbf{x}, t) \equiv V(\mathbf{x})$ a product ansatz

$$\psi(\mathbf{x}, t) \equiv \psi(\mathbf{x})\,\phi(t) \tag{2.24}$$

leads to[12] the time-independent-Schrödinger-equation

$$E\psi(\mathbf{x}) = (H\psi)(\mathbf{x}), \tag{2.25}$$

with

$$\phi(t) = \mathrm{e}^{-\mathrm{i}Et/\hbar}. \tag{2.26}$$

[12] With "leads to" we mean: We can solve the time-dependent Schrödinger-equation iff we can solve the time-independent Schrödinger-equation.

Proof 2.15 See Appendix, Proofs, page 494.

Corollary 2.16 The product ansatz above yields stationary-states.

Proof 2.16 See Appendix, Proofs, page 495.

Hypothesis 2.17 The product-ansatz in Equation (2.24) gives the „correct“ solution of the Schrödinger-equation, iff the state of interest is a stationary-state that can be described in the wavefunction-formalism.

Remark 2.17.1 Notice that the canonically quantized Hamiltonian of a single particle in $d_{\mathbf{x}} \in \{1, 2, 3\}$ dimensions with Hamilton-function given as $H = \frac{p^2}{2m} + V(\mathbf{x})$ is thus given by

$$H = -\frac{\hbar^2}{2m}\Delta_{\mathbf{x}} + V(\mathbf{x}). \tag{2.27}$$

Definition 2.18 The time-dependent Pauli equation for an N-particle system reads

$$i\frac{\partial}{\partial t}\psi(\mathbf{x}_1, s_1; \dots; \mathbf{x}_N, s_N; t) = \hat{H}\,\psi(\mathbf{x}_1, s_1; \dots; \mathbf{x}_N, s_N; t), \tag{2.28}$$

where the Hamiltonian is

$$\hat{H} = \sum_{j=1}^{N}\left[\frac{1}{2m_j}\left(-i\nabla_j - q_j\mathbf{A}(\mathbf{x}_j, t)\right)^2 + q_j\phi(\mathbf{x}_j, t) - \frac{q_j}{2m_j}\,\sigma_j \cdot \mathbf{B}(\mathbf{x}_j, t)\right] + \hat{V}_{\text{int}}. \tag{2.29}$$

Here, σ_j are the Pauli matrices acting on the spin degree of freedom of particle j, $\mathbf{A}$ and ϕ denote the vector and scalar potentials, and $\mathbf{B} = \nabla \times \mathbf{A}$ is the magnetic field.

Remark 2.18.1 For a system of N electrons (all of mass m and charge $-e$), this simplifies to

$$\hat{H} = \sum_{j=1}^{N}\left[\frac{1}{2m}\left(-i\nabla_j + e\mathbf{A}(\mathbf{x}_j, t)\right)^2 - e\phi(\mathbf{x}_j, t) + \frac{e}{2m}\,\sigma_j \cdot \mathbf{B}(\mathbf{x}_j, t)\right] + \sum_{i<j}\frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|}. \tag{2.30}$$

Remark 2.18.2 The single-particle Pauli-equation reads

$$\mathrm{i}\hbar\partial_t\psi = \left(\frac{1}{2m}\left[(\mathbf{p} - q\mathbf{A})^2 - q\hbar\boldsymbol{\sigma}\cdot\mathbf{B}\right] + q\phi\right)\psi \tag{2.31}$$

with $\psi(\mathbf{x}, t) \equiv \left(\psi_\uparrow, \psi_\downarrow\right)^{\mathrm{T}}(\mathbf{x}, t)$ etc.

Remark 2.18.3 Analogously one speaks about *Pauli*-particles.

Fact 2.19 A time-independent vector potential $\mathbf{A}(\mathbf{x})$ leads to a time-independent Hamiltonian $\hat{H}$ in the Pauli equation, and thus allows for a product ansatz of the form $\psi(\mathbf{x}_1, s_1; \ldots; \mathbf{x}_N, s_N; t) = \psi(\mathbf{x}_1, s_1; \ldots; \mathbf{x}_N, s_N)\phi(t)$, which yields the time-independent Pauli equation for a spatial wavefunction ψ.

2.3. The Postulates (for Wavefunction-States)

I A *wavefunction-state* of a physical system is a normalized solution $\psi(\bullet, t)$ of the underlying Schrödinger- / Pauli-equation, s.t. for each $t \in \mathbb{R}$, the coordinates[13] of the vector are complex-valued

$$\begin{aligned} \mathbf{x} &\mapsto \psi(\mathbf{x}, t) \equiv \langle \mathbf{x} | \psi_t \rangle \in \mathbb{C} \quad \text{for Schrödinger-equations} \\ x &\mapsto \psi(x, t) \equiv \langle x | \psi_t \rangle \in \mathbb{C} \quad \text{for Pauli-equations} \end{aligned} \tag{2.32}$$

and the vector is normalized, i.e. $\langle \psi_t | \psi_t \rangle = 1$.

II a) For any measurable quantity[14] there is an observable A.

b) The outcome of a measurement of A, i.e. the measured quantity, is one of the eigenvalues α_n of A.

c) Let $\{|\phi_{n,i}\rangle\}_{i=1,\dots,m}$ denote an orthonormal basis of the eigenspace of the eigenvalue (of A) α_n. A measurement of the observable A with a system in the state $|\psi_t\rangle$ gives the measured value α_n with probability

$$p_n = \sum_{i=1}^{m} |\langle \phi_{n,i} | \psi_t \rangle|^2. \tag{2.33}$$

Remark 2.19.1 For states that are not representated by wavefunctions, one obtains generalizations of the postulates. We will elaborate on this at a later point (when we acutally need it).

Remark 2.19.2 For wavefunctions obeying the Pauli-equation, the *Born-probability-interpretation* can be summarized as follows:

$$|\psi(x_1, x_2, \dots, x_N)|^2 \prod_{j=1}^{N} \mathrm{d}\mathbf{x}_j = \left\{ \begin{array}{l} \text{The probability for finding the } N \text{ particles in the } 3N\text{-dimensional volume } \prod_{j=1}^{N} \mathrm{d}\mathbf{x}_j, \\ \text{surrounding the point } (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) \\ \text{in the } 3N\text{-dimensional configuration space.} \end{array} \right\}.$$

For wavefunctions obeying the Schrödinger-equation, the same interpretation holds, but with $x_i \mapsto \mathbf{x}_i$ on the left hand side of the equation.

Remark 2.19.3 One finds these postulates in different books in all kinds of colours. It is, in my opinion, very difficult, if not impossible, to give a pedagogical and simultaneously complete introduction / description of quantum mechanics.

Notation 2.20 Further one finds the *expectation-value* of the observable A in the state $|\psi_t\rangle$ as

$$\langle A \rangle = \langle \psi_t | A | \psi_t \rangle. \tag{2.34}$$

[13] Notice that, depending on the system (with or without spin) and the number of particles, these coordinates are vectors with entries as many as $\mathbf{x}$ has.

[14] For example position, momentum, spin, angular-momentum, etc. There are also more complicated observables, such as Fermi-surfaces (through ARPES-measurements). Proving that these observables are indeed observables in the mathematical sense is a non-trivial, but straightforward task.

2.4. Time-Dependencies in Many-Body Quantum Mechanics

Notation 2.21 Let $\mathcal{H}$ denote the Hilbert-space (of a single- or many-particle) quantum system with a (possibly spin-dependent) time-independent Hamiltonian H (in the Schrödinger-picture) and consider the time-evolution in the Schrödinger- / Pauli-equation

$$\mathrm{i}\hbar\partial_t|\psi(t)\rangle = H|\psi(t)\rangle.$$

Definition 2.22 For arbitrary times $t_\mathrm{i}, t_\mathrm{f} \in \mathbb{R}$ we define the time-evolution operator $U(t_\mathrm{f}, t_\mathrm{i})$ of the system as

$$U(t_\mathrm{f}, t_\mathrm{i}) = \exp -\frac{\mathrm{i}}{\hbar}\left(t_\mathrm{f} - t_\mathrm{i}\right) H.$$

Theorem 2.23 The time-evolution operator defined above gives a formal solution to the Schrödinger-equation for a given initial-condition.

Proof 2.23 By taking the derivative, one sees that one indeeds obtains a solution for a given initial condition.

Definition 2.24 Let $X \equiv X_\mathrm{S} \equiv X_\mathrm{S}(t)$ be a possibly time-dependent operator, then one defines the corresponding Heisenberg-operator as

$$X_\mathrm{H}(t) := U(t,0)^\dagger\, X\, U(t,0).$$

Theorem 2.25 One immediately concludes the Heisenberg equation of motions

$$\frac{\mathrm{d}}{\mathrm{d}t}X_\mathrm{H}(t) = -\frac{\mathrm{i}}{\hbar}[X,H]_\mathrm{H}(t) + \left(\frac{\partial X_\mathrm{S}}{\partial t}\right)_\mathrm{H}(t) \tag{2.35}$$

Proof 2.25 See Appendix, Proofs, page 495.

Definition 2.26 In the so-called *Schrödinger-picture* one evaluates expectation-values of an observable X as

$$\langle X\rangle(t) \equiv \langle\psi_t|X|\psi_t\rangle, \tag{2.36}$$

In the *Heisenberg-picture* one evaluates expectation-values of an observable as

$$\langle X\rangle(t) \equiv \langle\psi_{t=0}|X_\mathrm{H}(t)|\psi_{t=0}\rangle \tag{2.37}$$

whereas $|\psi_{t=0}\rangle$ refers to some (known) state at time equal zero.

Remark 2.26.1 For pure states, both pictures are equivalent.

Remark 2.26.2 Sometimes it turns out to be useful to switch to yet another picture, the so-called „interaction-picture“. As the number of occasions where this is useful is rare (e.g. „Fermi's golden rule“, or „one-body-Green-functions for interacting systems“) we will not introduce it at this point.

3. Crystals

We focus on „crystalline solids“ (elaborated below) in this lecture.

3.1. Crystals, Lattices and Bases

Definition 3.1 For $d_{\mathbf{x}} \in \{1,2,3\}$ and linearly independent vectors $\bigcup_{j=1}^{d_{\mathbf{x}}} \left\{\mathbf{a}_j\right\}$ we introduce the corresponding *infinite point lattice*

$$\mathrm{L}_\infty \equiv \left\{ \mathbf{R}_\mathbf{n} \equiv \sum_{i=1}^{d_{\mathbf{x}}} n_i \mathbf{a}_i \quad | \quad \mathbf{n} \in \mathbb{Z}^{d_{\mathbf{x}}} \right\} \subset \mathbb{R}^{d_{\mathbf{x}}}. \tag{3.1}$$

Remark 3.1.1 The vectors $\bigcup_{j=1}^{d_{\mathbf{x}}} \left\{\mathbf{a}_j\right\}$ are usually called *lattice vectors* or *basis (vectors)*.

Definition 3.2 We define the *unit-cell* UC of a lattice w.r.t. the basis $\bigcup_{j=1}^{d_{\mathbf{x}}} \left\{\mathbf{a}_j\right\}$ as the set

$$\mathrm{UC} \equiv \mathrm{span}_{[0,1]} \bigcup_{j=1}^{d_{\mathbf{x}}} \left\{\mathbf{a}_j\right\} \subset \mathbb{R}^{d_{\mathbf{x}}} \tag{3.2}$$

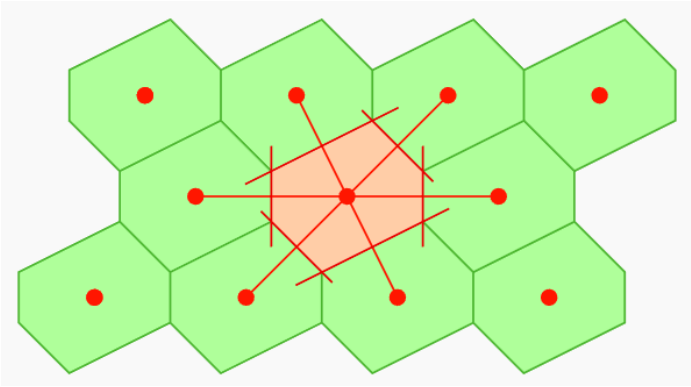
and we define its volume as

$$\mathrm{vol}(\mathrm{UC}) = \int \mathrm{d}^{d_{\mathbf{x}}}\mathbf{r}\; 1_{\mathrm{UC}}(\mathbf{r}). \tag{3.3}$$

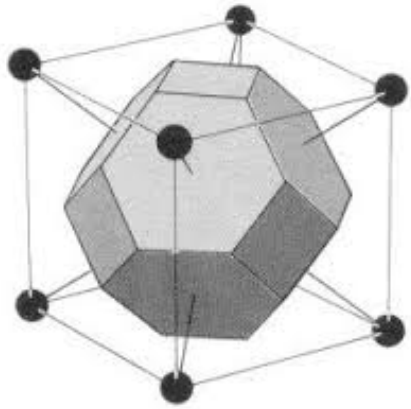
Definition 3.3 The *Wigner-Seitz-cell* around the lattice point $\mathbf{R}_\mathbf{m}$ is defined as the set

$$A_{\mathbf{R}_\mathbf{m}} \equiv A(\mathbf{R}_\mathbf{m}) \equiv A_\mathbf{m} = \left\{ \mathbf{r} \in \mathbb{R}^d \,|\, \forall \mathbf{n} \neq \mathbf{m} \,:\, |\mathbf{r} - \mathbf{R}_\mathbf{m}| < |\mathbf{r} - \mathbf{R}_\mathbf{n}| \right\}. \tag{3.4}$$

Remark 3.3.1 Therefore, all points in $A_{\mathbf{R}_\mathbf{m}}$ are closer to the point $\mathbf{R}_\mathbf{m}$ than to the neighboring grid-points.



(a) 2D construction for an „oblique-lattice“.



(b) 3D construction for a „bcc-lattice“.

Figure 3.1.: (a) 2D and (b) 3D constructions of a Wigner-Seitz-cell.

Definition 3.4 In one dimension, $d_{\mathbf{x}} = 1$, there exists only one kind of (*Bravais-*)lattice: Fixing the lattice constant a determines the lattice completely.

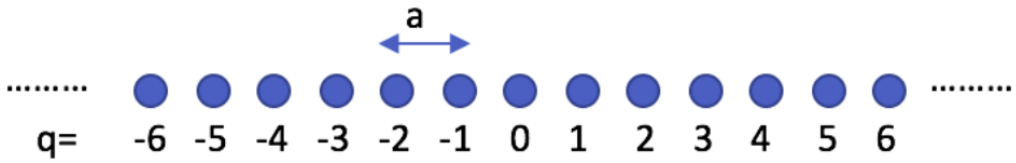


Figure 3.2.: One dimensional lattice (schematically).

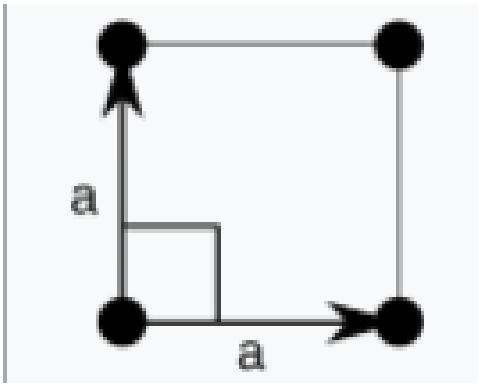
Definition 3.5 In two dimension, $d_{\mathbf{x}} = 2$, one introduces 5 so-called *(infinite) Bravais-lattices*[1], by considering the following cases of unit-vector combinations: Let $\varphi = \angle(\mathbf{a}_1, \mathbf{a}_2)$. Then one introduces …

1. *Square lattice*

   One choice of basis vectors is:

   $$\mathbf{a}_1 = (a, 0), \qquad \mathbf{a}_2 = (0, a),$$

   where $a = b$, and the angle $\varphi = 90°$.



The square lattice.

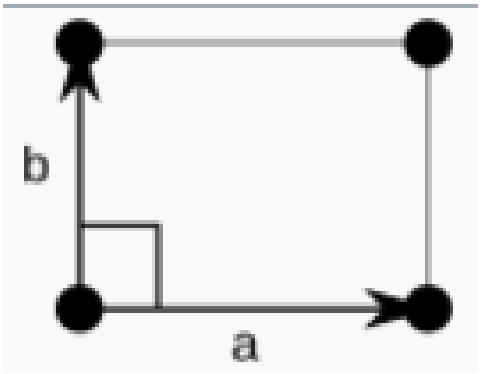
2. *Rectangular lattice*

[1] International Tables A page 720: There are 5 Bravais-Lattices in two dimensions.

One choice of basis vectors is:

$$\mathbf{a}_1 = (a, 0), \qquad \mathbf{a}_2 = (0, b),$$

where $a \neq b$, and the angle $\varphi = 90°$.



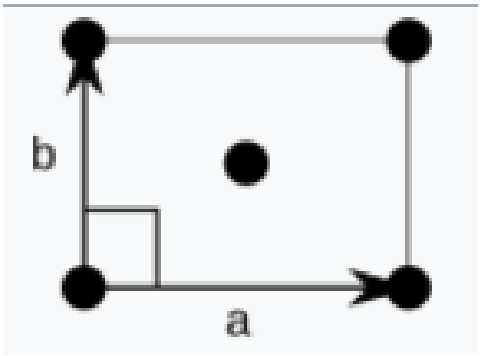
The rectangular lattice.

3. *Centered rectangular lattice*

One choice of basis vectors is:

$$\mathbf{a}_1 = \left(\frac{a}{2}, \frac{b}{2}\right), \qquad \mathbf{a}_2 = (a, 0),$$

where $a \neq b$, and the angle $\varphi \neq 90°$.



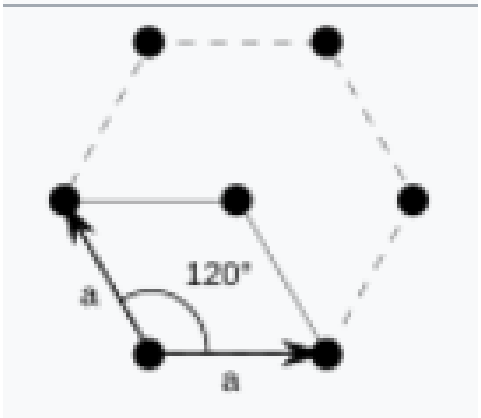
The centered rectangular lattice.

4. *Triangular (hexagonal) lattice*

One choice of basis vectors is:

$$\mathbf{a}_1 = (a, 0), \qquad \mathbf{a}_2 = \left(-\frac{a}{2}, \frac{\sqrt{3}}{2}a\right),$$

and the angle $\varphi = 120°$.



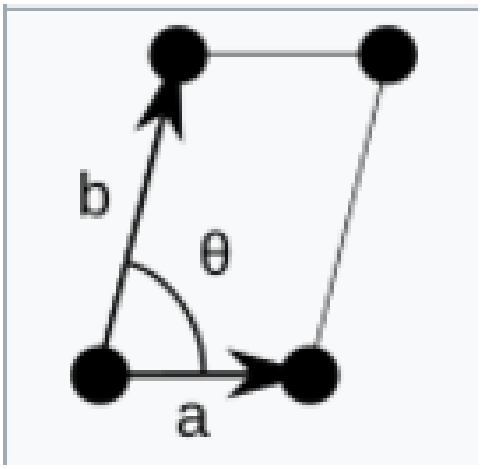
The triangular lattice.

5. *Oblique lattice*

One choice of basis vectors is:

$$\mathbf{a}_1 = (a, 0), \qquad \mathbf{a}_2 = (b\cos\varphi,\ b\sin\varphi),$$

where $a \neq b$, and $0° < \varphi < 180°$.



The oblique lattice.

Definition 3.6 In three dimensions, $d_{\mathbf{x}} = 3$, one introduces 14 so-called *Bravais-lattices*, by considering the following cases of unit-vector combinations: We denote the angles as

$$\alpha = \angle(\mathbf{a}_2, \mathbf{a}_3), \quad \beta = \angle(\mathbf{a}_1, \mathbf{a}_3), \quad \gamma = \angle(\mathbf{a}_1, \mathbf{a}_2) \tag{3.5}$$

and introduce the notation

$$\mathbf{a}_1 = \mathbf{a}, \quad \mathbf{a}_2 = \mathbf{b}, \quad \mathbf{a}_3 = \mathbf{c} \tag{3.6}$$

then one introduces the different lattices[2] …

1: the *triclinic lattice*: $a \neq b \neq c, \quad \alpha \neq \beta \neq \gamma$,

2-3: The *monoclinic* lattices

a) the *monoclinic primitive lattice*: $a \neq b \neq c, \quad \alpha = \gamma = 90° \neq \beta$

b) the *monoclinic base-centered lattice*: $a \neq b \neq c, \quad \alpha = \gamma = 90° \neq \beta$

4-7: The *orthorhombic* lattices

a) the *orthorhombic primitive lattice*: $a \neq b \neq c, \quad \alpha = \beta = \gamma = 90°$

b) the *orthorhombic base-centered lattice*: $a \neq b \neq c, \quad \alpha = \beta = \gamma = 90°$

c) the *orthorhombic body-centered lattice*: $a \neq b \neq c, \quad \alpha = \beta = \gamma = 90°$

d) the *orthorhombic face-centered lattice*: $a \neq b \neq c, \quad \alpha = \beta = \gamma = 90°$

8: the *hexagonal lattice*: $a = b \neq c, \quad \alpha = \beta = 90°, \quad \gamma = 120°$

9: the *trigonal lattice*: $a = b = c, \quad \alpha = \beta = \gamma \neq 90°$

10-11: The *tetragonal* lattices

a) the *tetragonal primitive lattice*: $a = b \neq c, \quad \alpha = \beta = \gamma = 90°$

b) the *tetragonal body-centered lattice*: $a = b \neq c, \quad \alpha = \beta = \gamma = 90°$

12-14: The *cubic* lattices

[2]Notice that e.g. the equations $a \neq b \neq c$ allow (strictly speaking) for the case $a = c \neq b$. But this is just poorly written in the books.

a) the *cubic primitive lattice*: $a = b = c, \quad \alpha = \beta = \gamma = 90°$

b) the *cubic body-centered lattice*: $a = b = c, \quad \alpha = \beta = \gamma = 90°$

c) the *cubic face-centered lattice*: $a = b = c, \quad \alpha = \beta = \gamma = 90°$

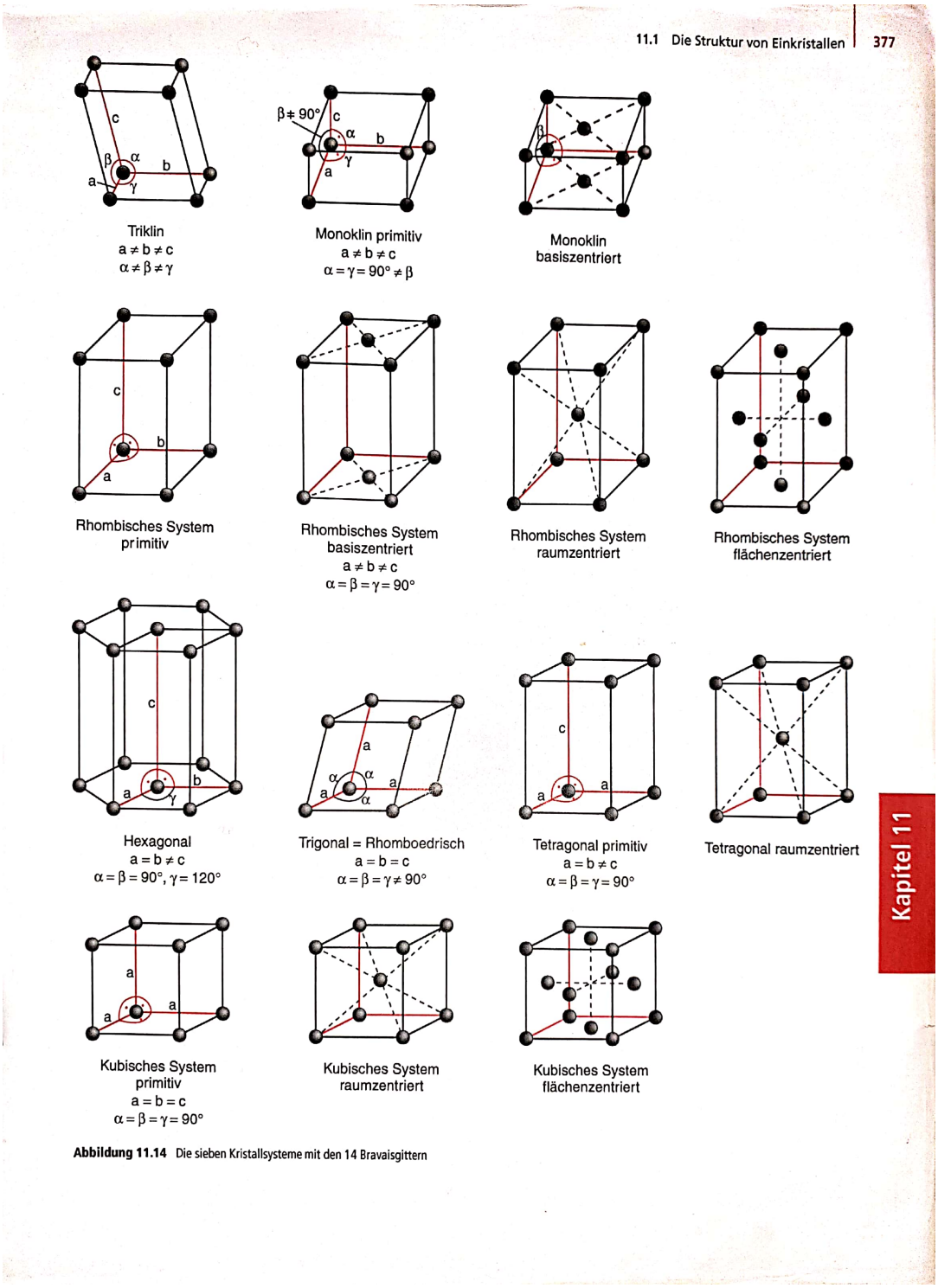


Figure 3.3.: Excerpt from Wolfang Demtröders Experimentalphysik 3.

Quoting from [Ashcroft]:

The seven crystal systems and fourteen Bravais lattices described above exhaust the possibilities. This

is far from obvious [...]. However, it is of no practical importance to understand why these are the only distinct cases. It is enough to know why the categories exist, and what they are.

Definition 3.7 We define an *infinite crystal* C_∞ by taking an infinite Bravais-lattice L_∞, and enlarge the number of points in the following way

$$\mathrm{C}_\infty \equiv \left\{ \boldsymbol{R}_{\mathbf{n}\kappa} \equiv \mathbf{R}_\mathbf{n} + \boldsymbol{R}_\kappa \equiv R_{\mathbf{n},\kappa,\alpha} \;\middle|\; \mathbf{R}_\mathbf{n} \in \mathrm{L}_\infty \quad \wedge \quad \kappa \in \{1, 2, \dots r\} \quad \wedge \quad \alpha \in \{1, \dots, d_\mathbf{x}\} \right\} \subset \mathbb{R}^{d_\mathbf{x}} \tag{3.7}$$

with *atomic basis-vectors* $\{\boldsymbol{R}_1, \dots, \boldsymbol{R}_r\}$ satisfying the equation

$$\boldsymbol{R}_\mu \in \{\boldsymbol{R}_1, \dots, \boldsymbol{R}_r\} \subset \mathrm{UC}\,. \tag{3.8}$$

Remark 3.7.1 The *atomic basis-vectors* $\{\boldsymbol{R}_1, \dots, \boldsymbol{R}_r\}$ represent the individual positions of the different atoms within the unit cell, and must not be confused with the primitive-vectors of the underlying lattice.

Remark 3.7.2 Notice that therefore, every infinite Bravais-lattice can be interpreted as a crystal with a trivial mono-atomic basis, i.e. $r = 1$ and $\boldsymbol{R}_1 = 0$.

Remark 3.7.3 A simple mnemonic for the definitions reads

$$\text{Crystal} = \text{Lattice} + \text{Basis}. \tag{3.9}$$

Remark 3.7.4 Note further, that this decomposition is not unique. For example potassium in its crystalline-form at room-temperature can be considered as a fcc-lattice with a mono-atomic basis *or* as a sc-lattice with a diatomic basis.

Remark 3.7.5 There are little pitfalls in the phraseology of the community... Graphene's crystal-structure is an example. It's realized as a triangular lattice with two basis-atoms. Because of the point-structure that one ends up with, one usually calls this crystal the *honeycomb-lattice*, although it is neither a Bravais-lattice, nor an infinite point-lattice in the sense above.

Definition 3.8 We call the lattice vectors $\bigcup_{j=1}^{d_\mathbf{x}} \{\mathbf{a}_j\}$ *primitive*, if r in Equation (3.7) is minimal. The corresponding unit-cell is called a *primitive unit-cell*.

Remark 3.8.1 A *primitive unit-cell* is the smallest unit cell that one can obtain for a crystal.

Definition 3.9 For a Bravais-lattice L_∞ with basis $\bigcup_{j=1}^{d_\mathbf{x}} \{\mathbf{a}_j\}$ we introduce the corresponding *reciprocal basis* in different dimensions

- $d = 1:\quad \mathbf{b}_1 = 2\pi \dfrac{\mathbf{a}_1}{|\mathbf{a}_1|}.$
- $d = 2:\quad \mathbf{b}_1 = 2\pi \dfrac{(-a_{2y}, a_{2x})}{|\mathbf{a}_1 \wedge \mathbf{a}_2|}, \quad \mathbf{b}_2 = 2\pi \dfrac{(a_{1y}, -a_{1x})}{|\mathbf{a}_1 \wedge \mathbf{a}_2|}.$
- $d = 3:\quad \mathbf{b}_1 = 2\pi \dfrac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}, \qquad \mathbf{b}_2 = 2\pi \dfrac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}, \qquad \mathbf{b}_3 = 2\pi \dfrac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}.$

Subsequently we define the corresponding *infinite reciprocal lattice* RL_∞ as

$$\mathrm{RL}_\infty \equiv \left\{ \mathbf{G} \in \mathbb{R}^{d_\mathbf{x}} \;\middle|\; \mathbf{G} = \sum_{j=1}^{d_\mathbf{x}} n_j \mathbf{b}_j \quad \text{with} \quad \mathbf{n} \in \bigtimes_{j=1}^{d_\mathbf{x}} \mathbb{Z} \right\} = \mathrm{span}_{\mathbb{Z}^{d_\mathbf{x}}} \bigcup_{j=1}^{d_\mathbf{x}} \{\mathbf{b}_j\}. \tag{3.10}$$

Remark 3.9.1 Recall that the wedge-product and the triple-product measure the (signed) volume of the parallelogram and the parallelepiped spanned by the vectors they are being applied on.

Corollary 3.10 It holds that

$$\mathrm{RL}_\infty \equiv \left\{ \mathbf{G} \in \mathbb{R}^{d_\mathbf{x}} \;\middle|\; \forall \mathbf{R} \in \mathrm{L}_\infty : \mathbf{G} \cdot \mathbf{R} \in 2\pi\mathbb{Z} \right\}. \tag{3.11}$$

Proof 3.10 With the anticommutativity-rules for the triple-product, one immediately sees that these vectors fulfill the defining condition.

Definition 3.11 The *first Brillouin-zone* FBZ is defined as

$$\mathrm{FBZ} = \left\{ \mathbf{r} \in \mathbb{R}^{d_\mathbf{x}} \;\middle|\; \forall \mathbf{G}_\mathbf{n} \in \mathrm{RL}_\infty : |\mathbf{r} - 0| < |\mathbf{r} - \mathbf{G}_\mathbf{n}| \right\}. \tag{3.12}$$

Remark 3.11.1 Therefore, the first Brillouin-zone is the Wigner-Seitz-cell of the origin of the reciprocal lattice.

Definition 3.12 A *unit-cell-periodic-function* or also *lattice-periodic function* is a smooth function

$$\begin{aligned} f :& \mathbb{R}^{d_\mathbf{x}} \to \mathbb{C} \\ & \mathbf{x} \mapsto f(\mathbf{x}) \end{aligned}$$

satisfying

$$f(\mathbf{x} + \mathbf{R}_\mathbf{n}) = f(\mathbf{x}) \quad \text{for } \mathbf{R}_\mathbf{n} \in \mathrm{L}_\infty. \tag{3.13}$$

Remark 3.12.1 Examples include ....

- The potential $\mathbf{x} \mapsto V(\mathbf{x}) \in \mathbb{R}$ that a "Bloch-electron"[3] experiences is a lattice-periodic function.
- A "Bloch-wavefunction"[4] $\mathbf{x} \mapsto \psi_{n,\mathbf{k}}(\mathbf{x}) \in \mathbb{C}$ can be factorized into a plane-wave $e^{i\mathbf{xk}}$ and a lattice-periodic function $u_{nm\mathbf{k}}(\mathbf{x})$.
- The "charge-density"[5] $\mathbf{x} \mapsto \rho(\mathbf{x}) \in \mathbb{R}$ is a lattice-periodic function.

Corollary 3.13 For a lattice-periodic function f it follows

$$f(\mathbf{x}) = \sum_{\mathbf{G} \in \mathrm{RL}_\infty} f_{\mathbf{G}}\, e^{i\mathbf{G}\cdot\mathbf{x}} \tag{3.14}$$

with expansion coefficients defined by

$$f_{\mathbf{G}} = \frac{1}{\mathrm{Vol(UC)}} \int_{\mathrm{UC}} \mathrm{d}^{d_\mathbf{x}}\mathbf{x}\, f(\mathbf{x})\, e^{-i\mathbf{G}\cdot\mathbf{x}} \tag{3.15}$$

Proof 3.13 See Appendix, Proofs, page 497.

Symmetries in Crystals

Symmetry-considerations are not trivial matters. There are endless tables on which kind of lattices imply what kind of behaviour for different kinds of experiments. (Laue-backscattering, Raman-scattering etc.) These behaviours can be concluded from symmetry-considerations and group-theoretical methods corresponding to the underlying lattice. Those who are interested can search for "International Tables for Crystallography".

3.2. Boundaries, Equivalences and Fourier

Hypothesis 3.14 We consider a real material embedded into $\mathbb{R}^{d_\mathbf{x}}$ with some finite volume $0 < V_{d_\mathbf{x}} < \infty$ and some underlying crystal(-structure), and introduce the numbers $N_1, \ldots, N_{d_\mathbf{x}} \in \mathbb{N}$ such that the scalar-product ($d_\mathbf{x} = 1$), wedge-product ($d_\mathbf{x} = 2$) or triple-product ($d_\mathbf{x} = 3$) coincides the volume

$$\begin{aligned}
&\bullet\ d_\mathbf{x} = 1: \quad V_{d_\mathbf{x}=1} \equiv L = N_1 \sqrt{\mathbf{a}_1^2}. \\
&\bullet\ d_\mathbf{x} = 2: \quad V_{d_\mathbf{x}=2} \equiv A = N_1 N_2\, \mathbf{a}_1 \wedge \mathbf{a}_2 = N_1 N_2\, \mathrm{Det} \begin{pmatrix} a_{1,x} & a_{1,y} \\ a_{2,x} & a_{2,y} \end{pmatrix}. \\
&\bullet\ d_\mathbf{x} = 3: \quad V_{d_\mathbf{x}=3} \equiv V = N_1 N_2 N_3\, \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) = N_1 N_2 N_3\, \mathrm{Det} \begin{pmatrix} a_{1,x} & a_{1,y} & a_{1,z} \\ a_{2,x} & a_{2,y} & a_{2,z} \\ a_{3,x} & a_{3,y} & a_{3,z} \end{pmatrix}.
\end{aligned}$$

[3] This term will be defined later.
[4] This term will be defined later.
[5] This term will be defined later.

and we denote the total number of cells as

$$\prod_{i=1}^{d_{\mathbf{x}}} N_i = N_p \tag{3.16}$$

Remark 3.14.1 Recall that the wedge product captures the (signed) area spanned by the two vectors in the plane, whereas the triple-product is the (signed) volume of the parallelepiped defined by the three vectors given.

Remark 3.14.2 When people speak about infinite crystals, they are usually considering the so-called *thermodynamic limit* in which $V_{d_{\mathbf{x}}} \to \infty$ and $\prod_{i=1}^{d_{\mathbf{x}}} N_i \to \infty$ with the additional condition that the size of the unit-cell is a constant $\frac{1}{V_{d_{\mathbf{x}}}} \prod_{j=1}^{d_{\mathbf{x}}} N_j = \text{const}$. In almost every (DFT) computer simulation however, crystals have a finite size with "periodic boundaries" (see below.)[6] One obtains „good approximations“ to densities of states and other observables by setting at least $N_i \approx 40$, unless there are some symmetries to consider.

We envision to catch the following two birds with one stone:

1. If we consider a piece of solid, and if we „look“ far into the bulk of the underlying material, we observe that in the Schrödinger-equation the potential arising from the ionic cores on the lattice site that a single-electron experiences „looks“ (at least within a finite region inside the bulk) like a periodic[7] function.
2. If we consider a piece of solid, it has a finite size.

Fact 3.15 One can model both these attributes in harmony to each other, by introducing periodic boundary conditions for crystal as a whole and restricting attention to solutions of the Schrödinger-eq. (4.2) which are periodic with the finite Bravais-lattice. We therefore identify wavefunctions in the bulk of the crystal as wavefunctions on a three-torus.

Definition 3.16 On $\mathbb{R}^{d_{\mathbf{x}}}$ we define the following relation

$$\forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^{d_{\mathbf{x}}} \,:\, \mathbf{x} \sim_x \mathbf{y} \quad :\Longleftrightarrow \quad \exists \mathbf{n} \in \mathbb{Z}^{d_{\mathbf{x}}} \,:\, \mathbf{x} = \mathbf{y} + \sum_{i=1}^{d_{\mathbf{x}}} n_i N_i \mathbf{a}_i. \tag{3.17}$$

Introducing these periodic boundary conditions is known as *Born- von Karman-boundary-conditions*.

Lemma 3.17 This defines an equivalence-relation.

Proof 3.17 Reflexivity is clear. For symmetry, we note that

$$\mathbf{x} = \mathbf{y} + \sum_{i=1}^{d_{\mathbf{x}}} n_i N_i \mathbf{a}_i \Longleftrightarrow \mathbf{y} = \mathbf{x} + \sum_{i=1}^{d_{\mathbf{x}}} (-n_i) N_i \mathbf{a}_i. \tag{3.18}$$

[6] Exceptions: quasicrystals, crystals with impurities, open boundary conditions.
[7] Notice that there are many useful mathematical formulae for periodic functions.

For transitivity one adds the coefficients.

Remark 3.17.1 Recall that a set on which an equivalence-relation is defined, can be partitioned into its equivalence-classes. This is an integral insight, in the construction of the Hilbert-space and the finite point lattice, and the Fourier-transform.

Lemma 3.18 It holds

$$\mathbb{R}^{d_{\mathbf{x}}}/\sim_x \equiv \left\{ [\mathbf{x}] = \sum_{i=1}^{d_{\mathbf{x}}} [c_i \mathbf{a}_i] \quad \middle| \quad c_i \in [0, N_i) \right\} \subset \mathbb{R}^{d_{\mathbf{x}}}. \tag{3.19}$$

Proof 3.18 We have to show, that for $\tilde{\mathbf{x}} \in \mathbb{R}^{d_{\mathbf{x}}}$ there is a unique representative $[\mathbf{x}] \in \mathbb{R}^{d_{\mathbf{x}}}/\sim_x$, such that $\tilde{\mathbf{x}} \in [\mathbf{x}]$. For this, we note that the lattice-vectors, being linearly independent, form a basis of $\mathbb{R}^{d_{\mathbf{x}}}$. Therefore, we can decompose $\tilde{\mathbf{x}}$ as

$$\tilde{\mathbf{x}} = \sum_{i=1}^{d_{\mathbf{x}}} \tilde{c}_i \mathbf{a}_i \quad \text{with } \tilde{c}_i \in \mathbb{R}. \tag{3.20}$$

Now we define

$$c_i = \tilde{c}_i \bmod N_i \in [0, N_i) \tag{3.21}$$

and

$$\mathbf{x} = \sum_{i=1}^{d_{\mathbf{x}}} c_i \mathbf{a}_i \quad \text{with} [\mathbf{x}] \in \mathbb{R}^{d_{\mathbf{x}}}/\sim_x . \tag{3.22}$$

It follows further that $\tilde{\mathbf{x}} \sim_x \mathbf{x}$ and therefore $[\tilde{\mathbf{x}}] = [\mathbf{x}] \in \mathbb{R}^{d_{\mathbf{x}}}/\sim_x$.

Corollary 3.19 Since $L_\infty \subset \mathbb{R}^{d_{\mathbf{x}}}$, this induces also a partitioning of the lattice into equivalence classes as

$$\mathrm{L_f} \equiv \mathrm{L}_\infty / \sim_x \equiv \left\{ [\mathbf{R}_\mathbf{n}] = \sum_{i=1}^{d_{\mathbf{x}}} [n_i \mathbf{a}_i] \quad \middle| \quad 0 \le n_i < N_i \wedge n_i \in \mathbb{N} \right\} \tag{3.23}$$

where we introduced the *finite point lattice* $\mathrm{L_f}$.

Proof 3.19 Analogously to the proof of Lemma 3.18.

Remark 3.19.1 Analogously we introduce the *finite crystal* $\mathrm{C_f}$ as

$$\mathrm{C_f} \equiv \left\{ \boldsymbol{R}_{\mathbf{n}\kappa} \equiv \mathbf{R}_{\mathbf{n}} + \boldsymbol{R}_{\kappa} \equiv R_{\mathbf{n},\kappa,\alpha} \quad \middle| \quad \mathbf{R}_{\mathbf{n}} \in \mathrm{L_f} \quad \wedge \quad \kappa \in \{1, 2, \dots r\} \quad \wedge \quad \alpha \in \{1, \dots, d_{\mathbf{x}}\} \right\} \subset \mathbb{R}^{d_{\mathbf{x}}}. \tag{3.24}$$

In order to write down neat and simple expressions for the „discrete Fourier-transform“ (will be introduced later), it is also convenient to introduce yet another lattice.

Definition 3.20 For a Bravais-lattice L_∞ with infinite reciprocal lattice and corresponding vectors $\mathbf{b}_i$ as in TBD, we introduce the *fine infinite reciprocal lattice* FRL_∞ as

$$\mathrm{FRL}_\infty \equiv \left\{ \mathbf{q} \equiv \sum_{i=1}^{d_{\mathbf{x}}} \frac{n_i}{N_i} \mathbf{b}_i \quad \middle| \quad n_i \in \mathbb{Z} \right\} \subset \mathbb{R}^{d_{\mathbf{x}}} \tag{3.25}$$

Definition 3.21 On FRL_∞ we define the following relation

$$\forall \mathbf{q}, \mathbf{q}' \in \mathrm{FRL}_\infty \,:\, \mathbf{q} \sim_q \mathbf{q}' \quad :\Longleftrightarrow \quad \exists \mathbf{n} \in \mathbb{Z}^{d_{\mathbf{x}}} \,:\, \mathbf{q} = \mathbf{q}' + \sum_{i=1}^{d_{\mathbf{x}}} n_i N_i \mathbf{b}_i \tag{3.26}$$

Lemma 3.22 This is an equivalence relation on FRL_∞.

Proof 3.22 Analogously to the proof of Lemma 3.18.

Corollary 3.23 It holds

$$\mathrm{Q} \equiv \mathrm{FRL}_\infty \,/\, \sim_q \equiv \left\{ [\mathbf{q}] = \sum_{i=1}^{d_{\mathbf{x}}} \left[\frac{n_i}{N_i} \mathbf{b}_i \right] \quad \middle| \quad 0 \leq n_i < N_i \right\} \tag{3.27}$$

Proof 3.23 Analogously to the proof of Lemma 3.18.

Notation 3.24 This set Q above, is what within the physics-community called the *allowed wave-vectors within the first Brillouin-zone*. Oftentimes one re-centers the representatives of the equivalence-classes around the origin, mostly for aesthetic reasons. There are however exceptions where it has computational reasons, for example when one introduces approximations. Then, considering for example acoustic phonons, for which one has $\hbar\omega_{\mathbf{q}} \approx \mathrm{const.}\, q$ for $q \ll 1$ ("Goldstone-theorem"), it is favourable to consider this „symmetric“ choice of equivalence-classes.

Notation 3.25 Summing over these equivalence-classes is usually denoted with an unconspicious

$$\sum_{\mathbf{q}} f(\mathbf{q}) \tag{3.28}$$

instead of

$$\sum_{[\mathbf{q}]\in \mathrm{Q}} f(\mathbf{q}) \tag{3.29}$$

with functions, that are independent on the choice of representative.

In order to proceed we now switch to the physics-notation.

Notation 3.26 In physics, one introduces the notation for the actual position(-operators) of the ionic coordinates (their average oscillates around the corresponding points in the crystal)

$$\left\{ \boldsymbol{\tau}_{\mathbf{n}\kappa} \equiv \mathbf{R}_{\mathbf{n}\kappa} + \boldsymbol{\Delta\tau}_{\mathbf{n}\kappa} \quad \middle| \quad [\mathbf{R}_{\mathbf{n}}] \in \mathrm{L_f} \quad \wedge \quad \kappa \in \{1, 2, \dots r\} \right\}$$

one introduces their Fourier-transforms as another sequence of numbers

$$\left\{ \tau_{\mathbf{q}\kappa} \quad \middle| \quad [\mathbf{q}] \in \mathrm{Q} \quad \wedge \quad \kappa \in \{1, 2, \dots r\} \right\}$$

as finite sums

$$\tau_{\mathbf{q}\kappa} = \frac{1}{\sqrt{N}} \sum_{[\mathbf{R}_{\mathbf{n}}]\in \mathrm{L_f}} \tau_{\mathbf{n}\kappa}\, \mathrm{e}^{+\mathrm{i}\mathbf{q}\cdot\mathbf{R}_{\mathbf{n}}} \tag{3.30}$$

whereas $N \equiv N_p \equiv \prod_{i=1}^{d_{\mathbf{x}}} N_i$.

Remark 3.26.1 Notice that this definition is well-defined, as both sides are independent of the choice of the representative that one chooses.

Lemma 3.27 The inverse transformation reads

$$\tau_{\mathbf{n}\kappa} = \frac{1}{\sqrt{N}} \sum_{[\mathbf{q}]\in \mathrm{Q}} \tau_{\mathbf{q}\kappa}\, \mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{R}_{\mathbf{n}}} \tag{3.31}$$

Proof 3.27 With the geometric series (again).

High Symmetry Points

Fact 3.28 For each lattice, one introduces within the first Brillouin-zone so-called „*high-symmetry-points*“ in order to plot band-structures.

Remark 3.28.1 These high-symmetry-points for each individual crystal are not unique. In different literatures one finds different high-symmetry-points.

Remark 3.28.2 It will turn out later, that fundamental quantities as so-called “phononic dispersion-relations” and “electronic band-structures”, are (for each respective “branch” or “band”) actually functions which take arguments from the first Brillouin-zone of the underlying crystal. Let us use ξ as a generic symbol for such an object of interest with domain located within the first Brillouin-zone:

$$\begin{aligned} \xi : \ & \mathrm{Q} \longrightarrow \mathbb{R} \\ & \mathbf{q} \longmapsto \xi(\mathbf{q}) \end{aligned}$$

with $\mathrm{Q} \subset \mathrm{FBZ}$. As one can hardly draw the graph of a function that takes three-dimensional arguments, one usually depicts the values of these functions on **k**-path. What one then usually sees is a picture with the **k**-path on the abscissa with the corresponding values of ξ on the ordinate. Hence the picture advertised in the beginning.

Remark 3.28.3 One can also rewrite this using the usual tools (and notations) that one knows from math-lectures by introducing a concrete curve $[0,1] \ni s \mapsto \gamma(s) \in \mathrm{FBZ}$ that connects the different high-symmetry **k**-points and then interpreting the pictures as image of a composite mapping $[0,1] \ni s \mapsto \xi(\gamma(s)) \in \mathbb{R}$. However...

Remark 3.28.4 These high-symmetry-points are actually a topic on their own... The mentality is, to get a glimpse of for example the band-structure of a certain material. (Keep in mind that the band-structure is a four-dimensional object, taking three arguments and giving one number for each argument.) By reducing the dimension to a two-dimensional picture in a neat-fashion, one can partly try to draw conclusions about this material. (For example, if there is a band-gap along the high-symmetry-points, it indicates that there is a band-gap in the density of states, leading to the classification of the material being metallic or insulating. There are however exceptions when this does not work...

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High-throughput electronic band structure calculations: Challenges and tools

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Figure 3.4.: A paper that lists high symmetry points for the different Bravais-lattices.

The following protocol should be followed. Unit cells must first be reduced to standard primitives, then they should be appropriately relaxed (if needed). Before the static run, the cells should be reduced again to standard primitive (symmetry and orientation might have changed during the relaxation). The user should then perform the static run and then project the eigenvalues along the directions which are specified in the "kpath" option. If the user is running AFLOW and VASP, the web interface can also prepare a template input file "aflow.in" which performs all the mentioned tasks.

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Appendix A

The choice of lattice vectors implemented in AFLOW is given here. When the primitive lattice is the same as the conventional one, it is simply called "lattice". Variables a, b, c, α, β, γ denote the axial lengths and interaxial angles of the conventional lattice vectors, while k_a, k_b, k_c, k_α, k_β, k_γ are those of the primitive reciprocal lattice vectors $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$. The coordinates of symmetry **k**-points are given in fractions of $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$.

A.1. Cubic (CUB, cP)

Lattice (see Fig. 1 and Table 2)

$\mathbf{a}_1 = (a, 0, 0)$
$\mathbf{a}_2 = (0, a, 0)$
$\mathbf{a}_3 = (0, 0, a)$

A.2. Face-centered cubic (FCC, cF)

(See Fig. 2 and Table 3.)

Conventional lattice	Primitive lattice
$\mathbf{a}_1 = (a, 0, 0)$	$\mathbf{a}_1 = (0, a/2, a/2)$
$\mathbf{a}_2 = (0, a, 0)$	$\mathbf{a}_2 = (a/2, 0, a/2)$
$\mathbf{a}_3 = (0, 0, a)$	$\mathbf{a}_3 = (a/2, a/2, 0)$

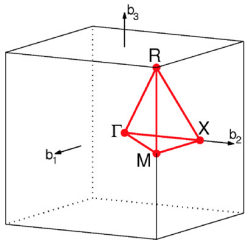


Fig. 1. Brillouin zone of CUB lattice. Path: Γ–X–M–Γ–R–$X|M$–R. An example of band structure using this path is given in Fig. 26.

Table 2
Symmetry **k**-points of CUB lattice.

$\times\mathbf{b}_1$	$\times\mathbf{b}_2$	$\times\mathbf{b}_3$		$\times\mathbf{b}_1$	$\times\mathbf{b}_2$	$\times\mathbf{b}_3$	
0	0	0	Γ	1/2	1/2	1/2	R
1/2	1/2	0	M	0	1/2	0	X

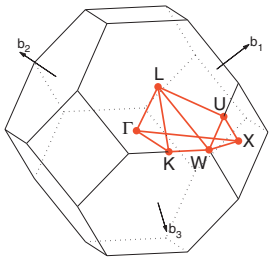


Fig. 2. Brillouin zone of FCC lattice. Path: Γ–X–W–K–Γ–L–U–W–L–$K|U$–X. An example of band structure using this path is given in Fig. 27.

Table 3
Symmetry **k**-points of FCC lattice.

$\times\mathbf{b}_1$	$\times\mathbf{b}_2$	$\times\mathbf{b}_3$		$\times\mathbf{b}_1$	$\times\mathbf{b}_2$	$\times\mathbf{b}_3$	
0	0	0	Γ	5/8	1/4	5/8	U
3/8	3/8	3/4	K	1/2	1/4	3/4	W
1/2	1/2	1/2	L	1/2	0	1/2	X

A.3. Body-centered cubic (BCC, cI)

(See Fig. 3 and Table 4.)

Conventional lattice	Primitive lattice
$\mathbf{a}_1 = (a, 0, 0)$	$\mathbf{a}_1 = (-a/2, a/2, a/2)$
$\mathbf{a}_2 = (0, a, 0)$	$\mathbf{a}_2 = (a/2, -a/2, a/2)$
$\mathbf{a}_3 = (0, 0, a)$	$\mathbf{a}_3 = (a/2, a/2, -a/2)$

A.4. Tetragonal (TET, tP)

Lattice (see Fig. 4 and Table 5)

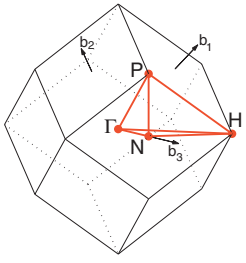


Fig. 3. Brillouin zone of BCC lattice. Path: Γ–H–N–Γ–P–$H|P$–N. An example of band structure using this path is given in Fig. 28.

Figure 3.5.: Excerpt of the paper above.

4. Quantum Mechanics of Crystals - Electrons and Cores

4.1. The General Problem

Notation 4.1 We consider a charge neutral *piece of solid material* and model it as a finite crystal as in Remark 3.19.1. Notice that this crystal has ...

- No defects, no impurities, no disorder, no surfaces, no interfaces, no grain-boundaries, no dislocations, no vacancies, ...
- a dimension $d_{\mathbf{x}} \in \{1, 2, 3\}$,
- an underlying crystal-structure, with lattice-vectors $\bigcup_{j=1}^{d_{\mathbf{x}}} \{\mathbf{a}_j\}$, and atomic basis-vectors $\{\boldsymbol{R}_1, \dots, \boldsymbol{R}_r\}$ according to Definition 3.7,
- a finite size, which will determine the numbers of unit-cells in each direction $N_1, \dots, N_{d_{\mathbf{x}}}$ and the total number of unit cells $\prod_{i=1}^{d_{\mathbf{x}}} N_i = N_p$ in Hypothesis 3.14,
- atoms or (inclusive) ionic cores with (individual) masses $\{\boldsymbol{M}_1, \dots, \boldsymbol{M}_r\}$ charges $\{Z_1\mathrm{e}, \dots, Z_r\mathrm{e}\}$ centered located on the crystal-points.
- $N_e = (Z_1 + \dots + Z_r) \prod_{j=1}^{d_{\mathbf{x}}} N_j$ (indistinguishable) electrons with (individual) mass m and charge $-\mathrm{e}$.

Remark 4.1.1 Notice that within these notations, this gives us a total of $rN_p = N_a$ ions to take care of, which results in $rd_{\mathbf{x}}N_p = d_{\mathbf{x}}N_a$ ionic coordinates. To distinguish the ionic coordinates from the lattice-points, we denote them (the coordinates) with[1] $\boldsymbol{\tau}$ (with proper indices that are clear in their meaning from the context).

Remark 4.1.2 Similarly, we have to take care of $d_{\mathbf{x}}N_e$ electronic coordinates[2]. Neglecting the spin-coordinate, we collect the spatial coordinates of the electrons and ionic cores in the collective vectors

$$\mathbf{r} \equiv (\mathbf{r}_1, \dots, \mathbf{r}_{N_e}) = \text{„electronic coordinates“}$$
$$\boldsymbol{\tau} \equiv (\boldsymbol{\tau}_1, \dots, \boldsymbol{\tau}_{N_a}) = \text{„ionic coordinates“}$$

[1] Notice that we denote the coordinates of the ions with another symbol than the lattice-vectors. This notation ("τ") was (probably) introduced by Feliciano Giustino (one of the main developers of the EPW-software) in his 2017-article „Electron-Phonon interactions from first principles“.

[2] We neglect the spin-coordinates for the moment. The fact, that in usual textbooks, for example, [Czycholl], the spin is being neglected is actually not really trivial. It is usually later re-implemented in the formulation of Bloch-wavefunctions by just „attaching“ the spin-part of a wavefunction to its spatial component. There are though exceptions, for example when the lattice-periodic potential possesses a non-trivial spin-dependence. Usual codes, for example [ELK, QE] possess an exchange-correlation functional with this property. This is the so-called „LSDA“-approximation.

Remark 4.1.3 From X-ray-spectroscopy, one can really conclude, that we are (in general) working with partially but not fully ionized cores. The ionic cares can be very well described with the orbital-model. Innermost shells are very similar to the shells of the generalized hydrogen-problem. One can however also compute their band-structure and sees that it is very flat.

Remark 4.1.4 With powder-diffraction (also called „Debye-Scherrer-method“) or with the „Laue-Backscattering-Method“ one can also conclude that the ions are really centered around lattice points.

Notation 4.2 We write for the kinetic-energy-operators

$$\mathrm{T}_e = \sum_{i=1}^{N_e} -\frac{\hbar^2}{2m}\Delta_{\mathbf{r}_i},$$
$$\mathrm{T}_a = \sum_{i=1}^{N_a} -\frac{\hbar^2}{2M_i}\Delta_{\boldsymbol{\tau}_i} = \sum_{\substack{\mathbf{R}_\mathbf{n}\in \mathrm{L_f} \\ \alpha\in\{1,\dots,d_\mathbf{x}\} \\ \kappa\in\{1,\dots,r\}}} -\frac{\hbar^2}{2M_\kappa}\frac{\partial^2}{\partial\tau^2_{\mathbf{n}\kappa\alpha}}$$

and for the interaction-operators

$$V_{e-e} \equiv \sum_{1\le i<j\le N_e} v_{e-e}(\mathbf{r}_i - \mathbf{r}_j)$$
$$V_{a-a} \equiv \sum_{1\le i<j\le N_a} v_{a_i-a_j}(\boldsymbol{\tau}_i - \boldsymbol{\tau}_j)$$
$$V_{e-a} \equiv \sum_{1\le i\le N_e}\sum_{1\le j\le N_a} v_{e-a_j}(\mathbf{r}_i - \boldsymbol{\tau}_j)$$

Remark 4.2.1 In modern density functional theory codes, one oftentimes approximates the interaction-potentials above through so-called „pseudopotentials“, instead of the proper Coulomb-interactions[3], which is mainly for computational convenience. (Leitmotiv: „Just solve it!“)

Hypothesis 4.3 Assuming the solid to be in a stationary state, the time-independent Schrödinger-equation now reads

[3]That would read in the current notation

$$\begin{aligned}
V_{e-e} &\equiv \sum_{1\le i<j\le N_e} v_{e-e}(\mathbf{r}_i - \mathbf{r}_j) && \approx \sum_{1\le i<j\le N_e} \frac{e^2}{4\pi\epsilon_0|\mathbf{r}_i - \mathbf{r}_j|} \\
V_{a-a} &\equiv \sum_{1\le i<j\le N_a} v_{a_i-a_j}(\boldsymbol{\tau}_i - \boldsymbol{\tau}_j) && \approx \sum_{1\le i<j\le N_a} \frac{Z_i Z_j e^2}{4\pi\epsilon_0|\boldsymbol{\tau}_i - \boldsymbol{\tau}_j|} \\
V_{e-a} &\equiv \sum_{1\le i\le N_e}\sum_{1\le j\le N_a} v_{e-a_j}(\mathbf{r}_i - \boldsymbol{\tau}_j) && \approx \sum_{1\le i\le N_e}\sum_{1\le j\le N_a} \frac{-Z_j e^2}{4\pi\epsilon_0|\mathbf{r}_i - \boldsymbol{\tau}_j|}
\end{aligned} \tag{4.1}$$

$$H\psi(\mathbf{r},\boldsymbol{\tau}) = E\psi(\mathbf{r},\boldsymbol{\tau}) \tag{4.2}$$

with

$$H \equiv \mathrm{T}_e + \mathrm{T}_a + \mathrm{V}_{e-e} + \mathrm{V}_{a-a} + \mathrm{V}_{e-a} \tag{4.3}$$

Remark 4.3.1 This Schrödinger-equation is impossible to solve exactly (neither analytically nor numerically) for crystals that are bigger than a couple of unit-cells in each direction. One needs to refer to approximation-schemes.

4.2. The Adiabatic / Born-Oppenheimer-Approximation

The general aim is to „decouple“ the dynamics (in the sense of a differential equation) of the electrons from the dynamics of the lattice.

Notation 4.4 We decompose the Hamiltonian above as

$$\begin{aligned} H &= \mathrm{T}_e + \mathrm{V}_{e-e} + \mathrm{V}_{a-a} + \mathrm{V}_{e-a} \quad + \quad \mathrm{T}_a \\ &\equiv \quad H_0 \quad + \quad V \end{aligned}$$

Definition 4.5 Applying now a perturbative treatment and neglecting the terms in equation (32.25) (see below) is called the *Born-Oppenheimer-Approximation* a.k.a *adiabatic approximation*

Notation 4.6 Let us assume, that for a fixed ion-configuration $\boldsymbol{\tau}$ we are able to determine all the orthonormal solutions

$$\left\{\mathbb{R}^{d_{\mathrm{x}}N_e} \ni \mathbf{r} \mapsto \phi_{\alpha,\boldsymbol{\tau}}(\mathbf{r}) \in \mathbb{C}\right\}_{\alpha\in\mathscr{A}} \tag{4.4}$$

of the equation

$$\left(H_0\phi_{\alpha,\boldsymbol{\tau}}\right)(\mathbf{r}) = \left(\left[\mathrm{T}_e + \mathrm{V}_{e-e} + \mathrm{V}_{a-a} + \mathrm{V}_{e-a}\right]\phi_{\alpha,\boldsymbol{\tau}}\right)(\mathbf{r}) = \epsilon_{\alpha,\boldsymbol{\tau}}\phi_{\alpha,\boldsymbol{\tau}}(\mathbf{r}) \tag{4.5}$$

Remark 4.6.1 This assumption, of being able to solve the electronic problem, was actually quite optimistic when it was proposed in 1927. In fact, even nowadays, only perturbative solutions to this problem exist.

Remark 4.6.2 In order to solve the problem

$$\left(H_0\phi_{\alpha,\boldsymbol{\tau}}\right)(\mathbf{r}) \equiv \epsilon_{\alpha,\boldsymbol{\tau}}\phi_{\alpha,\boldsymbol{\tau}}(\mathbf{r}) \tag{4.6}$$

perturbatively, it is nowadays usual to do a mean-field-approximation: Instead of considering the full electron-electron-interaction in Equation (4.1), one determines (with density functional theory) an effective single-particle-interaction, such that one has

$$\left(\left[\mathrm{T}_e + \mathrm{V}_{e-e} + \mathrm{V}_{a-a} + \mathrm{V}_{e-a}\right]\phi_{\alpha,\tau}\right)(\mathbf{r}) = \epsilon_{\alpha,\tau}\phi_{\alpha,\tau}(\mathbf{r}) \quad \overset{\text{Approximation}}{\Longleftrightarrow} \quad \left(\left[\mathrm{T}_e + \mathrm{V}_{\text{eff}} + \mathrm{V}_{a-a} + \mathrm{V}_{e-a}\right]\phi_{\alpha,\tau}\right)(\mathbf{r}) = \epsilon_{\alpha,\tau}\phi_{\alpha,\tau}(\mathbf{r}) \tag{4.7}$$

whereas the effective one-particle-potentials

$$\mathrm{V}_{\text{eff}}(\mathbf{r}) \equiv \sum_{i=1}^{N_e} \mathrm{V}_{\text{eff}}(\mathbf{r}_i) \equiv \sum_{i=1}^{N_e} \mathrm{V}_{\mathrm{H}}(\mathbf{r}_i) + \mathrm{V}_{\mathrm{XC}}(\mathbf{r}_i) \tag{4.8}$$

is composed of the so-called „Hartree“ and „exchange-correlation“-contributions. These potentials are determined through density functional theory, on which we will not elaborate further in this course.

Remark 4.6.3 With the procedure elucidated above, it becomes clear, that $\alpha \in \mathscr{A}$ represents a multi-index and the wavefunction $\mathbf{r} \mapsto \phi_{\alpha,\tau}(\mathbf{r})$ represents a Slater-determinant. These Slater-determinants are being build with single-particle-wavefunctions $\psi_{n\mathbf{k}\sigma}(x)$ (*Bloch-functions* or *Kohn-Sham-wavefunctions*, or, even more precise, *Bloch-Kohn-Sham-wavefunctions*) which will turn out to obey the one-particle Schrödinger-equation

$$\left(-\frac{\hbar^2}{2m}\Delta + V_{\mathrm{H}}(\mathbf{x}) + V_{\mathrm{XC}}(\mathbf{x}) + V_{\text{e-a}}(\mathbf{x}) + \text{const.}\right)\psi_{n\mathbf{k}\sigma}(\mathbf{x}) = E_{n\mathbf{k}}\psi_{n\mathbf{k}\sigma}(\mathbf{x}) \tag{4.9}$$

with $n \in \{1, 2, \ldots\}$, $\mathbf{k} \in \mathrm{Q}$ and $\sigma \in \{\downarrow, \uparrow\}$ in the absence of spin-orbit-coupling[4].

Remark 4.6.4 One notices, that in order to tackle the Schrödinger-equations of crystals, one divides the problem into further and further smaller (more or less managable) problems:

- We will be able to solve the time-independent Schrödinger-equation for the full (electronic and ionic system) in Equation (2.19) …

  …*if* we are able to solve the time-independent Schrödinger-equation for the effective electronic problem for some fixed ion-configuration in Equation (4.2).

- We will be able to solve the time-independent Schrödinger-equation for the effective electronic problem for some fixed ion-configuration in Equation (4.2) …

  …*if* we are able to find a (lattice-periodic) single-particle-potential that represents a good approximation to the electron-electron-interactions in Equation (4.7),

  …*and (inclusive) if* we are able solve the time-independent Schrödinger-equation for a single-electron moving in a lattice-periodic potential with an effective one-particle-interaction in Equation (4.9).

Remark 4.6.5 There are also problems with the procedure outlined above... For example band-gaps and energies might be calculated inaccurately by a poor approximation of the electron-electron-interactions. One cure / catchphrase is here the so-called „GW-approximation“, on which we will not elaborate further in this document.

[4] In the presence of spin-orbit coupling the energies acquire a spin-dependence $E_{n\mathbf{k}} \mapsto E_{n\mathbf{k}\sigma}$.

Remark 4.6.6 Although the laborious procedure outlined above results in „concrete“ (numerical) expressions for the wavefunctions, it will later on turn out to be appropriate to not work directly with the wavefunctions themselves, but with the matrix-elements (w.r.t. those wavefunctions above) of the Hamiltonian and a „density“ that represents „the state of the thermodynamic equilibrium in the grand canonical ensemble in absence of spontaneous symmetry breaking“. We will briefly touch this formalism, when we compute specific heats in the low-temperature-limit in the formalism of second-quantization.

Notation 4.7 Having determined the wave-functions $\left\{\mathbf{r} \mapsto \phi_{\alpha,\boldsymbol{\tau}}(\mathbf{r})\right\}_{\alpha\in\mathscr{A}}$ with eigenenergies $\left\{\epsilon_{\alpha,\boldsymbol{\tau}} \equiv \epsilon_{\alpha}(\boldsymbol{\tau})\right\}_{\alpha\in\mathscr{A}}$ for an (arbitrarily) fixed ion position τ, we now consider the full time-independent Schrödinger-equation

$$H\psi(\mathbf{r},\boldsymbol{\tau}) = E\psi(\mathbf{r},\boldsymbol{\tau}) \tag{4.10}$$

and expand the wavefunctions w.r.t. complete basis

$$\psi(\mathbf{r},\boldsymbol{\tau}) = \sum_{\alpha\in\mathscr{A}} \chi_{\alpha}(\boldsymbol{\tau})\phi_{\alpha,\boldsymbol{\tau}}(\mathbf{r}) \tag{4.11}$$

Theorem 4.8 The expansion in Equation (4.11) is a solution to the Schrödinger-Equation (4.10) in frame of the adiabatic approximation, if the coefficients $\chi_{\alpha}(\boldsymbol{\tau})$ fulfill the equation

$$\left(T_{\mathrm{a}} + \epsilon_{\alpha,\boldsymbol{\tau}}\right)\chi_{\alpha}(\boldsymbol{\tau}) = E\chi_{\alpha}(\boldsymbol{\tau}) \tag{4.12}$$

Proof 4.8 See Appendix, Proofs, page 500.

Remark 4.8.1 Since the electronic energies represent for each index α a mapping $\tau \mapsto \epsilon_{\alpha,\boldsymbol{\tau}} \equiv \epsilon_{\alpha}(\boldsymbol{\tau})$ one usually interpretes Equation (32.27) as the *ionic Schrödinger-equation*.

5. The Ionic Problem

5.1. The Schrödinger-Equation of the Ionic-System in the Harmonic-Approximation

We start with the effective Schrödinger-equation for the wavefunctions of the ions

$$H\,\chi(\boldsymbol{\tau}) = E\,\chi(\boldsymbol{\tau}) \qquad \text{with} \qquad H = \sum_{\substack{\mathbf{R}_{\mathbf{n}} \in \mathrm{L}_{\mathrm{f}} \\ \alpha \in \{1,\ldots,d_{\mathbf{x}}\} \\ \kappa \in \{1,\ldots,r\}}} -\frac{\hbar^2}{2M_\kappa}\frac{\partial^2}{\partial \tau_{\mathbf{n}\kappa\alpha}^2} + V_{\mathrm{eff}}(\boldsymbol{\tau}) \tag{5.1}$$

with an effective potential[1]

$$\boldsymbol{\tau} \mapsto V_{\mathrm{eff}}(\boldsymbol{\tau}) \in \mathbb{R} \tag{5.2}$$

that is the result of the solution to the electronic problem for different ion configurations $\boldsymbol{\tau}$.

Remark 5.0.1 Recall from Lemma **??** that we have the canonical commutation relations for the ionic coordinates

$$\left[\tau_{\mathbf{n}\kappa\alpha},\, p_{\tau_{\mathbf{n}'\kappa'\alpha'}}\right] = \mathrm{i}\hbar\delta_{\mathbf{n},\mathbf{n}'}\delta_{\kappa,\kappa'}\delta_{\alpha,\alpha'} \tag{5.3}$$

Intermezzo: Coordinate-Change

Lemma 5.1 If one changes coordinates as

$$x_i = x_i(x_1', \ldots, x_n') \tag{5.4}$$

then it follows for the derivatives of the corresponding coordinates that

$$\frac{\partial}{\partial x_i'} = \sum_{j=1}^{n} \frac{\partial x_j}{\partial x_i'}\frac{\partial}{\partial x_j} \tag{5.5}$$

Proof 5.1 See any textbook on calculus in more than one dimensions.

[1] Notice that we changed the notation of the effective potential, relative to the last section.

Hypothesis 5.2 We assume that there is an minimal equilibirum-position for the ions $\boldsymbol{\tau}$ s.t.

$$\min_{\boldsymbol{\tau}\in\mathbb{R}^{d_{\mathbf{x}}N_a}} V_{\text{eff}}(\boldsymbol{\tau}) \equiv V_{\text{eff}}(\mathbf{R}_{\text{eq}}) = \text{const.} \overset{\text{w.l.o.g.}}{=} 0 \quad \text{with} \quad \left(\nabla_{\boldsymbol{\tau}} V_{\text{eff}}\right)(\mathbf{R}_{\text{eq}}) = 0. \tag{5.6}$$

Notation 5.3 We change coordinates to the elongation of the ions from the individual lattice-sites

$$\Delta\boldsymbol{\tau}_{\mathbf{n}\kappa} \equiv \boldsymbol{\tau}_{\mathbf{n}\kappa} - \mathbf{R}_{\mathbf{n}\kappa} \quad \Longleftrightarrow \quad \Delta\tau_{\mathbf{n}\kappa\alpha} \equiv \boldsymbol{\tau}_{\mathbf{n}\kappa\alpha} - R_{\mathbf{n}\kappa\alpha}. \tag{5.7}$$

Lemma 5.4 The derivatives change according to the chain-rule

$$\frac{\partial}{\partial\tau_{\mathbf{n}\kappa\alpha}} \equiv \frac{\partial}{\partial\Delta\tau_{\mathbf{n}\kappa\alpha}}. \tag{5.8}$$

and that this transformation preserves the CCR; it holds

$$\left[\Delta\tau_{\mathbf{n}\kappa\alpha},\, p_{\Delta\tau_{\mathbf{n}'\kappa'\alpha'}}\right] = \mathrm{i}\hbar\delta_{\mathbf{n},\mathbf{n}'}\delta_{\kappa,\kappa'}\delta_{\alpha,\alpha'} \tag{5.9}$$

Proof 5.4 Follows immediately from the linearity of the commutator together with Lemma 5.1.

Corollary 5.5 Changing the coordinates and expanding the effective potential in a series up to the second-order simplifies the Hamiltonian to

$$\begin{aligned}
T_a &= \sum_{\substack{\mathbf{R}_{\mathbf{n}}\in\mathrm{L}_{\mathrm{f}}\\ \kappa\in\{1,\dots,r\}\\ \alpha\in\{1,\dots,d_{\mathbf{x}}\}}} -\frac{\hbar^2}{2M_\kappa}\frac{\partial^2}{\partial\Delta\tau^2_{\mathbf{n}\kappa\alpha}} \\
V_{\text{eff}}(\Delta\boldsymbol{\tau}) &\equiv V_{\text{eff}}(0) + \sum_{\substack{\mathbf{n}\in\mathrm{L}_{\mathrm{f}}\\ \kappa\in\{1,\dots,r\}\\ \alpha\in\{1,\dots,d_{\mathbf{x}}\}}} \left(\frac{\partial V_{\text{eff}}}{\partial\Delta\tau_{\mathbf{n}\kappa\alpha}}\right)(0)\,\Delta\tau_{\mathbf{n}\kappa\alpha} + \frac{1}{2}\sum_{\substack{\mathbf{n},\mathbf{n}'\in\mathrm{L}_{\mathrm{f}}\\ \kappa,\kappa'\in\{1,\dots,r\}\\ \alpha,\alpha'\in\{1,\dots,d_{\mathbf{x}}\}}} \left(\frac{\partial^2 V_{\text{eff}}}{\partial\Delta\tau_{\mathbf{n}\kappa\alpha}\partial\Delta\tau_{\mathbf{n}'\kappa'\alpha'}}\right)(0)\,\Delta\tau_{\mathbf{n}\kappa\alpha}\Delta\tau_{\mathbf{n}'\kappa'\alpha'} + \dots \\
&\approx 0 \qquad + 0 \qquad + \frac{1}{2}\sum_{\substack{\mathbf{n},\mathbf{n}'\in\mathrm{L}_{\mathrm{f}}\\ \kappa,\kappa'\in\{1,\dots,r\}\\ \alpha,\alpha'\in\{1,\dots,d_{\mathbf{x}}\}}} \left(\frac{\partial^2 V_{\text{eff}}}{\partial\Delta\tau_{\mathbf{n}\kappa\alpha}\partial\Delta\tau_{\mathbf{n}'\kappa'\alpha'}}\right)(0)\,\Delta\tau_{\mathbf{n}\kappa\alpha}\Delta\tau_{\mathbf{n}'\kappa'\alpha'}
\end{aligned}$$

Proof 5.5 Follows immediately by the assumptions and the Taylor-expansion.

Notation 5.6 From the Hesse-matrix at the equilibrium-position, one defines the *real-space-dynamical-matrix* as

$$D_{\mathbf{n}\kappa\alpha,\mathbf{n}'\kappa'\alpha'} \equiv \frac{1}{\sqrt{M_\kappa M_{\kappa'}}} \left(\frac{\partial^2 V_{\text{eff}}}{\partial \Delta\tau_{\mathbf{n}\kappa\alpha} \partial \Delta\tau_{\mathbf{n}'\kappa'\alpha'}} \right) (0). \tag{5.10}$$

Remark 5.6.1 Notice that …

- D is real-valued (the potential is real-valued),
- D is symmetric since the Schwarz-theorem applies

  $$\frac{\partial^2 V_{\text{eff}}}{\partial \Delta\tau_{\mathbf{n}\kappa\alpha} \partial \Delta\tau_{\mathbf{n}'\kappa'\alpha'}}(\bullet) = \frac{\partial^2 V_{\text{eff}}}{\partial \Delta\tau_{\mathbf{n}'\kappa'\alpha'} \partial \Delta\tau_{\mathbf{n}\kappa\alpha}}(\bullet),$$

  which implies for the dynamical matrix the relation

  $$D_{\mathbf{n}\kappa\alpha,\mathbf{n}'\kappa'\alpha'} = D_{\mathbf{n}'\kappa'\alpha',\mathbf{n}\kappa\alpha} \tag{5.11}$$

  meaning that the real-space-dynamical matrix is symmetric.
- D is positive definite, i.e. $\mathbf{v}^{\mathrm{T}} \cdot D \cdot \mathbf{v} > 0$ for $\mathbf{v} \neq 0$, since we assume an equilibrium-position that minimizes the potential energy.

At this point we are facing a crossroad. We can now continue with the solution of the Schrödinger-equation in two ways. The first is valuable for pedagogical reasons, and the other is valuable for computational (i.e. numerical) reasons. We will present both. In either way, we have to go through a series of coordinate-transformations, which is quite exhausting to keep track of.

5.1.1. Road 1 through Real-Space: A Poor Man's Phonons.

Notation 5.7 We introduce new coordinates as

$$\widetilde{u}_{\mathbf{n}\kappa\alpha} \equiv \sqrt{M_\kappa} \Delta\tau_{\mathbf{n}\kappa\alpha} \tag{5.12}$$

Lemma 5.8 We obtain for the new derivatives the relation

$$\frac{\partial}{\partial \widetilde{u}_{\mathbf{n}\kappa\alpha}} = \frac{1}{\sqrt{M_\kappa}} \frac{\partial}{\partial \Delta\tau_{\mathbf{n}\kappa\alpha}} \tag{5.13}$$

and this transformation preserves the CCR, i.e. it holds

$$\left[\widetilde{u}_{\mathbf{n}\kappa\alpha},\, p_{\widetilde{u}_{\mathbf{n}'\kappa'\alpha'}} \right] = \mathrm{i}\hbar \delta_{\mathbf{n},\mathbf{n}'} \delta_{\kappa,\kappa'} \delta_{\alpha,\alpha'} \tag{5.14}$$

Proof 5.8 Follows immediately from the linearity of the commutator, and the chain-rule for derivatives in Lemma 5.1.

Corollary 5.9 Switching to the new coordinates simplifies the Hamiltonian in the harmonic approximation to

$$\begin{aligned} H_{\text{harm}} &= T_{\text{ions}} + V_{\text{eff}}(\Delta\boldsymbol{\tau}) \\ &= \frac{1}{2} \sum_{\substack{\mathbf{R_n} \in \mathrm{L_f} \\ \kappa \in \{1,\dots,r\} \\ \alpha \in \{1,\dots,d\}}} -\hbar^2 \frac{\partial^2}{\partial \widetilde{u}^2_{\mathbf{n}\kappa\alpha}} + \frac{1}{2} \sum_{\substack{\mathbf{n},\mathbf{n}' \in \mathrm{L_f} \\ \kappa,\kappa' \in \{1,\dots,r\} \\ \alpha,\alpha' \in \{1,\dots,d\}}} D_{\mathbf{n}\kappa\alpha,\mathbf{n}'\kappa'\alpha'} \widetilde{u}_{\mathbf{n}\kappa\alpha} \widetilde{u}_{\mathbf{n}'\kappa'\alpha'} \\ &= \frac{1}{2} \mathbf{p}^{\mathrm{T}}_{\widetilde{\mathbf{u}}} \cdot \mathbb{1} \cdot \mathbf{p}_{\widetilde{\mathbf{u}}} + \frac{1}{2} \widetilde{\mathbf{u}}^{\mathrm{T}} \cdot D \cdot \widetilde{\mathbf{u}} \end{aligned}$$

Proof 5.9 Follows immediately by insertion and applying the correspondence principle backwards.

Lemma 5.10 Since the dynamical matrix is symmetric, one can find an orthogonal[2] matrix $C \in \mathrm{Mat}(\mathbb{R}^{d_{\mathbf{x}} N_a} \times \mathbb{R}^{d_{\mathbf{x}} N_a})$ s.t.

$$C D C^{\mathrm{T}} = \Omega = \mathrm{diag}(\omega_1^2, \omega_2^2, \dots, \omega^2_{d_{\mathbf{x}} N_a}) \tag{5.16}$$

with frequencies that are chosen to be positive $\omega_i \in \mathbb{R}_{>0}$.

Proof 5.10 See any textbook on linear algebra.

Notation 5.11 We introduce new coordinates as

$$\mathbf{u} \equiv C \widetilde{\mathbf{u}} \tag{5.17}$$

Lemma 5.12 We obtain new momenta as

$$\mathbf{p}_{\mathbf{u}} = C^{\mathrm{T}} \mathbf{p}_{\widetilde{\mathbf{u}}} \quad \Longleftrightarrow \quad \mathbf{p}_{\widetilde{\mathbf{u}}} = C \mathbf{p}_{\mathbf{u}} \tag{5.18}$$

and this coordinate-transformation is compatible with the CCR; it holds

$$\left[u_{\mathbf{n}\kappa\alpha},\, p_{u_{\mathbf{n}'\kappa'\alpha'}} \right] = \mathrm{i}\hbar \delta_{\mathbf{n},\mathbf{n}'} \delta_{\kappa,\kappa'} \delta_{\alpha,\alpha'} \tag{5.19}$$

Proof 5.12 Follows immediately from the linearity of the commutator, and the chain-rule for derivatives in Lemma 5.1.

[2]Recall that this means that the transpose of the matrix is its inverse

$$C \cdot C^{\mathrm{T}} = C^{\mathrm{T}} \cdot C = \mathbb{1}. \tag{5.15}$$

Corollary 5.13 Changing to the new coordinates brings the Hamiltonian into the diagonal form

$$H_{\text{harm.}} = \frac{1}{2}\mathbf{p}_{\mathbf{u}}^{\mathrm{T}} \cdot \mathbb{1} \cdot \mathbf{p}_{\mathbf{u}} + \frac{1}{2}\mathbf{u}^{\mathrm{T}} \cdot \Omega \cdot \mathbf{u}$$

Proof 5.13 By direct calculation, we obtain

$$\begin{aligned} H_{\text{harm.}} &= \frac{1}{2}\tilde{\mathbf{p}}^{\mathrm{T}} \cdot C^{\mathrm{T}} \cdot C \cdot \tilde{\mathbf{p}} + \frac{1}{2}\tilde{\mathbf{u}}^{\mathrm{T}} C^{\mathrm{T}} \cdot C \cdot D \cdot C^{\mathrm{T}} \cdot C\tilde{\mathbf{u}} \\ &= \frac{1}{2}\tilde{\mathbf{p}}^{\mathrm{T}} \cdot C^{\mathrm{T}} \cdot C \cdot \tilde{\mathbf{p}} + \frac{1}{2}\tilde{\mathbf{u}}^{\mathrm{T}} C^{\mathrm{T}} \cdot \Omega \cdot C\tilde{\mathbf{u}} \end{aligned}$$

Remark 5.13.1 Notice therefore, that within the harmonic approximation, the ionic system is can be described as a sum of harmonic oscillators

$$H_{\text{harm.}} = \frac{1}{2}\mathbf{p}_{\mathbf{u}}^{\mathrm{T}} \cdot \mathbb{1} \cdot \mathbf{p}_{\mathbf{u}} + \frac{1}{2}\mathbf{u}^{\mathrm{T}} \cdot \Omega \cdot \mathbf{u} = \frac{1}{2}\sum_{i=1}^{d_{\mathbf{x}}N_a} p_i^2 + \omega_i^2 u_i^2 \equiv \sum_{i=1}^{d_{\mathbf{x}}N_a} H_i$$

Corollary 5.14 Using the standard-techniques from the single-particle-harmonic-oscillator, i.e. introducing ladder-operators

$$b_j = \sqrt{\frac{\omega_j}{2\hbar}}u_j + \mathrm{i}\sqrt{\frac{1}{2\hbar\omega_j}}p_j, \qquad b_j^{\dagger} = \sqrt{\frac{\omega_j}{2\hbar}}u_j - \mathrm{i}\sqrt{\frac{1}{2\hbar\omega_j}}p_j \tag{5.20}$$

with commutation relations

$$[b_j, b_k^{\dagger}] = \delta_{j,k}, \qquad [b_j, b_k] = [b_j^{\dagger}, b_k^{\dagger}] = 0, \tag{5.21}$$

one arrives at the semi-final form the Hamilton-operator in the harmonic approximation

$$H_{\text{harm.}} = \sum_{j=1}^{d_{\mathbf{x}}N_a} \hbar\omega_j \left(b_j^{\dagger}b_j + \frac{1}{2}\right). \tag{5.22}$$

Proof 5.14 By using standard-theorems that we proved earlier in the lecture and on the exercise sheets, we immediately obtain the result.

Remark 5.14.1 We therefore see, that we can solve the effective Schrödinger-equation of the ionic problem iff we can diagonalize the real-space-dynamical-matrix D (which is a task that we can't for realistic system sizes). One circumvents this problem by going to reciprocal space.

5.1.2. Road 2 through Reciprocal-Space: State of the Art Description and Identities.

Theorem 5.15 Through the Coulomb-potential and the periodic boundary-conditions the dynamical matrix inherits the translational invariance

$$D_{\mathbf{n}\kappa\alpha,\,\mathbf{n}'\kappa'\alpha'} \equiv D_{\kappa\alpha,\,\kappa'\alpha'}(\mathbf{R}_{\mathbf{n}} - \mathbf{R}_{\mathbf{n}'}) \tag{5.23}$$

Proof 5.15 Follows from the distance-dependence of the Coulomb-interaction, when one explicitly writes down the sums.

Remark 5.15.1 Notice that this implies that the dynamical matrix is a function of the difference of the lattice-vectors, which implies the relations

$$D_{\mathbf{n}\kappa\alpha,\,\mathbf{n}'\kappa'\alpha'} = D_{\mathbf{n}-\mathbf{n}'\kappa\alpha,\,0\kappa'\alpha'} = D_{0\kappa\alpha,\,-(\mathbf{n}-\mathbf{n}')\kappa'\alpha'} \tag{5.24}$$

Notation 5.16 We change the coordinates and consider discrete Fourier-transforms with prefactor-conventions, to introduce the *Fourier-transformed Dynamical Matrix*

$$\begin{aligned}
\Delta\tau_{\mathbf{n}\kappa\alpha} \equiv \frac{1}{\sqrt{N_p}}\sum_{\mathbf{q}\in \mathrm{Q}} \Delta\tau_{\mathbf{q}\kappa\alpha}\mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{R}_{\mathbf{n}}} \qquad &\Longleftrightarrow \qquad \Delta\tau_{\mathbf{q}\kappa\alpha} \equiv \frac{1}{\sqrt{N_p}}\sum_{\mathbf{R}_{\mathbf{n}}\in \mathrm{L_f}} \Delta\tau_{\mathbf{n}\kappa\alpha}\mathrm{e}^{+\mathrm{i}\mathbf{q}\cdot\mathbf{R}_{\mathbf{n}}} \\
D_{\kappa\alpha,\,\kappa'\alpha'}(\mathbf{R}_{\mathbf{n}} - \mathbf{R}_{\mathbf{n}'}) \equiv \frac{1}{N_p}\sum_{\mathbf{q}\in \mathrm{Q}} D_{\kappa\alpha,\,\kappa'\alpha'}(\mathbf{q})\mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\left(\mathbf{R}_{\mathbf{n}}-\mathbf{R}_{\mathbf{n}'}\right)} \qquad &\Longleftrightarrow \qquad D_{\kappa\alpha,\,\kappa'\alpha'}(\mathbf{q}) \equiv \sum_{\mathbf{R}_{\mathbf{n}}\in \mathrm{L_f}} D_{\kappa\alpha,\,\kappa'\alpha'}(\mathbf{R}_{\mathbf{n}})\mathrm{e}^{+\mathrm{i}\mathbf{q}\cdot\mathbf{R}_{\mathbf{n}}}
\end{aligned} \tag{5.25}$$

Remark 5.16.1 One might wonder how it comes that one uses in two subsequent lines two different prefactor-conventions for the definition of the Fourier-transform (of a quantity). It is this choice in particular that makes the resulting final expression for the Hamiltonian look „particularly simple“. This charm has prevailed and these two prefactor-conventions are therefore in all the books and more importantly in all the codes for first principles and ab initio calculations and one has to get used to them.

Remark 5.16.2 Notice that since $\Delta\tau_{\mathbf{n}\kappa\alpha} = \Delta\tau^{\dagger}_{\mathbf{n}\kappa\alpha}$ (as an operator) it follows that

$$\Delta\tau^{\dagger}_{\mathbf{q}\kappa\alpha} = \frac{1}{\sqrt{N_p}}\sum_{\mathbf{R}_{\mathbf{n}}\in \mathrm{L_f}} \Delta\tau^{\dagger}_{\mathbf{n}\kappa\alpha}\mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{R}_{\mathbf{n}}} = \frac{1}{\sqrt{N_p}}\sum_{\mathbf{R}_{\mathbf{n}}\in \mathrm{L_f}} \Delta\tau_{\mathbf{n}\kappa\alpha}\mathrm{e}^{+\mathrm{i}(-\mathbf{q})\cdot\mathbf{R}_{\mathbf{n}}} = \Delta\tau_{-\mathbf{q}\kappa\alpha} \tag{5.26}$$

(as an operator again) and one obtains the further auxiliary-identity

$$\Delta\tau_{\mathbf{n}\kappa\alpha} = \Delta\tau^{\dagger}_{\mathbf{n}\kappa\alpha} = \frac{1}{\sqrt{N_p}}\sum_{\mathbf{q}\in \mathrm{Q}} \Delta\tau^{\dagger}_{\mathbf{q}\kappa\alpha}\mathrm{e}^{+\mathrm{i}\mathbf{q}\cdot\mathbf{R}_{\mathbf{n}}} = \frac{1}{\sqrt{N_p}}\sum_{\mathbf{q}\in \mathrm{Q}} \Delta\tau_{-\mathbf{q}\kappa\alpha}\mathrm{e}^{+\mathrm{i}\mathbf{q}\cdot\mathbf{R}_{\mathbf{n}}} \tag{5.27}$$

which will turn out to be good to use in the following.

Lemma 5.17 The derivatives change accordingly again:

$$\frac{\partial}{\partial \Delta\tau_{\mathbf{n}\kappa\alpha}} = \frac{1}{\sqrt{N_p}} \sum_{\mathbf{q}\in \mathrm{Q}} \mathrm{e}^{+\mathrm{i}\mathbf{q}\mathbf{R}_\mathbf{n}} \frac{\partial}{\partial \Delta\tau_{\mathbf{q}\kappa\alpha}} \quad \Longleftrightarrow \quad \frac{\partial}{\partial \Delta\tau_{\mathbf{q}\kappa\alpha}} = \frac{1}{\sqrt{N_p}} \sum_{\mathbf{R}_\mathbf{n}\in \mathrm{L_f}} \mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{R}_\mathbf{n}} \frac{\partial}{\partial \Delta\tau_{\mathbf{n}\kappa\alpha}} \tag{5.28}$$

and this transformation preserves the CCR, i.e. one has

$$\begin{aligned} \left[\Delta\tau_{\mathbf{q}\kappa\alpha},\, \frac{\partial}{\partial \Delta\tau_{\mathbf{q}'\kappa'\alpha'}}\right] &= \frac{1}{N_p} \sum_{\mathbf{R}_\mathbf{n},\mathbf{R}_{\mathbf{n}'}\in \mathrm{L_f}} \mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{R}_\mathbf{n}} \mathrm{e}^{+\mathrm{i}\mathbf{q}'\mathbf{R}_{\mathbf{n}'}} \left[\Delta\tau_{\mathbf{n}\kappa\alpha},\, \frac{\partial}{\partial \Delta\tau_{\mathbf{n}'\kappa'\alpha'}}\right] \\ &= \frac{\delta_{\kappa,\kappa'}\delta_{\alpha,\alpha'}}{N_p} \sum_{\mathbf{R}_\mathbf{n}\in \mathrm{L_f}} \mathrm{e}^{\mathrm{i}R_\mathbf{n}\cdot(\mathbf{q}-\mathbf{q}')} \\ &= \delta_{\mathbf{q},\mathbf{q}'}\delta_{\kappa,\kappa'}\delta_{\alpha,\alpha'} \end{aligned} \tag{5.29}$$

Proof 5.17 Follows immediately from the linearity of the commutator, and the chain-rule for derivatives in Lemma 5.1.

Corollary 5.18 It follows for the Hamiltonian

$$T_{\mathrm{ions}} + V_{\mathrm{eff}}(\tau) \approx \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ \kappa\in\{1,\dots,r\} \\ \alpha\in\{1,\dots,d_\mathbf{x}\}}} -\frac{\hbar^2}{2M_\kappa} \frac{\partial}{\partial \Delta\tau_{-\mathbf{q}\kappa\alpha}} \frac{\partial}{\partial \Delta\tau_{\mathbf{q}\kappa\alpha}} + \frac{1}{2} \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ \kappa,\kappa'\in\{1,\dots,r\} \\ \alpha,\alpha'\in\{1,\dots,d_\mathbf{x}\}}} \Delta\tau_{-\mathbf{q}\kappa\alpha} \frac{D_{\kappa\alpha,\,\kappa'\alpha'}(\mathbf{q})}{\sqrt{M_\kappa M_{\kappa'}}^{-1}} \Delta\tau_{\mathbf{q}\kappa'\alpha'}.$$

Proof 5.18 See Appendix, p. 65.

Lemma 5.19 For each $\mathbf{q} \in \mathrm{Q}$ the matrix $D(\mathbf{q})$ with matrix entries $D_{\kappa\alpha,\kappa'\alpha'}(\mathbf{q})$ is hermitian.

Proof 5.19 See Appendix, p. 501.

Corollary 5.20 Since $D(\mathbf{q})$ is hermitian, there is a unitary matrix $U(\mathbf{q})$ consisting of orthonormal eigenvectors (as columns) that diagonalizes the dynamical matrix

$$U^\dagger(\mathbf{q}) D(\mathbf{q}) U(\mathbf{q}) = \mathrm{diag}\left(\omega_1^2(\mathbf{q}), \dots, \omega_{rd_\mathbf{x}}^2(\mathbf{q})\right). \tag{5.30}$$

Proof 5.20 This proof is carried out in any textbook on linear algebra.

Notation 5.21 Recall from any linear algebra course, that the matrix-entries of $U(\mathbf{q})$ are given by the orthonormal eigenvectors of the dynamical matrix $D(\mathbf{q})$. We introduce for each $\mathbf{q} \in \mathrm{Q}$ its eigenvectors as

$$\left\{\mathbf{e}_{:,1}(\mathbf{q}), \mathbf{e}_{:,2}(\mathbf{q}), \ldots, \mathbf{e}_{:,rd_{\mathbf{x}}}(\mathbf{q})\right\}.$$

This gives the equation for their components

$$\sum_{\kappa'\alpha'} D_{\kappa\alpha,\kappa'\alpha'}(\mathbf{q}) e_{\kappa'\alpha',\nu}(\mathbf{q}) = \omega_\nu^2(\mathbf{q}) e_{\kappa\alpha,\nu}(\mathbf{q}) \quad \Longleftrightarrow \quad D(\mathbf{q})\mathbf{e}_{:,\nu}(\mathbf{q}) = \omega_\nu^2(\mathbf{q})\mathbf{e}_{:,\nu}(\mathbf{q}) \tag{5.31}$$

Lemma 5.22 The unitarity of the transformation-matrix $U(\mathbf{q})$ implies the relations

$$\begin{aligned} \sum_{\kappa\alpha} e^*_{\kappa\alpha,\nu}(\mathbf{q}) e_{\kappa\alpha,\nu'}(\mathbf{q}) &= \delta_{\nu\nu'} \\ \sum_{\nu} e^*_{\kappa\alpha,\nu}(\mathbf{q}) e_{\kappa'\alpha',\nu}(\mathbf{q}) &= \delta_{\kappa',\kappa}\delta_{\alpha',\alpha} \end{aligned} \tag{5.32}$$

whereas the first relation merely resembles the orthonormality of the eigenvectors w.r.t. the standard scalar-product on the complex numbers, and the second equation is a version of the completeness-relation for the eigenvectors.

Proof 5.22 See any textbook on linear algebra.

Lemma 5.23 For the eigenvectors and eigenvalues of the dynamical matrix in reciprocal space one finds the relations

$$\omega^2_{-\mathbf{q}\nu} = \omega^2_{\mathbf{q}\nu}, \quad e_{\kappa\alpha,\nu}(-\mathbf{q}) = e^*_{\kappa\alpha,\nu}(\mathbf{q}). \tag{5.33}$$

Proof 5.23 See Appendix, p. 501.

Notation 5.24 For reasons that will become clear in a moment, we introduce coordinates according to

$$\Delta\tau_{\mathbf{q}\kappa\alpha} = \sum_{\nu'} e_{\kappa\alpha,\nu'}(\mathbf{q}) \frac{u_{\mathbf{q}\nu'}}{\sqrt{M_\kappa}}, \quad \Longleftrightarrow \quad u_{\mathbf{q}\nu} = \sum_{\kappa'\alpha'} e^*_{\kappa'\alpha',\nu}(\mathbf{q}) \sqrt{M_{\kappa'}} \Delta\tau_{\mathbf{q}\kappa'\alpha'} \tag{5.34}$$

Lemma 5.25 We will prove …

- that the inverse-relation in Equation (5.34) is correct,
- the auxiliary-identity

$$\Delta\tau^\dagger_{\mathbf{q}\kappa\alpha} = \sum_{\nu'} e^*_{\kappa\alpha,\nu'}(\mathbf{q}) \frac{u^\dagger_{\mathbf{q}\nu'}}{\sqrt{M_\kappa}} = \Delta\tau_{-\mathbf{q}\kappa\alpha}, \tag{5.35}$$

- the derivatives change according to

$$\frac{\partial}{\partial \Delta\tau_{\mathbf{q}\kappa\alpha}} = \sum_{\nu'} e^{*}_{\kappa\alpha,\nu'}(\mathbf{q})\sqrt{M_\kappa}\frac{\partial}{\partial u_{\mathbf{q}\nu'}} \quad \Longleftrightarrow \quad \frac{\partial}{\partial u_{\mathbf{q}\nu}} = \sum_{\kappa'\alpha'} e_{\kappa'\alpha'\nu}(\mathbf{q})\frac{1}{\sqrt{M_{\kappa'}}}\frac{\partial}{\partial \Delta\tau_{\mathbf{q}\kappa'\alpha'}}. \tag{5.36}$$

- and this transformation preserves the CCR, i.e. one has

$$[u_{\mathbf{q}\nu},\ \frac{\partial}{\partial u_{\mathbf{q}'\nu'}}] = -\delta_{\nu,\nu'}\delta_{\mathbf{q},\mathbf{q}'} \tag{5.37}$$

Proof 5.25 See Appendix, p. 502.

Lemma 5.26 Summarizing all the coordinate-changes, we obtain in total

$$\tau_{\mathbf{n}\kappa\alpha} = R_{\mathbf{n}\kappa\alpha} + \frac{1}{\sqrt{N_p}}\sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ \nu'\in\{1,\dots,rd_{\mathbf{x}}\}}} e_{\kappa\alpha,\nu'}(\mathbf{q})\frac{\mathrm{e}^{\mathrm{i}\mathbf{q}\mathbf{R}_{\mathbf{n}}}}{\sqrt{M_\kappa}}u_{\mathbf{q}\nu'} \quad \Longleftrightarrow \quad u_{\mathbf{q}\nu} = \frac{1}{\sqrt{N_p}}\sum_{\substack{\mathbf{R}_{\mathbf{n}}\in \mathrm{L_f} \\ \kappa'\alpha'}} e^{*}_{\kappa'\alpha',\nu}(\mathbf{q})\sqrt{M_{\kappa'}}\mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{R}_{\mathbf{n}}}\left(\tau_{\mathbf{n}\kappa'\alpha'} - R_{\mathbf{n}\kappa'\alpha'}\right) \tag{5.38}$$

which implies the equations

$$\frac{1}{\partial \tau_{\mathbf{n}\kappa\alpha}} = \frac{1}{\sqrt{N_p}}\sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ \nu'\in\{1,\dots,rd_{\mathbf{x}}\}}} e^{*}_{\kappa'\alpha',\nu'}(\mathbf{q})\sqrt{M_\kappa}\mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{R}_{\mathbf{n}}}\frac{\partial}{\partial u_{\mathbf{q}\nu'}} \quad \Longleftrightarrow \quad \frac{\partial}{\partial u_{\mathbf{q}\nu}} = \frac{1}{\sqrt{N_p}}\sum_{\substack{\mathbf{R}_{\mathbf{n}}\in \mathrm{L_f} \\ \kappa'\alpha'}} e_{\kappa'\alpha',\nu}(\mathbf{q})\frac{\mathrm{e}^{+\mathrm{i}\mathbf{q}\mathbf{R}_{\mathbf{n}}}}{\sqrt{M_{\kappa'}}}\frac{\partial}{\partial \tau_{\mathbf{n}\kappa'\alpha'}}$$

Proof 5.26 See Appendix, p. 503.

Corollary 5.27 It follows

$$T_{\text{ions}} + V_{\text{eff}}(\tau) \approx \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} -\frac{\hbar^2}{2}\frac{\partial}{\partial u_{-\mathbf{q}\nu}}\frac{\partial}{\partial u_{\mathbf{q}\nu}} + \frac{\omega_\nu^2}{2}(\mathbf{q})\, u_{-\mathbf{q}\nu}u_{\mathbf{q}\nu}.$$

Proof 5.27 See Appendix, p. 505.

Definition 5.28 We introduce the ladder-operators

$$a_{\mathbf{q}\nu} = \sqrt{\frac{\omega_\nu(\mathbf{q})}{2\hbar}}\left(u_{\mathbf{q}\nu} + \frac{\hbar}{\omega_\nu(\mathbf{q})}\frac{\partial}{\partial u_{-\mathbf{q}\nu}}\right), \qquad a^{\dagger}_{\mathbf{q}\nu} = \sqrt{\frac{\omega_\nu(\mathbf{q})}{2\hbar}}\left(u_{-\mathbf{q}\nu} - \frac{\hbar}{\omega_\nu(\mathbf{q})}\frac{\partial}{\partial u_{+\mathbf{q}\nu}}\right) \tag{5.39}$$

Remark 5.28.1 Although this is simply a neat rewriting of operators, one oftentimes calls this step *canonical quantization* of position operators or *second quantization*.

Lemma 5.29 The ladder-operators fulfill the CCR

$$[a_{\mathbf{q}\nu},\, a^\dagger_{\mathbf{q}'\nu'}] = \delta_{\nu,\nu'}\delta_{\mathbf{q},\mathbf{q}'}, \qquad [a_{\mathbf{q}\nu},\, a_{\mathbf{q}'\nu'}] = [a^\dagger_{\mathbf{q}\nu},\, a^\dagger_{\mathbf{q}'\nu'}] = 0 \tag{5.40}$$

and one finds the inversion formulae

$$u_{\mathbf{q}\nu} = \sqrt{\frac{\hbar}{2\omega_\nu(\mathbf{q})}}\left(a_{\mathbf{q}\nu} + a^\dagger_{-\mathbf{q}\nu}\right), \qquad \frac{\partial}{\partial u_{\mathbf{q}\nu}} = \sqrt{\frac{\omega_\nu(\mathbf{q})}{2\hbar}}\left(a_{-\mathbf{q}\nu} - a^\dagger_{\mathbf{q}\nu}\right) \tag{5.41}$$

Proof 5.29 See Appendix, p. 507.

Corollary 5.30 Inserting this in the Hamiltonian above yields the final expression

$$H = \sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} \hbar\omega_\nu(\mathbf{q})\left(a^\dagger_{\mathbf{q}\nu}a_{\mathbf{q}\nu} + \frac{1}{2}\right). \tag{5.42}$$

Proof 5.30 See Appendix, p. 508.

Remark 5.30.1 Notice that we used $\omega_\nu(-\mathbf{q}) = \omega_\nu(+\mathbf{q})$ within the proof.

Lemma 5.31 Notice the important formula that is an integral component on any derivation of electron-phonon-couplings:

$$\Delta\tau_{\mathbf{n}\kappa\alpha} = \frac{1}{\sqrt{N_p}} \sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ \nu'\in\{1,\dots,rd_{\mathbf{x}}\}}} \sqrt{\frac{\hbar}{2M_\kappa\omega_{\nu'}(\mathbf{q})}} e_{\kappa\alpha,\nu'}(\mathbf{q})\, \mathrm{e}^{\mathrm{i}\mathbf{q}\mathbf{R}_{\mathbf{n}}}\left(a_{\mathbf{q}\nu'} + a^\dagger_{-\mathbf{q}\nu'}\right) \tag{5.43}$$

Proof 5.31 See Appendix, p. 509.

5.2. Electron-Phonon-Coupling

Cf. Waste-Folder 6, topic 10: For Felicianos derivation of electron-phonon-coupling.

5.3. Summary

The Main Tricks

By using a Taylor-expansion around the crystal-coordinates one has to simply diagonalize a matrix in order to solve the Schrödinger-equation (within the harmonic approximation). By going to reciprocal space, we have reduced the problem

$$\text{“Diagonalizing a symmetric } rd_{\mathbf{x}}N_p \times rd_{\mathbf{x}}N_p \text{ -matrix”} \tag{5.44}$$

with $N_p \in [10^{20}, 10^{24}]$ to the *equivalent* problem

$$\text{“Diagonalizing } N_p \text{ hermitian } rd_{\mathbf{x}} \times rd_{\mathbf{x}} \text{ -matrices”} \tag{5.45}$$

with $rd_{\mathbf{x}} \leq 100$ (in general...).

Thus the problem of

> *"Solving the effective Schrödinger-equation for the wavefunctions of the ions with an effective potential that is the result of the solution to the electronic problem for different ion configurations"*

turned out to be equivalent[3] (within the validity of the harmonic-approximation) to the problem

> *"Solving the Schrödinger-equation of harmonic-oscillators and simultaneously diagonalizing* $rd_{\mathbf{x}} \times rd_{\mathbf{x}}$*-matrices for different values of* $\mathbf{q} \in \mathrm{Q}$.

Eigen-energies and eigenstates of the ionic Schrödinger-equation

Let us now introduce an enumeration of the cross-product

$$\left\{ \lambda_1, \lambda_2, \dots, \lambda_{rd_{\mathbf{x}}N_p} \right\} \equiv \{1, 2, \dots, rd_{\mathbf{x}}\} \times \mathrm{Q}$$

such that $\lambda \equiv (j, \mathbf{q})$. Now each harmonic oscillator H_{λ} appearing in the harmonic-approximation can be diagonalized individually with standard-techniques, such that the total Hamiltonian

$$H \approx H_{\substack{\text{ionic} \\ \text{harmonic}}} = \sum_{\substack{\mathbf{q} \in \mathrm{Q} \\ \nu \in \{1,\dots,rd_{\mathbf{x}}\}}} \hbar\omega_{\nu}(\mathbf{q}) \left(a^{\dagger}_{\mathbf{q}\nu} a_{\mathbf{q}\nu} + \frac{1}{2} \right) \equiv \sum_{\lambda \in \{1,2,\dots,rd_{\mathbf{x}}N_p\}} \hbar\omega_{\lambda} \left(a^{\dagger}_{\lambda} a_{\lambda} + \frac{1}{2} \right). \tag{5.46}$$

can be diagonalized with a product-ansatz. This yields a basis for the underlying Hilbert-space

$$\bigotimes_{j=1}^{rd_{\mathbf{x}}N_p} L^2(\mathbb{R}) \simeq L^2(\mathbb{R}^{rd_{\mathbf{x}}N_p}) \equiv \mathscr{H}$$

a basis by products of wavefunctions

[3] In the sense: If we have found the solutions, i.e. wavefunctions, to the latter problem, then we can find solutions to the prior problem by simply changing the coordinates and expanding w.r.t. these wavefunctions.

$$\mathscr{B} = \left\{ |\Psi_{n_{\lambda_1}, n_{\lambda_2}, \ldots, n_{\lambda_{rd_{\mathbf{x}}N_p}}}\rangle \equiv |n_{\lambda_1}, n_{\lambda_2}, \ldots, n_{\lambda_{rd_{\mathbf{x}}N_p}}\rangle \,|\, n_{\lambda_\bullet} \in \{0, 1, 2, \ldots, \infty\} \right\} \tag{5.47}$$

We thus conclude that the total energies that the system can have (corresponding to the individual eigenstates that the system can be in) are

$$E_{n_{\lambda_1}, n_{\lambda_2}, \ldots, n_{\lambda_{rd_{\mathbf{x}}N_p}}} = \sum_{j=1}^{rd_{\mathbf{x}}N_p} \hbar\omega_{\lambda_j} \left(n_{\lambda_j} + \frac{1}{2} \right) \equiv \sum_{\mathbf{q} \in \mathrm{Q}} \sum_{\nu=1}^{rd_{\mathbf{x}}} \hbar\omega_{\nu\mathbf{q}} \left(n_{\nu\mathbf{q}} + \frac{1}{2} \right). \tag{5.48}$$

Remark 5.31.1 Notice that each of these wavefunctions has $rd_{\mathbf{x}}N_p$-positional-arguments! However... Usually one does not work so much about the ionic wavefunctions themselves anymore in solid-state-theory. It will turn out that the energies are quite enough to get a good picture of what is happening inside a solid in a lot of situations.

Definition of Phonons

Definition 5.32 For each $\nu \in \{1, 2, \ldots, rd_{\mathbf{x}}\}$ one categorizes the *phonon-branches* as mappings

$$\mathrm{Q} \ni \mathbf{q} \mapsto \omega_\nu(\mathbf{q}) \in \mathbb{R}_{>0}. \tag{5.49}$$

Remark 5.32.1 A phonon branch ω_ν is called *acoustical* (or *optical*), if

$$\lim_{\mathbf{q}\to 0} \omega_\nu(\mathbf{q}) = 0 \qquad \left(\text{or} \quad \lim_{\mathbf{q}\to 0} \omega_\nu(\mathbf{q}) \neq 0 \right). \tag{5.50}$$

Fact 5.33 For a crystal, there are $d_{\mathbf{x}}$ acoustical phonon-branches and $rd_{\mathbf{x}} - d_{\mathbf{x}}$ optical branches. (Without Proof.)

Notation 5.34 Without loss of generality we enumerate the phonon-branches

$$\{\omega_1, \ldots, \omega_{d_{\mathbf{x}}}, \omega_{d_{\mathbf{x}}} + 1, \ldots, \omega_{rd_{\mathbf{x}}}\} \tag{5.51}$$

in such a way, that

- the first $d_{\mathbf{x}}$ branches are acoustical,
- the remaining $rd_{\mathbf{x}} - d_{\mathbf{x}}$ branches are optical.

Interpretation of Phonons as Quasiparticles

For this we borrow the words from Alexander Altland in his book about condensed matter field theory:

Consider a standard harmonic oscillator (HO) Hamiltonian [...]. The HO has, of course, the status of a single-particle problem. However, the equidistance of its energy levels suggests an alternative interpretation. One can think of a given energy state ϵ_n as an accumulation of n elementary entities, or quasi-particles, each having energy ω. What can be said about the features of these new objects? First, they are structureless, i.e. the only "quantum number" identifying the quasi-particles is their energy ω (otherwise n-particle states formed of the quasi-particles would not be equidistant). This implies that the quasi-particles must be bosons. (The same state ω can be occupied by more than one particle [...].

About the rewritten form of the HO-Hamiltonian

$$H_{\mathrm{HO}} = \frac{p^2}{2m} + \frac{m\omega^2}{2}x^2 = \omega\left(a^\dagger a + \frac{1}{2}\right) \tag{5.52}$$

[...] its "real" advantage is that it naturally affords a many-particle interpretation. To this end, let us declare $|0\rangle$ to represent a "vacuum" state, i.e. a state with zero particles present. Next, imagine that $a^\dagger|0\rangle$ is a state with a single featureless particle [...] of energy ω. Similarly $\left(a^\dagger\right)^n|0\rangle$ is considered as a many-body state with n particles, i.e. within the new picture [...]. [...] While, at first sight, this may look unfamiliar, the new interpretation is internally consistent. Moreover, it achieves what we had asked for above, i.e. it allows an interpretation of the HO states as a superposition of independent structureless entities. Physically, the quasi-particles [...] are identified with the phonon modes of the solid.

6. The Electronic Problem

To Be Done... Bloch-Theorem and reference to Slater-determinants solving the non-interacting problem.

6.1. The Many-Electron Problem

6.2. The One-Electron Problem (Bloch-Theorem)

6.3. Density Functional Theory - Kohn-Sham-Equations

Part II.

Green-Function-Techniques

Motivation and Overview

After this part of the notes you will understand ...

- what Hans Bethe meant, when he said[1] that

  > *"[The fact that] Particles can be created and annihilated, is the bread and butter of todays physics and has remained so."*

  and why this is usually visualized through pictures like the one in Figure 6.1.

- How Green-Functions (in this work) are defined by combining two big pillars of modern physics, namely *Quantum Many Body Physics* and *Equilibrium Statistical Physics*.

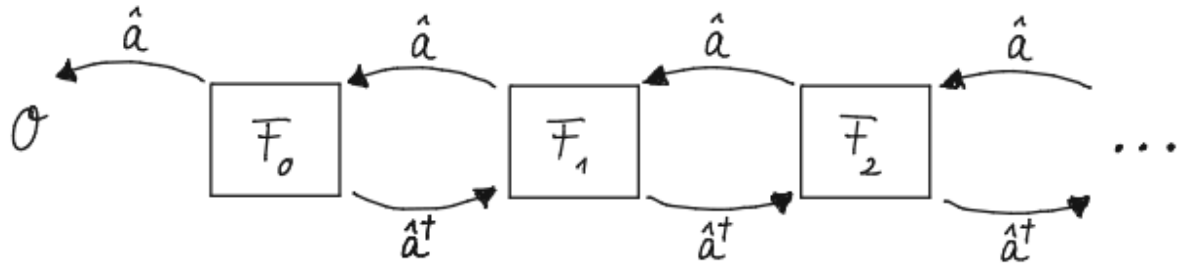
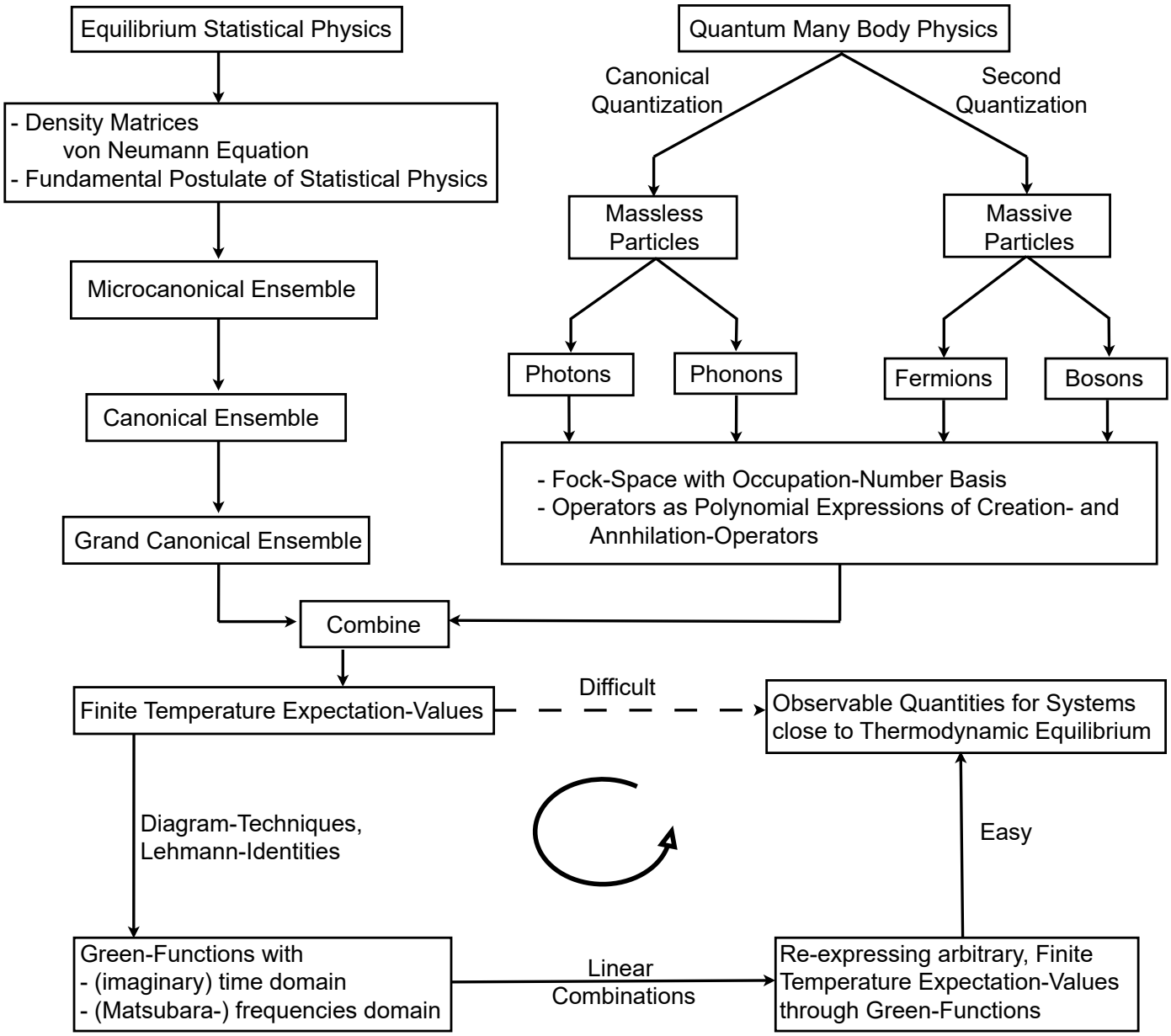


Figure 6.1.: Particles being creataed and annihilated, mapping from one sub-Hilbert-space to another.

[1] Hans Bethe lecture held at MIT Nov. 21 1977 `https://www.youtube.com/watch?v=E61UR4Lbifo`, timestamp: 01h 11min

Outline of the Presentation



7. Fundamentals I - Hilbert-Spaces, States and Operators

7.1. The Many-Body-Formalism for Distinguishable Objects

Fact 7.1 Let $\mathcal{H}_1, \dots, \mathcal{H}_n$ denote the single-particle-Hilbert-spaces with respective scalar-products of n (pairwise) distinguishable *objects*[1]. Then the Hilbert-space $\mathscr{H}$ of the total system is given as tensor product

$$\mathscr{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_n \equiv \bigotimes_{j=1}^{n} \mathcal{H}_j \tag{7.1}$$

with sesqui-linear scalar-product defined on product-states as

$$\langle \psi_1 \otimes \cdots \otimes \psi_n, \psi_1' \otimes \cdots \otimes \psi_n' \rangle_{\mathscr{H}} := \langle \psi_1, \psi_1' \rangle_{\mathcal{H}_1} \cdots \langle \psi_n, \psi_n' \rangle_{\mathcal{H}_n} \equiv \prod_{j=1}^{n} \langle \psi_j, \psi_j' \rangle_{\mathcal{H}_j}. \tag{7.2}$$

which is extended by linearity on the entire tensor-product.

Remark 7.1.1 Notice also that if $e_1^i, e_2^i, \dots, e_{\mathrm{d}_i}^i$ denote bases of $\mathcal{H}_i$, then the products

$$\left\{ e_{l_1}^1 \otimes \cdots \otimes e_{l_n}^n \quad \middle| \quad (l_1, \dots, l_n) \in \bigtimes_{j=1}^{n} \mathbb{N}_{\mathrm{d}_j} \right\} \tag{7.3}$$

form a basis of $\mathscr{H}$.

Fact 7.2 Phonons, photons and electrons are pairwise distinguishable from another.

[1] We are using the term "object", in order to represent a "wave" or a "particle" object.

7.2. The Many-Body-Formalism for Indistinguishable Particles (Second Quantization, Algebraic Formalism)

7.2.1. Algebras in Many Particle Physics

Definition 7.3 Let $\mathbb{K}$ be a field and $\mathcal{A}$ be a vector space over $\mathbb{K}$ equipped with an additional binary operation

$$\begin{aligned} \odot : \mathcal{A} \times \mathcal{A} &\to \mathcal{A} \\ (x\,,\, x') &\mapsto x \odot x'. \end{aligned} \tag{7.4}$$

Then $\mathcal{A}$ is an *associative algebra over* $\mathbb{K}$, if for all $x, y, z \in \mathcal{A}$ and $a, b \in \mathbb{K}$ the following identities hold

1. Right distributivity: $(x + y) \odot z = x \odot z + y \odot z$,
2. Left distributivity: $z \odot (x + y) = z \odot x + z \odot y$,
3. Compatibility with scalars: $(ax) \odot (by) = (ab)(x \odot y)$,
4. Associativity[2]: $(x \odot y) \odot z = x \odot (y \odot z)$.

Remark 7.3.1 For $x, y \in \mathcal{A}$ one calls $x \odot y$ the product of x and y and the binary operation is oftentimes referred to as *multiplication*. An associative algebra over a field $\mathbb{K}$ is sometimes called a *associative* $\mathbb{K}$*-algebra*, and $\mathbb{K}$ is called the *base-field*.

Remark 7.3.2 The algebra $\mathcal{A}$ is called *unitary*, if there exists an element $1 \in \mathcal{A}$ such that

$$\forall x \in \mathcal{A} : 1 \odot x = x \odot 1 = x. \tag{7.5}$$

Remark 7.3.3 When we construct the Fock-space in Definition 7.6, the product will be denoted by the so-called "zeta-product" $\odot \equiv \textcircled{\zeta}$. This will stress the interpretation of objects in the Fock-space as wavefunctions with coordinate-representations. In the constructions of the so-called "ζ-algebra" and the "polynomial algebra" in Definitions 7.15, 16.1 we will use the usual product symbol.

Definition 7.4 Let $\mathcal{A}$ be a vector-space over the field $\mathbb{K}$ with a basis. We define[3] the *associative, unitary algebra generated by* $\mathbb{K} \oplus \mathcal{A}$, as all formal polynomial expressions that one can build with the elements (or, equivalently, the basis elements) of $\mathcal{A}$, given coefficients from the field $\mathbb{K}$ and obeying the relations in Definition 7.3.

The initial situation (which one encounters quite naturally for particle-like objects in physics) is as follows.

[2] This requirement is not unique in the literature. There are non-associative algebras. We will however not be concerned with them.

[3] We don't give this object a symbol, because we will make use of this object three times. Depending on the situation it will be referenced with a different symbol. In order to avoid confusion, we leave out a symbol in this definition.

Notation 7.5 Let $\mathcal{H} = \text{span}_{\mathbb{C}} \left\{ |1\rangle, |2\rangle, \dots |\mathrm{d}_{\mathcal{H}}\rangle \right\}$ be a single-particle Hilbert-space with (not neccessarily, but oftentimes orthonormal) basis, corresponding to wavefunctions

$$\langle\, x \mid i \,\rangle \equiv \psi_i(x). \tag{7.6}$$

Definition 7.6 We define the *Fock-space* $\mathscr{F}_\zeta \equiv \mathscr{F}_\zeta(\mathcal{H})$ of the complex vector space $\mathcal{H}$ as the associative, unitary algebra generated by $\mathbb{C} \oplus \mathcal{H}$ with binary operation $\textcircled{\zeta}$ which we call ζ*-product* and relations

$$\forall |\psi\rangle, |\psi'\rangle \in \mathcal{H} : \quad |\psi\rangle \,\textcircled{\zeta}\, |\psi'\rangle - \zeta |\psi'\rangle \,\textcircled{\zeta}\, |\psi\rangle = 0. \tag{7.7}$$

Remark 7.6.1 One distinguishes two cases:

- For $\zeta = -1$, the Fock-space is called the *exterior algebra* and it is commonly denoted with $\wedge(\mathcal{H})$.
- For $\zeta = +1$, the Fock-space is called the *symmetric algebra* and commonly denoted with $\mathrm{S}(\mathcal{H})$.

Remark 7.6.2 We will occasioanlly denote the vectors and the algebra-product in a different way (without the Bra-Ket-Notation, or with adapted Bra-Ket-Notation) as

$$|\psi\rangle \,\textcircled{\zeta}\, |\psi'\rangle \equiv |\psi \,\textcircled{\zeta}\, \psi'\rangle = \psi \,\textcircled{\zeta}\, \psi'. \tag{7.8}$$

We do this out of notational convenience, for example if double-bra-kets appear otherwise, as in Equations (7.15), (7.31). The meaning of the notation will be clear from the respective context.

Theorem 7.7 The Fock space factorizes into subspaces s.t.

$$\mathscr{F}_\zeta(\mathcal{H}) = \mathscr{F}_\zeta^0(\mathcal{H}) \oplus \mathscr{F}_\zeta^1(\mathcal{H}) \oplus \mathscr{F}_\zeta^2(\mathcal{H}) \oplus \dots \equiv \begin{cases} \bigoplus_{n=0}^{\mathrm{d}_{\mathcal{H}}} \wedge^n(\mathcal{H}) & \text{for } \zeta = -1 \\ \bigoplus_{n=0}^{\infty} \mathrm{S}^n(\mathcal{H}) & \text{for } \zeta = +1 \end{cases} \tag{7.9}$$

with convention $\mathscr{F}_\zeta^0(\mathcal{H}) \equiv \mathbb{C}$ and dimensions

$$\dim_{\mathbb{C}} \mathscr{F}_\zeta^n(\mathcal{H}) = \begin{cases} \binom{\mathrm{d}_{\mathcal{H}}}{n} & \text{for } \zeta = -1 \\ \binom{\mathrm{d}_{\mathcal{H}} + n - 1}{n} & \text{for } \zeta = +1 \end{cases} \tag{7.10}$$

Proof 7.7 See Appendix, Proofs, page 510.

Remark 7.7.1 Note further the identity for fermions

$$\dim_{\mathbb{C}} \mathscr{F}^n_{-1}(\mathcal{H}) = \binom{\mathrm{d}_{\mathcal{H}}}{n} = \binom{\mathrm{d}_{\mathcal{H}}}{\mathrm{d}_{\mathcal{H}} - n} = \dim_{\mathbb{C}} \mathscr{F}^{\mathrm{d}_{\mathcal{H}} - n}_{-1}(\mathcal{H}) \tag{7.11}$$

Corollary 7.8 For $0 \leq n^2 \ll \mathrm{d}_{\mathcal{H}}$, one finds the asymptotic behaviour

$$\dim_{\mathbb{C}} \mathscr{F}^n_{\zeta}(\mathcal{H}) \approx \frac{1}{n!} \left(\dim_{\mathbb{C}} \mathcal{H}\right)^n . \tag{7.12}$$

Proof 7.8 Follows by expanding the binomial coefficients, cancelling terms and using the asymptotic behaviour of the factorials.[4] Write $d \equiv \mathrm{d}_{\mathcal{H}}$ and keep n fixed. By Theorem 7.7,

$$\binom{d}{n} = \frac{d(d-1)\cdots(d-n+1)}{n!} = \frac{d^n}{n!} \prod_{k=0}^{n-1} \left(1 - \frac{k}{d}\right),$$

$$\binom{d+n-1}{n} = \frac{(d+n-1)\cdots(d+1)d}{n!} = \frac{d^n}{n!} \prod_{k=0}^{n-1} \left(1 + \frac{k}{d}\right).$$

Both products tend to 1 for $n^2/d \to 0$, which proves the claim for $n^2 \ll \mathrm{d}_{\mathcal{H}}$.

Lemma 7.9 It follows for the dimension of the Fock-space

$$\dim_{\mathbb{C}} \mathscr{F}_{\zeta}(\mathcal{H}) = \begin{cases} 2^{\mathrm{d}_{\mathcal{H}}} & \text{for } \zeta = -1, \\ \infty & \text{for } \zeta = +1. \end{cases} \tag{7.13}$$

Proof 7.9 The bosonic case is trivial. For the dimension of the fermionic Fock-space one finds

$$\dim_{\mathbb{C}} \Lambda(\mathcal{H}) = \sum_{n=0}^{\mathrm{d}_{\mathcal{H}}} \binom{\mathrm{d}_{\mathcal{H}}}{n} = 2^{\mathrm{d}_{\mathcal{H}}}. \tag{7.14}$$

as a special case of the binomial theorem $(1+1)^d = \sum_n \binom{d}{n} 1^n 1^{d-n}$.

Fact 7.10 By specifiying the product of the algebra, we can interprete it's elements as many-particle-wavefunctions. As the single-particle-wavefunctions are already defined by assumption, this procedure happens inductively.

Definition 7.11 Consider two elements $\psi \in \mathscr{F}^p_{\zeta}(\mathcal{H})$ and $\phi \in \mathscr{F}^q_{\zeta}(\mathcal{H})$ of the corresponding degree subspaces in the algebra. We define the *coordinate-representation* of the corresponding wave-function for $p+q$ particles as

[4] Cf., for example, [64].

$$\begin{aligned}\left\langle x_1, \dots, x_{p+q} \,|\, \psi \,\textcircled{\zeta}\, \phi \right\rangle &\equiv \left(\psi \,\textcircled{\zeta}\, \phi\right)(x_1, \dots, x_{p+q}) \\ &:= \frac{1}{p!q!} \sum_{\pi \in \mathrm{S}_{p+q}} \mathrm{sign}(\pi)^{1-\theta(\zeta)} \psi(x_{\pi(1)}, \dots, x_{\pi(p)}) \phi(x_{\pi(p+1)}, \dots, x_{\pi(p+q)}).\end{aligned} \tag{7.15}$$

Remark 7.11.1 Notice that, depending on the nature of the single-particle wavefunctions (scalar-wavefunctions that solve a Schrödinger-equation or spinor-wavefunctions that solve a Pauli-equation) the concrete meaning of the "coordinates" $x_\bullet$ is being specified from the context.

Corollary 7.12 For $\psi_i \in \mathscr{F}^k_\zeta(\mathcal{H})$, $\phi \in \mathscr{F}^l_\zeta(\mathcal{H})$, $\chi \in \mathscr{F}^m_\zeta(\mathcal{H})$ one finds for the ζ-product the following rules for the wavefunctions w.r.t. their coordinate representation:

1. $\left(\psi_1 + \psi_2\right) \textcircled{\zeta}\, \phi = \psi_1 \textcircled{\zeta}\, \phi + \psi_2 \textcircled{\zeta}\, \phi$ (linearity),
2. $(\psi \textcircled{\zeta}\, \phi) \textcircled{\zeta}\, \chi = \psi \textcircled{\zeta}\, (\phi \textcircled{\zeta}\, \chi)$ (associativity),
3. $\psi \textcircled{\zeta}\, \phi = \zeta^{kl} \phi \textcircled{\zeta}\, \psi$ (Koszul-sign-rule).

Proof 7.12 See Appendix, Proofs, page 512.

Remark 7.12.1 Notice that the third equation gives the compatibility of the ζ-product with eq. (7.7).

Definition 7.13 On the direct sum $\mathcal{H} \oplus \mathcal{H}^*$ we define the *ζ-bilinearform* B_ζ as mapping

$$\begin{aligned}B_\zeta : \mathcal{H} \oplus \mathcal{H}^* \times \mathcal{H} \oplus \mathcal{H}^* &\longrightarrow \mathbb{C} \\ (|v\rangle + \langle\phi|\,,\, |v'\rangle + \langle\phi'|) &\mapsto B_\zeta(|v\rangle + \langle\phi|\,,\, |v'\rangle + \langle\phi'|) \equiv \langle\phi|v'\rangle - \zeta\langle\phi'|v\rangle\end{aligned}$$

Lemma 7.14 Notice that this bilinearform is (anti-)symmetric depending on the statistics of the system:

$$\forall u, u' \in \mathcal{H} \oplus \mathcal{H}^* : \quad B_\zeta(u, u') + \zeta B_\zeta(u', u) = 0 \tag{7.16}$$

Proof 7.14 See Appendix, Proofs, page 512.

Definition 7.15 We define the *ζ-algebra* $\mathscr{A}_\zeta(\mathcal{H} \oplus \mathcal{H}^*, B_\zeta)$ as the associative algebra generated by $\mathbb{C} \oplus \mathcal{H} \oplus \mathcal{H}^*$ with relations

$$\forall u, u' \in \mathcal{H} \oplus \mathcal{H}^* : \quad uu' - \zeta u'u = B_\zeta(u, u') \tag{7.17}$$

Remark 7.15.1 Again, one distinguishes two cases:

- For $\zeta = -1$, the underlying algebra is a so-called *Clifford-algebra*.
- For $\zeta = +1$, the underlying algebra is a so-called *Weyl-algebra*.

Definition 7.16 We define the *statistical commutator*, or ζ*-commutator* as

$$\left[A, B\right]_\zeta \equiv AB - \zeta BA. \tag{7.18}$$

Remark 7.16.1 This definition is a little bit tricky since it is a magnet for confusion and errors. We are following the prefactor-convention from [4, p. 44], [38, p. 13], in contrast to the prefactor-convention from [7, p. 43], [38, p. 15].[5].

Remark 7.16.2 Notice that this definition becomes generalized later on in Definition 8.12.

Lemma 7.17 A useful identity relates the ordinary commutator to statistical commutators

$$[A, BC] = [A, B]_\zeta C + \zeta B[A, C]_\zeta. \tag{7.19}$$

Proof 7.17 See Appendix, Proofs, page 512.

7.2.2. Representation and Scalar-Product on the Fock-Space

In order to define operators on the Fock-space, we will define a representation

$$\begin{aligned} \mathscr{A}_\zeta(\mathcal{H} \oplus \mathcal{H}^*, B_\zeta) \times \mathscr{F}_\zeta &\longrightarrow \mathscr{F}_\zeta \\ (x\,,\,\xi) &\longmapsto x \cdot \xi. \end{aligned} \tag{7.20}$$

We will do so inductively.

Fact 7.18 Since $\mathscr{A}_\zeta(\mathcal{H} \oplus \mathcal{H}^*, B_\zeta)$ is generated by $\mathbb{C} \oplus \mathcal{H} \oplus \mathcal{H}^*$, it suffices to specify the *action / multiplication* in Equation (7.20) for

$$\text{(1) scalars:} \quad x \equiv k \in \mathbb{C} \subset \mathscr{A}_\zeta(\mathcal{H} \oplus \mathcal{H}^*, B_\zeta) \tag{7.21}$$

$$\text{(2) vectors:} \quad x = |\psi\rangle \equiv c^+_{|\psi\rangle} \in \mathcal{H} \subset \mathscr{A}_\zeta(\mathcal{H} \oplus \mathcal{H}^*, B_\zeta) \tag{7.22}$$

$$\text{(3) dual-vectors:} \quad x = \langle\psi| \equiv c_{\langle\psi|} \in \mathcal{H}^* \subset \mathscr{A}_\zeta(\mathcal{H} \oplus \mathcal{H}^*, B_\zeta) \tag{7.23}$$

whereas *multiplication by scalars* is given by the structure of a complex vector space.

[5] Notice that there is an inconsistency within the book from Negele and Orland!

Definition 7.19 *Multiplication by vectors* is defined by the statistical product computed inside the algebra

$$c^+_{|\psi\rangle} \cdot |\xi\rangle \equiv c^+_{|\psi\rangle}\,|\xi\rangle \;:=\; |\,\psi\,\rangle \,\textcircled{\zeta}\, |\,\xi\,\rangle \equiv |\,\psi \,\textcircled{\zeta}\, \xi\,\rangle. \tag{7.24}$$

Remark 7.19.1 The notation $c^+_{|\psi\rangle}$ is used in order to dinstinguish the algebra element $|\psi\rangle \equiv |\psi\rangle + 0 \in \mathscr{A}_\zeta(\mathcal{H} \oplus \mathcal{H}^*, B_\zeta)$ from its concrete realization as a linear operator $c^+_{|\psi\rangle}$ on $\mathscr{F}_\zeta$.

Remark 7.19.2 Note also that this multiplication increases the degree of a state in a statistical sense (in physics language: the number of particles):

- For $\zeta = +1$ we obtain a mapping $c^+_{|\psi\rangle} :\ \mathrm{S}^l(\mathcal{H}) \to \mathrm{S}^{l+1}(\mathcal{H})$.
- For $\zeta = -1$ we obtain a mapping $c^+_{|\psi\rangle} :\ \Lambda^l(\mathcal{H}) \to \Lambda^{l+1}(\mathcal{H}) \cup \{0\}$, that either increases the degree of a state, or maps it to zero.

Remark 7.19.3 Notice further, that one immediately finds the linearity

$$c^+_{\lambda|\psi\rangle+\lambda'|\psi'\rangle} = \lambda c^+_{|\psi\rangle} + \lambda' c^+_{|\psi'\rangle}. \tag{7.25}$$

for $\lambda, \lambda' \in \mathbb{C}$.

Definition 7.20 *Multiplication by co-vectors* is defined recursively and denoted as

$$\begin{array}{lll} c_{\langle\phi|} \cdot 1 & := 0 & \\ c_{\langle\phi|} \cdot |\psi\rangle & := B_\zeta(\langle\phi|,\, |\psi\rangle) = \langle\phi|\psi\rangle & \text{for } |\psi\rangle \in \mathcal{H} \subset \mathscr{F}_\zeta \\ c_{\langle\phi|} \cdot |\xi \,\textcircled{\zeta}\, \eta\rangle & := \left(c_{\langle\phi|} \cdot |\xi\rangle\right) \,\textcircled{\zeta}\, |\eta\rangle + \zeta^l |\xi\rangle \,\textcircled{\zeta}\, \left(c_{\langle\phi|} \cdot |\eta\rangle\right) & \text{for } |\xi\rangle, |\eta\rangle \in \mathscr{F}_\zeta \end{array} \tag{7.26}$$

whereas $|\,\xi\,\rangle \in \mathscr{F}^l_\zeta(\mathcal{H})$ in the last equation.

Remark 7.20.1 Here, again, the notation $c_{\langle\phi|}$ is used in order to dinstinguish the algebra element $\langle\phi| \equiv 0 + \langle\phi| \in \mathscr{A}_\zeta(\mathcal{H} \oplus \mathcal{H}^*, B_\zeta)$ from its concrete realization as a linear operator $c_{\langle\phi|}$ on $\mathscr{F}_\zeta$.

Remark 7.20.2 Notice that due to linearity, we obtain the action

$$\left(k + c^+_{|\psi\rangle} + c_{\langle\phi|}\right) \cdot |\xi\rangle \equiv k|\xi\rangle + c^+_{|\psi\rangle}\,|\xi\rangle + c_{\langle\phi|}|\xi\rangle \tag{7.27}$$

Remark 7.20.3 Notice that the commutation relations in Equation (7.17) imply the relations

$$1_{\mathscr{F}_\zeta}\langle\phi|\psi\rangle = c_{\langle\phi|}c^+_{|\psi\rangle} - \zeta c^+_{|\psi\rangle}c_{\langle\phi|}$$
$$0 = c_{\langle\phi|}c_{\langle\phi'|} - \zeta c_{\langle\phi'|}c_{\langle\phi|} = c^+_{|\upsilon\rangle}c^+_{|\upsilon'\rangle} - \zeta c^+_{|\psi'\rangle}c^+_{|\psi\rangle}$$

Notation 7.21 Let us fix an orthonormal basis $\mathcal{H} = \mathrm{span}_{\mathbb{C}}\left\{|1\rangle, |2\rangle, \ldots |\mathrm{d}_{\mathcal{H}}\rangle\right\}$ of the single-particle Hilbert-space with dual basis $\mathcal{H}^* = \mathrm{span}_{\mathbb{C}}\left\{\langle 1|, \langle 2|, \ldots \langle \mathrm{d}_{\mathcal{H}}|\right\}$, and let us write $\langle i| \equiv |c_{\langle i|} \equiv c_i$ and $|i\rangle \equiv c^+_{|i\rangle} \equiv c^+_i$.

Lemma 7.22 Using the duality-relation $\langle i|j\rangle = \delta_{ij}$ we obtain the relations (7.17) in the form

$$[c_i, c^+_j]_\zeta = \delta_{ij}, \quad [c_i, c_j]_\zeta = [c^+_i, c^+_j]_\zeta = 0 \tag{7.28}$$

Proof 7.22 We insert special elements into the relations (7.17), following [65, Eqs. (3.17), (3.21)]. For $u = 0 + \langle i|$ and $u' = |j\rangle + 0$ the definition of B_ζ gives $B_\zeta(u, u') = \langle i|j\rangle - \zeta \cdot 0 = \delta_{ij}$, i.e. $c_i c^+_j - \zeta c^+_j c_i = \delta_{ij}$. For $u = 0 + \langle i|$, $u' = 0 + \langle j|$ and for $u = |i\rangle + 0$, $u' = |j\rangle + 0$ one has $B_\zeta(u, u') = 0$, since B_ζ only pairs vectors with co-vectors. This gives $[c_i, c_j]_\zeta = 0$ and $[c^+_i, c^+_j]_\zeta = 0$.

Remark 7.22.1 In the next subsection, we will elucidate how c_i and c^+_i will be acting as linear operators on the Fock-space with its canonical Hermitian scalar-product. In that setting, the operator $c^+_i \equiv c^\dagger_i$ will turn out to be the „Hermitian adjoint“ of c_i.

Theorem 7.23 Equations (7.26), (7.24) define a representation of the algebra $\mathscr{A}_\zeta(\mathcal{H} \oplus \mathcal{H}^*, B_\zeta)$ on the complex vector-space $\mathscr{F}_\zeta$.

Proof 7.23 See Appendix, Proofs, page 512.

We follow [65, Sects. 2.8 and 3.3, pp. 39 f. and 63 f.], where the cases $\zeta = -1$ and $\zeta = +1$ are treated separately and the commutation relations of the creation and annihilation operators are left as problems (Eqs. (2.55), (3.28) there). Throughout, $\psi, \psi', \psi_k \in \mathcal{H}$ and $\phi, \phi' \in \mathcal{H}^*$, where we write $\phi(\psi) = \langle\phi|\psi\rangle$, and we abbreviate $c_\phi \equiv c_{\langle\phi|}$, $c^+_\psi \equiv c^+_{|\psi\rangle}$.

Step 1 (Annihilation operators on products, well-definedness). Choosing $\xi = \psi_1$ (degree $l = 1$) in the last line of Equation (7.26) gives $c_\phi(\psi_1 \,\textcircled{\zeta}\, \eta) = \langle\phi|\psi_1\rangle\,\eta + \zeta\,\psi_1 \,\textcircled{\zeta}\, (c_\phi\eta)$. By induction on n it follows that

$$c_\phi\left(\psi_1 \,\textcircled{\zeta}\, \cdots \,\textcircled{\zeta}\, \psi_n\right) = \sum_{k=1}^{n} \zeta^{k-1}\langle\phi|\psi_k\rangle\,\psi_1 \,\textcircled{\zeta}\, \cdots \,\textcircled{\zeta}\, \widehat{\psi_k} \,\textcircled{\zeta}\, \cdots \,\textcircled{\zeta}\, \psi_n, \tag{7.29}$$

where the hat denotes omission. Conversely, one may read the right-hand side as the definition of c_ϕ. Being multilinear in $\psi_1, \ldots, \psi_n$, it is well-defined on the tensor algebra $\bigoplus_n \mathcal{H}^{\otimes n}$, of which $\mathscr{F}_\zeta(\mathcal{H})$ is the quotient by the two-sided ideal generated by the elements $r = \psi \otimes \psi' - \zeta\psi' \otimes \psi$. Splitting the sum into $k \le l$ and $k > l$ shows that it obeys the ζ-Leibniz rule of Equation (7.26), and it annihilates the generators of the ideal:

$$c_\phi(r) = \langle\phi|\psi\rangle\psi' + \zeta\langle\phi|\psi'\rangle\psi - \zeta\langle\phi|\psi'\rangle\psi - \zeta^2\langle\phi|\psi\rangle\psi' = 0.$$

By the Leibniz rule, c_ϕ therefore maps the ideal into itself and descends to a well-defined linear operator on $\mathscr{F}_\zeta(\mathcal{H})$, which is the one of Equation (7.26). Zirnbauer calls it a *derivation* (bosons, p. 63) resp. defines it by the *anti-Leibniz rule* (fermions, p. 40). Notice also that $\phi \mapsto c_\phi$ and $\psi \mapsto c_\psi^+$ are linear.

Step 2 (Relations between the operators). We show, as operators on $\mathscr{F}_\zeta(\mathcal{H})$,

$$\text{(a)}\quad c_\psi^+ c_{\psi'}^+ - \zeta c_{\psi'}^+ c_\psi^+ = 0, \qquad \text{(b)}\quad c_\phi c_\psi^+ - \zeta c_\psi^+ c_\phi = \langle\phi|\psi\rangle\, 1_{\mathscr{F}_\zeta}, \qquad \text{(c)}\quad c_\phi c_{\phi'} - \zeta c_{\phi'} c_\phi = 0.$$

(a) By associativity and the relations (7.7), $c_\psi^+ c_{\psi'}^+ \xi = \psi \textcircled{\zeta} \psi' \textcircled{\zeta} \xi = \zeta\, \psi' \textcircled{\zeta} \psi \textcircled{\zeta} \xi = \zeta c_{\psi'}^+ c_\psi^+ \xi$.

(b) The Leibniz rule with the degree-one factor ψ gives $c_\phi c_\psi^+ \xi = c_\phi(\psi \textcircled{\zeta} \xi) = \langle\phi|\psi\rangle\,\xi + \zeta\, \psi \textcircled{\zeta} (c_\phi \xi) = \langle\phi|\psi\rangle\,\xi + \zeta c_\psi^+ c_\phi \xi$.

(c) Let $D = c_\phi c_{\phi'} - \zeta c_{\phi'} c_\phi$. Since annihilation operators lower the degree and annihilate $1 \in \mathscr{F}_\zeta^0$, D vanishes on $\mathscr{F}_\zeta^0 \oplus \mathscr{F}_\zeta^1$. Using (b) twice and $\zeta^2 = 1$ one finds

$$\begin{aligned} D c_\psi^+ &= c_\phi \left(\langle\phi'|\psi\rangle + \zeta c_\psi^+ c_{\phi'} \right) - \zeta c_{\phi'} \left(\langle\phi|\psi\rangle + \zeta c_\psi^+ c_\phi \right) \\ &= \langle\phi'|\psi\rangle c_\phi + \zeta \left(\langle\phi|\psi\rangle + \zeta c_\psi^+ c_\phi \right) c_{\phi'} - \zeta\langle\phi|\psi\rangle c_{\phi'} - \left(\langle\phi'|\psi\rangle + \zeta c_\psi^+ c_{\phi'} \right) c_\phi = c_\psi^+ D. \end{aligned}$$

Since $\mathscr{F}_\zeta^{n+1}$ is spanned by elements $\psi \textcircled{\zeta} \eta = c_\psi^+ \eta$ with $\eta \in \mathscr{F}_\zeta^n$, induction on the degree gives $D(\psi \textcircled{\zeta} \eta) = c_\psi^+ D\eta = 0$.

Step 3 (Representation). For $u = \psi + \phi$ and $u' = \psi' + \phi'$ in $\mathcal{H} \oplus \mathcal{H}^*$ set $\rho(u) = c_\psi^+ + c_\phi$. With (a)–(c) and $[Y, X]_\zeta = -\zeta[X, Y]_\zeta$ we obtain [65, p. 64]

$$\rho(u)\rho(u') - \zeta\rho(u')\rho(u) = [c_\psi^+, c_{\psi'}^+]_\zeta + [c_\psi^+, c_{\phi'}]_\zeta + [c_\phi, c_{\psi'}^+]_\zeta + [c_\phi, c_{\phi'}]_\zeta = -\zeta\langle\phi'|\psi\rangle + \langle\phi|\psi'\rangle = B_\zeta(u, u')\, 1_{\mathscr{F}_\zeta}.$$

Since $\mathscr{A}_\zeta(\mathcal{H} \oplus \mathcal{H}^*, B_\zeta)$ is the associative, unitary algebra generated by $\mathbb{C} \oplus \mathcal{H} \oplus \mathcal{H}^*$ subject only to the relations (7.17), the linear map $k + u \mapsto k\, 1_{\mathscr{F}_\zeta} + \rho(u)$ extends uniquely to a homomorphism of unitary algebras $\rho : \mathscr{A}_\zeta(\mathcal{H} \oplus \mathcal{H}^*, B_\zeta) \to \mathrm{End}(\mathscr{F}_\zeta)$ (products of generators are mapped to compositions of operators, which is compatible with the relations by the computation above). With $x \cdot \xi := \rho(x)\xi$ all conditions of a representation (cf. the appendix) hold: $\rho(x)$ is linear, $1 \cdot \xi = \xi$, and $x_1 \cdot (x_2 \cdot \xi) = \rho(x_1)\rho(x_2)\xi = \rho(x_1 x_2)\xi = (x_1 x_2) \cdot \xi$, where the compatibility with the product is automatic since the composition of linear operators is associative [65, p. 40].

Theorem 7.24 One obtains the identities

$$\begin{aligned} c_j^\dagger \cdot \left(c_{i_1}^\dagger c_{i_2}^\dagger \cdots c_{i_l}^\dagger |\,0\,\rangle \right) &= c_j^\dagger c_{i_1}^\dagger c_{i_2}^\dagger \cdots c_{i_l}^\dagger |\,0\,\rangle \\ c_j \cdot \left(c_{i_1}^\dagger c_{i_2}^\dagger \cdots c_{i_l}^\dagger |\,0\,\rangle \right) &= \delta_{ji_1} c_{i_2}^\dagger c_{i_3}^\dagger \cdots c_{i_l}^\dagger |\,0\,\rangle \quad + \quad \zeta\delta_{ji_2} c_{i_1}^\dagger c_{i_3}^\dagger \cdots c_{i_l}^\dagger |\,0\,\rangle \quad + \quad \ldots \quad + \quad \zeta^{l-1}\delta_{ji_l} c_{i_1}^\dagger c_{i_2}^\dagger \cdots c_{i_{l-1}}^\dagger |\,0\,\rangle \\ &= \sum_{k=1}^{l} \zeta^{k+1} \delta_{j,i_k} c_{i_1}^\dagger \cdots c_{i_{k-1}}^\dagger c_{i_{k+1}}^\dagger \cdots c_{i_l}^\dagger |\,0\,\rangle \\ &= \sum_{k=1}^{l} \zeta^{k+1} \delta_{j,i_k} c_{i_1}^\dagger \cdots \widehat{c_{i_k}^\dagger} \cdots c_{i_l}^\dagger |\,0\,\rangle. \end{aligned}$$

Proof 7.24 See Appendix, Proofs, page 513.

These are Equations (3.30), (3.31), (3.34), (3.35) in [65, pp. 64 f.]. Since $|0\rangle = 1$ is the unit of $\mathscr{F}_\zeta$, Definition (7.24) and associativity give $c^\dagger_{i_1} c^\dagger_{i_2} \cdots c^\dagger_{i_l} |0\rangle = |i_1\rangle \zeta |i_2\rangle \zeta \cdots \zeta |i_l\rangle$, and applying $c^\dagger_j$ puts the factor $|j\rangle$ in front, which is the first identity. The second identity is Equation (7.29) for $\phi = \langle j|$ and $\psi_k = |i_k\rangle$, with $\langle j|i_k\rangle = \delta_{j,i_k}$ and $\zeta^{k-1} = \zeta^{k+1}$ (as $\zeta^2 = 1$). In particular, the annihilation operators annihilate the vacuum, $c_j|0\rangle = 0$ [65, Eq. (3.32)].

Definition 7.25 We introduce a mapping on the subspace

$$\langle \cdot, \cdot \rangle_{\mathscr{F}^n_\zeta} : \mathscr{F}^n_\zeta \times \mathscr{F}^n_\zeta \to \mathbb{C} \tag{7.30}$$

by defining it through permanents ($\zeta = +1$) and determinants ($\zeta = -1$) as

$$\begin{aligned} \left\langle \psi_1 \zeta \cdots \zeta \psi_n, \psi'_1 \zeta \cdots \zeta \psi'_n \right\rangle_{\mathscr{F}_\zeta(\mathcal{H})} &:= \sum_{\pi \in \mathrm{S}_n} \mathrm{sign}(\pi)^{1-\theta(\zeta)} \prod_{j=1}^{n} \left\langle \psi_n, \psi'_{\pi(n)} \right\rangle_{\mathcal{H}} \\ &= \begin{vmatrix} \langle \psi_1, \psi'_1 \rangle_{\mathcal{H}} & \cdots & \langle \psi_1, \psi'_n \rangle_{\mathcal{H}} \\ \vdots & \ddots & \vdots \\ \langle \psi_n, \psi'_1 \rangle_{\mathcal{H}} & \cdots & \langle \psi_n, \psi'_n \rangle_{\mathcal{H}} \end{vmatrix}_\zeta \end{aligned} \tag{7.31}$$

and sesqui-linear continuation.

Corollary 7.26 This mapping is a well-defined hermitian scalar-product on $\mathscr{F}^n_\zeta$, meaning that it is sesqui-linear, positive definite.

Proof 7.26 See Appendix, Proofs, page 513.

Zirnbauer states that the scalar products (3.36), (3.38) have all properties required of a Hermitian scalar product [65, Sect. 3.4, p. 66]; we supply the proof. First, the product in Equation (7.31) has to be read as $\prod_{j=1}^n \langle \psi_j, \psi'_{\pi(j)} \rangle_{\mathcal{H}}$ (the index n in the factors is a typo). We write $s_\zeta(\pi) := \mathrm{sign}(\pi)^{1-\theta(\zeta)}$, i.e. $s_{-1} = \mathrm{sign}$ and $s_{+1} \equiv 1$. Then s_ζ is multiplicative, $s_\zeta(\pi^{-1}) = s_\zeta(\pi)$, and $s_\zeta(\tau) = \zeta$ for every transposition τ. For an $n \times n$ matrix M let $|M|_\zeta = \sum_\pi s_\zeta(\pi) \prod_j M_{j,\pi(j)}$ (determinant for $\zeta = -1$, permanent for $\zeta = +1$). By substituting $\pi \to \tau\pi$ resp. $\pi \to \pi^{-1}$ in the sum one finds: (i) interchanging two rows or two columns of M multiplies $|M|_\zeta$ by ζ; (ii) $|M^T|_\zeta = |M|_\zeta$; (iii) $|M|_\zeta$ is linear in each row and in each column.

Step 1 (Well-defined and sesqui-linear). By (iii), the right-hand side of Equation (7.31) is anti-linear in each ψ_j and linear in each ψ'_k. Hence it defines a sesqui-linear form on $\mathcal{H}^{\otimes n} \times \mathcal{H}^{\otimes n}$. The space $\mathscr{F}^n_\zeta$ is the quotient of $\mathcal{H}^{\otimes n}$ by the span of all tensors that contain a factor $\psi \otimes \psi' - \zeta \psi' \otimes \psi$ in two adjacent slots. On such tensors the form vanishes, since by (i) the interchange of the two corresponding rows (resp. columns) produces a factor ζ, such that the two contributions cancel, $X - \zeta \cdot \zeta X = 0$. Hence the form descends to $\mathscr{F}^n_\zeta \times \mathscr{F}^n_\zeta$.

Step 2 (Hermitian). Interchanging the two arguments replaces the matrix $M_{jk} = \langle \psi_j, \psi'_k \rangle$ by $M'_{jk} = \langle \psi'_j, \psi_k \rangle = \overline{M_{kj}}$, so by (ii) $|M'|_\zeta = \overline{|M|_\zeta}$.

Step 3 (Positive definite). Let $\{|i\rangle\}$ be an orthonormal basis of $\mathcal{H}$. For a non-decreasing sequence $I = (i_1 \le \ldots \le i_n)$ let $e_I = |i_1\rangle \zeta \cdots \zeta |i_n\rangle$, and let $n_i(I)$ be the number of occurrences of i in I. By the relations (7.7),

every product of n basis vectors equals $\pm e_I$ for some non-decreasing I; for $\zeta = -1$ repeated factors give zero, as $\psi \circledast_\zeta \psi = -\psi \circledast_\zeta \psi$. Thus the e_I span $\mathscr{F}_\zeta^n$. Moreover,

$$\langle e_I, e_J \rangle = \sum_{\pi \in S_n} s_\zeta(\pi) \prod_{a=1}^{n} \delta_{i_a, j_{\pi(a)}} = \delta_{IJ} \prod_i n_i(I)!, \tag{7.32}$$

since a non-zero term requires J to be a rearrangement of I, i.e. $J = I$ for non-decreasing sequences, and then exactly the $\prod_i n_i(I)!$ permutations that only permute equal indices contribute, each with $s_\zeta(\pi) = 1$ (for $\zeta = -1$ all $n_i \leq 1$, such that only $\pi = \mathrm{id}$ contributes). This generalizes $\langle v^n, v'^n \rangle = n! \langle v, v' \rangle^n$ [65, p. 66]. For $\Psi = \sum_I a_I e_I$ we thus obtain $\langle \Psi, \Psi \rangle = \sum_I |a_I|^2 \prod_i n_i(I)! \geq 0$, with equality if and only if all $a_I = 0$, i.e. $\Psi = 0$.

Remark 7.26.1 We continue this hermitian scalar-product on $\mathscr{F}_\zeta^n$ in the canonical way on the entire Fock-space $\mathscr{F}_\zeta$, by defining the scalar-product of different particle-number subspaces to vanish. Equipped with a scalar-product, the Fock-space is a Hilbert-space.

7.2.3. Occupation-Number States and Bra-Ket-Isomorphism

Definition 7.27 We introduce the *statistical occupation-numbers* as set

$$\mathbb{N}_\zeta = \begin{cases} \{0, 1\} & \text{for } \zeta = -1, \\ \{0, 1, 2, \ldots, \infty\} & \text{for } \zeta = +1. \end{cases} \tag{7.33}$$

Definition 7.28 We define the *occupation-number-states* as elements of the Fock-space

$$\mathscr{B}_\zeta = \left\{ \frac{\left(c_1^\dagger\right)^{n_1}}{\sqrt{n_1!}} \cdots \frac{\left(c_{\mathrm{d}_\mathcal{H}}^\dagger\right)^{n_{\mathrm{d}_\mathcal{H}}}}{\sqrt{n_{\mathrm{d}_\mathcal{H}}!}} |\,0\,\rangle =: |n_1, \ldots, n_{\mathrm{d}_\mathcal{H}}\rangle \;\middle|\; n_1, \ldots, n_{\mathrm{d}_\mathcal{H}} \in \mathbb{N}_\zeta \right\} \subset \mathscr{F}_\zeta. \tag{7.34}$$

with the so-called *vacuum-state* a.k.a *the empty state*

$$|\,0\,\rangle \equiv |\mathrm{vac.}\rangle \equiv 1 \in \mathbb{C}. \tag{7.35}$$

Remark 7.28.1 In the *physics-jargon*, one usually says that such a state possesses n_1 particles in the first state, n_2 particles in the second state, etc.

Remark 7.28.2 Notice that this definition comes with different prefactor-conventions in the literature. We are following the convention of [62], in contrast to, for example, the convention of [51].

Recall now that in a complex vector space with sesqui-linear scalar-product there is a canonically defined operation of taking the hermitian adjoint[6] of an operator, denoted by the symbol †.

[6]The hermitian adjoint of an operator A w.r.t. a scalar-product is defined such that the following equation

Corollary 7.29 One has

$$\left(c_i^+\right)^\dagger = c_i \Longleftrightarrow c_i^+ = c_i^\dagger. \tag{7.37}$$

Proof 7.29 See Appendix, Proofs, page 513.

This is the Problem at the end of [65, Sect. 3.4, p. 66]. With the adjoint defined as in the footnote above, we have to show $\langle c_i^+\xi, \eta\rangle = \langle \xi, c_i\eta\rangle$ for all $\xi, \eta \in \mathscr{F}_\zeta$. By (anti-)linearity it suffices to take $\xi = \psi_1 \textcircled{\zeta} \cdots \textcircled{\zeta} \psi_{n-1} \in \mathscr{F}_\zeta^{n-1}$ and $\eta = \psi_1' \textcircled{\zeta} \cdots \textcircled{\zeta} \psi_m' \in \mathscr{F}_\zeta^m$. For $m \neq n$ both sides vanish, since different particle-number subspaces are orthogonal. For $m = n$, the left-hand side is $|M|_\zeta$ for the matrix with first row $\langle i|\psi_k'\rangle$ and further rows $\langle \psi_a, \psi_k'\rangle$, since $c_i^+\xi = |i\rangle \textcircled{\zeta} \psi_1 \textcircled{\zeta} \cdots \textcircled{\zeta} \psi_{n-1}$. We expand along the first row (Laplace expansion; its cofactor signs, $(-1)^{1+k}$ for determinants and 1 for permanents, both equal ζ^{k-1}) and use Equation (7.29) with $\phi = \langle i|$:

$$\begin{aligned}\langle c_i^+\xi, \eta\rangle &= \sum_{k=1}^n \zeta^{k-1}\langle i|\psi_k'\rangle \left\langle \xi, \psi_1' \textcircled{\zeta} \cdots \textcircled{\zeta} \widehat{\psi_k'} \textcircled{\zeta} \cdots \textcircled{\zeta} \psi_n' \right\rangle \\ &= \left\langle \xi, \sum_{k=1}^n \zeta^{k-1}\langle i|\psi_k'\rangle\, \psi_1' \textcircled{\zeta} \cdots \textcircled{\zeta} \widehat{\psi_k'} \textcircled{\zeta} \cdots \textcircled{\zeta} \psi_n' \right\rangle = \langle \xi, c_i\eta\rangle.\end{aligned}$$

Hence $(c_i^+)^\dagger = c_i$, and taking the adjoint once more, $c_i^+ = c_i^\dagger$. The argument covers fermions ($(c_j^+)^\dagger = c_j$) and bosons ($(a_j^+)^\dagger = a_j$) simultaneously.

Fact 7.30 The Hermitian scalar-product on the single-particle-Hilbert-space $\langle\cdot,\cdot\rangle : \mathcal{H}\times\mathcal{H} \longrightarrow \mathbb{C}$ determines a one-to-one-correspondence between the Hilbert-space and the dual-space known as *ket-bra-bijection* a.k.a. *Riesz-isomorphism*

$$\begin{aligned}\mathrm{J}_\mathcal{H} &: \mathcal{H} \longrightarrow \mathcal{H}^* \\ &\lambda|\,\psi\,\rangle \mapsto \mathrm{J}_\mathcal{H}(\lambda\psi) \equiv \lambda^*\langle\,\psi\,| \equiv \lambda^*\langle\,\psi\,|\,\bullet\,\rangle\end{aligned}$$

for $\lambda \in \mathbb{C}$.

We will introduce this one-to-one-correspondence as well for the Fock-space.

Lemma 7.31 It holds $\mathscr{F}_\zeta(\mathcal{H})^* \simeq \mathscr{F}_\zeta(\mathcal{H}^*)$ as a vector-space.

Proof 7.31 See Appendix, Proofs, page 514.

Cf. [65, Sect. 3.4, p. 67], where the identification $\wedge(V)^* \cong \wedge(V^*)$ is used. For $\phi_1, \ldots, \phi_n \in \mathcal{H}^*$ and $\psi_1, \ldots, \psi_n \in \mathcal{H}$ we define the pairing

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$$TBD \qquad \langle A\xi, \eta\rangle = \langle \xi, A^\dagger\eta\rangle \quad \text{for all } \xi, \eta \tag{7.36}$$

is fulfilled.

$$\left(\phi_1 \circledast \cdots \circledast \phi_n\right)\left(\psi_1 \circledast \cdots \circledast \psi_n\right) := \left|\left(\phi_j(\psi_k)\right)_{j,k}\right|_\zeta ,$$

and set the pairing between different degrees to zero. Exactly as in Step 1 of the proof of Corollary 7.26 (now bilinear instead of sesqui-linear), this is a well-defined bilinear pairing $\mathscr{F}_\zeta^n(\mathcal{H}^*) \times \mathscr{F}_\zeta^n(\mathcal{H}) \to \mathbb{C}$, i.e. a linear map $\Theta_n : \mathscr{F}_\zeta^n(\mathcal{H}^*) \to \mathscr{F}_\zeta^n(\mathcal{H})^*$. With the dual bases $\{\langle i|\}, \{|j\rangle\}$, the vectors e_I of Step 3 there, and $f_I = \langle i_1| \circledast \cdots \circledast \langle i_n|$, the computation (7.32) gives $f_I(e_J) = \delta_{IJ} \prod_i n_i(I)!$. Hence Θ_n is injective: if $\Theta_n(\sum_I a_I f_I) = 0$, evaluating at e_J gives $a_J = 0$. Since $\dim \mathscr{F}_\zeta^n(\mathcal{H}^*) = \dim \mathscr{F}_\zeta^n(\mathcal{H}) = \dim \mathscr{F}_\zeta^n(\mathcal{H})^* < \infty$ by Theorem 7.7 (as $\dim \mathcal{H}^* = \dim \mathcal{H}$), each Θ_n is an isomorphism.

For $\zeta = -1$, the Fock-space is finite-dimensional and $\mathscr{F}_{-1}(\mathcal{H})^* = \bigoplus_n \mathscr{F}_{-1}^n(\mathcal{H})^* \simeq \bigoplus_n \mathscr{F}_{-1}^n(\mathcal{H}^*) = \mathscr{F}_{-1}(\mathcal{H}^*)$. For $\zeta = +1$, the full algebraic dual of the infinite direct sum $\mathrm{S}(\mathcal{H}) = \bigoplus_n \mathrm{S}^n(\mathcal{H})$ is the direct *product* $\prod_n \mathrm{S}^n(\mathcal{H})^*$, which is strictly larger than $\bigoplus_n \mathrm{S}^n(\mathcal{H})^* \simeq \mathrm{S}(\mathcal{H}^*)$. In this case the Lemma has to be read for the graded (restricted) dual $\bigoplus_n \mathscr{F}_\zeta^n(\mathcal{H})^*$, i.e. for linear functionals that are non-zero only on finitely many particle-number subspaces. These are all functionals used in the following, e.g. $\langle 0|c_{i_n} \cdots c_{i_1}$.

Definition 7.32 We introduce the *ket-bra-correspondence of the Fock-space* as

$$\begin{aligned} \mathrm{J}_{\mathscr{F}} &: \mathscr{F}_\zeta(\mathcal{H}) \longrightarrow \mathscr{F}_\zeta(\mathcal{H}^*) \\ &\lambda |\,\psi_1\,\rangle \circledast \ldots \circledast |\,\psi_n\,\rangle \mapsto \lambda^* \,\mathrm{J}_{\mathcal{H}}(\psi_1) \circledast \ldots \circledast \mathrm{J}_{\mathcal{H}}(\psi_n) = \lambda^* \langle\,\psi_1\,| \circledast \ldots \circledast \langle\,\psi_n\,| \end{aligned}$$

with $\lambda \in \mathbb{C}$.

Corollary 7.33 In *physics-notation*, this implies the ket-bra-correspondence

$$\mathscr{F}(\mathcal{H}) \ni \quad \left(c_1^\dagger\right)^{n_1} \ldots \left(c_{\mathrm{d}_\mathcal{H}}^\dagger\right)^{n_{\mathrm{d}_\mathcal{H}}} |0\rangle \quad \mapsto \quad \mathrm{J}_{\mathscr{F}}\left(\left(c_1^\dagger\right)^{n_1} \ldots \left(c_{\mathrm{d}_\mathcal{H}}^\dagger\right)^{n_{\mathrm{d}_\mathcal{H}}} |0\rangle\right) = \langle 0| c_{\mathrm{d}_\mathcal{H}}^{n_{\mathrm{d}_\mathcal{H}}} \cdots c_1^{n_1} \quad \in \mathscr{F}(\mathcal{H}^*) \tag{7.38}$$

with $\lambda \in \mathbb{C}$.

Proof 7.33 Throughout, $n_1, \ldots, n_{\mathrm{d}_\mathcal{H}}$ are *finite* occupation-numbers, i.e. $n_i \in \{0,1\}$ for $\zeta = -1$ and $n_i \in \{0,1,2,\ldots\}$ for $\zeta = +1$ (for $n_i = \infty$ the expression $\left(c_i^\dagger\right)^{n_i}$ is not defined). Recall from Theorem 7.7 that every $\xi \in \mathscr{F}_\zeta(\mathcal{H})$ is a *finite* sum of elements of the subspaces $\mathscr{F}_\zeta^n(\mathcal{H})$. Hence c_i and $c_i^\dagger$ map $\mathscr{F}_\zeta(\mathcal{H})$ into itself, so all expressions below are well-defined, also for $\zeta = +1$, where these operators are unbounded. We abbreviate $\langle \cdot, \cdot \rangle \equiv \langle \cdot, \cdot \rangle_{\mathscr{F}_\zeta(\mathcal{H})}$ and use $c_i^+ = c_i^\dagger$ (Corollary 7.29).

Step 1: Bras as functionals. Under the identification of Lemma 7.31, i.e. $\mathscr{F}_\zeta(\mathcal{H}^*) \simeq \mathscr{F}_\zeta(\mathcal{H})^*$, an element $\varphi_1 \circledast \ldots \circledast \varphi_n \in \mathscr{F}_\zeta^n(\mathcal{H}^*)$ acts on $\xi_1 \circledast \ldots \circledast \xi_m \in \mathscr{F}_\zeta^m(\mathcal{H})$ by the permanent / determinant of the matrix $\left(\varphi_j(\xi_k)\right)_{j,k}$ if $n = m$, and by 0 if $n \neq m$; this is extended linearly. For $\varphi_j = \mathrm{J}_{\mathcal{H}}(\psi_j) = \langle\,\psi_j\,|$ one has $\varphi_j(\xi_k) = \langle \psi_j, \xi_k \rangle_{\mathcal{H}}$, so this is precisely the right-hand-side of Equation (7.31). Since both $\mathrm{J}_{\mathscr{F}}$ and $\psi \mapsto \langle \psi, \cdot\,\rangle$ are anti-linear, it follows that

$$\left(\mathrm{J}_{\mathscr{F}}(\psi)\right)(\xi) = \langle\,\psi\,,\,\xi\,\rangle \qquad \text{for all } \psi, \xi \in \mathscr{F}_\zeta(\mathcal{H}). \tag{7.39}$$

Step 2: Meaning of the right-hand-side. In *physics-notation*, a bra followed by an operator B denotes the composition of the bra with B, i.e. $\langle\, \psi \mid B \equiv \mathrm{J}_{\mathscr{F}}(\psi) \circ B$. With Equation (7.39) and $\psi = |\, 0\,\rangle$ this means

$$(\langle 0|\, B)\,(\xi) = \langle\, |\, 0\,\rangle\,,\ B\,\xi\,\rangle \qquad \text{for all } \xi \in \mathscr{F}_\zeta(\mathcal{H}). \tag{7.40}$$

Step 3: Adjoint of a product. Let $A_1, \ldots, A_m$ be operators on $\mathscr{F}_\zeta(\mathcal{H})$ that have adjoints $A_1^\dagger, \ldots, A_m^\dagger$, i.e. $\langle A_j x, y\rangle = \langle x, A_j^\dagger y\rangle$ for all $x, y \in \mathscr{F}_\zeta(\mathcal{H})$. Moving one factor at a time to the right slot gives

$$\langle\, A_1 A_2 \cdots A_m\, x\,,\ y\,\rangle = \left\langle\, A_2 \cdots A_m\, x\,,\ A_1^\dagger\, y\,\right\rangle = \ldots = \left\langle\, x\,,\ A_m^\dagger \cdots A_2^\dagger A_1^\dagger\, y\,\right\rangle, \tag{7.41}$$

i.e. $\left(A_1 \cdots A_m\right)^\dagger = A_m^\dagger \cdots A_1^\dagger$: taking the adjoint *reverses the order* of the factors. (Formally, this is an induction on m.)

Step 4: Conclusion. Write the creation-string as a product of $m = n_1 + \ldots + n_{\mathrm{d}_\mathcal{H}}$ single creation operators,

$$A := \left(c_1^\dagger\right)^{n_1} \cdots \left(c_{\mathrm{d}_\mathcal{H}}^\dagger\right)^{n_{\mathrm{d}_\mathcal{H}}} = \underbrace{c_1^\dagger \cdots c_1^\dagger}_{n_1} \cdots \underbrace{c_{\mathrm{d}_\mathcal{H}}^\dagger \cdots c_{\mathrm{d}_\mathcal{H}}^\dagger}_{n_{\mathrm{d}_\mathcal{H}}}. \tag{7.42}$$

By Corollary 7.29, $\left(c_i^\dagger\right)^\dagger = c_i$. Hence Equation (7.41) yields

$$A^\dagger = \underbrace{c_{\mathrm{d}_\mathcal{H}} \cdots c_{\mathrm{d}_\mathcal{H}}}_{n_{\mathrm{d}_\mathcal{H}}} \cdots \underbrace{c_1 \cdots c_1}_{n_1} = c_{\mathrm{d}_\mathcal{H}}^{n_{\mathrm{d}_\mathcal{H}}} \cdots c_1^{n_1}. \tag{7.43}$$

Combining Equations (7.39), (7.41) (with $x = |\, 0\,\rangle$, $y = \xi$) and (7.40) (with $B = A^\dagger$), we find for all $\xi \in \mathscr{F}_\zeta(\mathcal{H})$

$$\mathrm{J}_{\mathscr{F}}\left(A\,|\, 0\,\rangle\right)(\xi) = \langle\, A\,|\, 0\,\rangle\,,\ \xi\,\rangle = \left\langle\, |\, 0\,\rangle\,,\ A^\dagger\,\xi\,\right\rangle = \left(\langle 0|\, c_{\mathrm{d}_\mathcal{H}}^{n_{\mathrm{d}_\mathcal{H}}} \cdots c_1^{n_1}\right)(\xi). \tag{7.44}$$

Two linear functionals on $\mathscr{F}_\zeta(\mathcal{H})$ that agree on every ξ are equal. By Lemma 7.31 they are therefore also equal as elements of $\mathscr{F}_\zeta(\mathcal{H}^*)$, which proves the claim.

Theorem 7.34 The states defined in Equation (7.34) are an orthonormal basis $\mathscr{F}_\zeta(\mathcal{H})$

Proof 7.34 See Appendix, Proofs, page 514.

Cf. [65, Eqs. (3.37), (3.39), p. 66], where the statement is given without proof. The occupation-numbers are finite ($n_i = \infty$ is excluded, cf. the proof of Corollary 7.33). Applying the creation operators from right to left (Definition (7.24)) gives

$$\left(c_1^\dagger\right)^{n_1} \cdots \left(c_{\mathrm{d}_\mathcal{H}}^\dagger\right)^{n_{\mathrm{d}_\mathcal{H}}} |0\rangle = \underbrace{|1\rangle \,\zeta\, \cdots \,\zeta\, |1\rangle}_{n_1} \,\zeta\, \cdots \,\zeta\, \underbrace{|\,\mathrm{d}_\mathcal{H}\rangle \,\zeta\, \cdots \,\zeta\, |\,\mathrm{d}_\mathcal{H}\rangle}_{n_{\mathrm{d}_\mathcal{H}}} = e_{I(n)},$$

where $I(n)$ is the non-decreasing sequence that contains each i exactly n_i times (notation of Step 3 of the proof of Corollary 7.26). Hence $|n_1, \ldots, n_{\mathrm{d}_\mathcal{H}}\rangle = \left(\prod_i n_i!\right)^{-1/2} e_{I(n)}$.

Spanning. By Step 3 of the proof of Corollary 7.26, the e_I with non-decreasing I of length n span $\mathscr{F}_\zeta^n$, and every such I equals $I(n)$ for exactly one tuple of occupation-numbers with $\sum_i n_i = n$ (for $\zeta = -1$, strictly increasing sequences correspond to $n_i \in \{0,1\}$). Together with $\mathscr{F}_\zeta = \bigoplus_n \mathscr{F}_\zeta^n$ (Theorem 7.7), the states (7.34) span $\mathscr{F}_\zeta$.

Orthonormality. By Equation (7.32),

$$\langle n_1, \dots, n_{\mathrm{d}_\mathcal{H}} | m_1, \dots, m_{\mathrm{d}_\mathcal{H}} \rangle = \frac{\langle e_{I(n)}, e_{I(m)} \rangle}{\sqrt{\prod_i n_i! \prod_i m_i!}} = \prod_i \delta_{n_i, m_i},$$

which also holds for $\sum_i n_i \neq \sum_i m_i$ by the orthogonality of different particle-number subspaces. Orthonormal vectors are linearly independent, so the states form an orthonormal basis.

7.2.4. Operators on the Fock-Space

One-Body-Operators

Notation 7.35 Let $L \in \mathrm{End}(\mathcal{H})$ be a linear operator on the single-particle-Hilbert-space $\mathcal{H}$.

Definition 7.36 *The second quantized version of* L is given as element of the ζ-algebra (which we denote by the same symbol for notational simplicity):

$$\mathrm{End}(\mathcal{H}) \ni \quad L \quad \mapsto \quad L^{2\mathrm{Q}} \equiv \sum_{j=1}^{\mathrm{d}_\mathcal{H}} c^+_{L|j\rangle}\, c_j \quad \in \mathscr{A}_\zeta(\mathcal{H} \oplus \mathcal{H}^*, B_\zeta) \tag{7.45}$$

Remark 7.36.1 For notational simplicity, one oftentimes simply drops the upper index and writes $L^{2\mathrm{Q}} \equiv L$ as it is clear from the context what is meant. The same hodls true for other operators in second quantization.

Corollary 7.37 On the one-particle-subspace of the Fock-space, this mapping acts precisely as its first quantized version, i.e. TBMathematised.

With the identification $\mathscr{F}_\zeta^1(\mathcal{H}) = \mathcal{H}$ one has

$$L^{2\mathrm{Q}}|\psi\rangle = L|\psi\rangle \qquad \text{for all } |\psi\rangle \in \mathcal{H}.$$

More generally, $L^{2\mathrm{Q}}$ acts on products of single-particle states as

$$L^{2\mathrm{Q}}\left(\psi_1 \,\textcircled{\zeta}\, \cdots \,\textcircled{\zeta}\, \psi_n\right) = \sum_{k=1}^{n} \psi_1 \,\textcircled{\zeta}\, \cdots \,\textcircled{\zeta}\, \psi_{k-1} \,\textcircled{\zeta}\, (L\psi_k) \,\textcircled{\zeta}\, \psi_{k+1} \,\textcircled{\zeta}\, \cdots \,\textcircled{\zeta}\, \psi_n. \tag{7.46}$$

Proof 7.37 See Appendix, Proofs, page 514.

We follow [65, Sect. 3.5, Fact and Proof on pp. 67 f.], where the fermionic case is shown and the bosonic one is said to work „the same albeit for some sign changes“; we treat both at once. Since $\{|j\rangle\}$ is an orthonormal basis, $\sum_j \langle j|\psi\rangle|j\rangle = |\psi\rangle$. With $c_j|\psi\rangle = \langle j|\psi\rangle \cdot 1$ (Equation (7.26)) one finds

$$L^{2Q}|\psi\rangle = \sum_j c^+_{L|j\rangle}\left(\langle j|\psi\rangle \cdot 1\right) = \sum_j \langle j|\psi\rangle\, L|j\rangle = L|\psi\rangle.$$

For products we use Equation (7.29) and move the created factor $L|j\rangle$ (of degree one) past the $k-1$ single-particle factors in front of slot k. By the Koszul-sign-rule (Corollary 7.12) this produces another factor ζ^{k-1}, and $\zeta^{2(k-1)} = 1$:

$$\begin{aligned} L^{2Q}\left(\psi_1 \textcircled{\zeta} \cdots \textcircled{\zeta} \psi_n\right) &= \sum_j \sum_{k=1}^{n} \zeta^{k-1} \langle j|\psi_k\rangle \left(L|j\rangle\right) \textcircled{\zeta} \psi_1 \textcircled{\zeta} \cdots \textcircled{\zeta} \widehat{\psi_k} \textcircled{\zeta} \cdots \textcircled{\zeta} \psi_n \\ &= \sum_{k=1}^{n} \psi_1 \textcircled{\zeta} \cdots \textcircled{\zeta} \Big(\sum_j \langle j|\psi_k\rangle\, L|j\rangle \Big) \textcircled{\zeta} \cdots \textcircled{\zeta} \psi_n = \sum_{k=1}^{n} \psi_1 \textcircled{\zeta} \cdots \textcircled{\zeta} (L\psi_k) \textcircled{\zeta} \cdots \textcircled{\zeta} \psi_n. \end{aligned}$$

Remark 7.37.1 This implies, that the second-quantized-version of L is mathematically considered to be a so-called *derivation*[7].

Lemma 7.38 This is an hermitian operator on the Fock-space.

Proof 7.38 See Appendix, Proofs, page 514.

The statement is to be read as: if L is hermitian, then so is L^{2Q}. More generally, $(L^{2Q})^\dagger = (L^\dagger)^{2Q}$. To see this, we use Lemma 7.39, $\overline{\langle i|L|j\rangle} = \langle j|L^\dagger|i\rangle$, and $(c_i^\dagger c_j)^\dagger = c_j^\dagger c_i$. The latter follows from Corollary 7.29 and the reversal of the order of factors under the adjoint (Step 3 of the proof of Corollary 7.33). Then

$$(L^{2Q})^\dagger = \sum_{i,j} \overline{\langle i|L|j\rangle}\, (c_i^\dagger c_j)^\dagger = \sum_{i,j} \langle j|L^\dagger|i\rangle\, c_j^\dagger c_i = (L^\dagger)^{2Q}.$$

For $L = L^\dagger$ this gives $(L^{2Q})^\dagger = L^{2Q}$. (For $\zeta = +1$, the adjoint relation $\langle A\xi, \eta\rangle = \langle \xi, A^\dagger\eta\rangle$ is understood for all $\xi, \eta \in \mathscr{F}_\zeta$, i.e. for finite sums of states with finite particle-numbers, on which these unbounded operators are defined.)

Lemma 7.39 Switching to standard-physics-notation, we obtain the second-quantized version of the one-body-operator L as

[7] TBElaborated? A linear map D on an algebra is called a *derivation*, if it obeys the Leibniz rule $D(xy) = (Dx)y + x(Dy)$, cf. [65, p. 63]. By Equation (7.46), $L^{2Q}(\xi \textcircled{\zeta} \eta) = (L^{2Q}\xi) \textcircled{\zeta} \eta + \xi \textcircled{\zeta} (L^{2Q}\eta)$ for all $\xi, \eta \in \mathscr{F}_\zeta(\mathcal{H})$, i.e. L^{2Q} is the unique derivation of $\mathscr{F}_\zeta(\mathcal{H})$ that extends L from $\mathcal{H} = \mathscr{F}^1_\zeta(\mathcal{H})$ [65, Fact on p. 67]. In contrast, the annihilation operators obey the ζ-twisted Leibniz rule of Equation (7.26).

$$\mathrm{End}(\mathcal{H}) \ni \quad L \quad \mapsto \quad L^{2Q} \equiv \sum_{i,j=1}^{d_{\mathcal{H}}} \langle i|L|j\rangle\, c_i^\dagger c_j \quad \in \mathscr{A}_\zeta(\mathcal{H}\oplus\mathcal{H}^*, B_\zeta). \tag{7.47}$$

Proof 7.39 See Appendix, Proofs, page 514.

Cf. [65, Eq. (3.42), p. 68]. Expanding $L|j\rangle = \sum_i |i\rangle\langle i|L|j\rangle$ in the orthonormal basis and using the linearity of $|\psi\rangle \mapsto c^+_{|\psi\rangle}$ gives $c^+_{L|j\rangle} = \sum_i \langle i|L|j\rangle\, c_i^+$. Hence $L^{2Q} = \sum_{i,j}\langle i|L|j\rangle\, c_i^+ c_j$, and $c_i^+ = c_i^\dagger$ by Corollary 7.29.

Definition 7.40 We define the *number-operator* as the second-quantized version of the identity-operator on the single-particle-Hilbert-space, i.e.

$$\mathrm{End}(\mathcal{H}) \ni \quad \mathbb{1} \quad \mapsto \quad \mathbb{1}^{2Q} \equiv \sum_{j=1}^{d_{\mathcal{H}}} c_j^\dagger c_j \equiv N \quad \in \mathscr{A}_\zeta(\mathcal{H}\oplus\mathcal{H}^*, B_\zeta). \tag{7.48}$$

Corollary 7.41 For basis-states as in equation (7.34) we have

$$\hat{N}|n_1,\dots,n_{d_{\mathcal{H}}}\rangle = \sum_{j=1}^{d_{\mathcal{H}}} n_j |n_1,\dots,n_{d_{\mathcal{H}}}\rangle. \tag{7.49}$$

Proof 7.41 TBD

By Equation (7.46) with $L = \mathbb{1}$, $N(\psi_1 \zeta \cdots \zeta \psi_n) = n\,\psi_1 \zeta \cdots \zeta \psi_n$, i.e. N acts as $n\cdot\mathbb{1}$ on $\mathscr{F}^n_\zeta$. The state $|n_1,\dots,n_{d_{\mathcal{H}}}\rangle$ is obtained from $|0\rangle \in \mathscr{F}^0_\zeta$ by applying $\sum_j n_j$ creation operators, so it lies in $\mathscr{F}^n_\zeta$ with $n = \sum_j n_j$, which proves the claim. Finer, for the projector $P_j = |j\rangle\langle j|$ Lemma 7.39 gives $P_j^{2Q} = c_j^\dagger c_j$, the *occupation number operator* [65, p. 69]. Since $P_j|i\rangle = \delta_{ij}|i\rangle$, Equation (7.46) counts the factors $|j\rangle$ in $e_{I(n)}$ (notation of the proof of Theorem 7.34), i.e.

$$c_j^\dagger c_j\, |n_1,\dots,n_{d_{\mathcal{H}}}\rangle = n_j\, |n_1,\dots,n_{d_{\mathcal{H}}}\rangle, \qquad N = \sum_j c_j^\dagger c_j.$$

Lemma 7.42 For fermionic or bosonic operators, one finds in both cases the identity

$$[a_j^\dagger a_k, a_l^\dagger a_l] = a_j^\dagger a_l \delta_{k,l} - a_l^\dagger a_k \delta_{l,j} \tag{7.50}$$

Proof 7.42 Cf. Gross, AQM2013, Sheet 5, Exercise 1 a), c). (TBDigitalized)

(The exercise sheet of Gross is not contained in the Zirnbauer folder; we give a direct proof, cf. [65, Eq. (3.18)] for a related identity.) We write $a_j \equiv c_j$ and use the relations (7.28). Lemma 7.17 with $A = a_m^\dagger$, $B = a_j^\dagger$, $C = a_k$ gives

$$[a_m^\dagger, a_j^\dagger a_k] = [a_m^\dagger, a_j^\dagger]_\zeta\, a_k + \zeta\, a_j^\dagger\, [a_m^\dagger, a_k]_\zeta = 0 + \zeta\, a_j^\dagger \left(-\zeta [a_k, a_m^\dagger]_\zeta\right) = -\delta_{km}\, a_j^\dagger,$$

and analogously $[a_n, a_j^\dagger a_k] = [a_n, a_j^\dagger]_\zeta\, a_k + \zeta\, a_j^\dagger\, [a_n, a_k]_\zeta = \delta_{nj}\, a_k$. Hence $[a_j^\dagger a_k, a_m^\dagger] = \delta_{km} a_j^\dagger$ and $[a_j^\dagger a_k, a_n] = -\delta_{jn} a_k$, and with the Leibniz rule $[X, YZ] = [X, Y]Z + Y[X, Z]$ of the ordinary commutator we obtain, for fermions and bosons alike,

$$[a_j^\dagger a_k, a_m^\dagger a_n] = \delta_{km}\, a_j^\dagger a_n - \delta_{jn}\, a_m^\dagger a_k. \tag{7.51}$$

For $m = n = l$ this is the claimed identity.

Two-Body-Operators

Notation 7.43 Let $V \in \mathrm{End}(\mathcal{H} \otimes \mathcal{H})$ be a linear operator on the tensor product of two single-particle Hilbert-spaces.

Definition 7.44 The *second quantized version of* V is given as an element of the ζ-algebra

$$\mathrm{End}(\mathcal{H} \otimes \mathcal{H}) \ni \quad V \quad \mapsto \quad V^{2\mathrm{Q}} \equiv \frac{1}{2} \sum_{ijkl} \langle i,\, j|L|k,\, l\rangle\, c_i^\dagger c_j^\dagger c_l c_k \quad \in \mathscr{A}_\zeta(\mathcal{H} \oplus \mathcal{H}^*, B_\zeta). \tag{7.52}$$

Remark 7.44.1 Notice also the peculiarity that the two latest indices in the expression are contra-symmetrically exchanged in order to be a derivation of its first-quantized version.

Corollary 7.45 On the two-particle-subspace the second-quantized-version of V acts precisely as its first-quantized-version. TBMathematised.

In the Definition above, L is to be read as V (Zirnbauer denotes two-body operators by L [AQM, Eqs. (3.45)–(3.49)]), with the matrix elements $\langle i, j|V|k, l\rangle := \langle |i\rangle \otimes |j\rangle, V(|k\rangle \otimes |l\rangle)\rangle_{\mathcal{H}\otimes\mathcal{H}}$ [65, Eq. (3.46)]. We identify $\mathscr{F}_\zeta^2(\mathcal{H})$ with the (anti-)symmetric two-particle wavefunctions via the coordinate representation (7.15), i.e. via the injective map

$$\iota :\ \mathscr{F}_\zeta^2(\mathcal{H}) \to \mathcal{H} \otimes \mathcal{H}, \qquad \psi \,\textcircled{\zeta}\, \phi \mapsto \psi \otimes \phi + \zeta\, \phi \otimes \psi,$$

and denote by $P(\psi \otimes \phi) = \phi \otimes \psi$ the exchange operator. Then

$$\iota \circ V^{2\mathrm{Q}}\Big|_{\mathscr{F}_\zeta^2} = \frac{1}{2}\,(1 + \zeta P)\, V \circ \iota,$$

and in particular $\iota(V^{2\mathrm{Q}}\Psi) = V\iota(\Psi)$ for all $\Psi \in \mathscr{F}_\zeta^2$, if V commutes with the exchange of the two particles, $[V, P] = 0$ (as, e.g., the Coulomb interaction of the next section).

Proof 7.45 See Appendix, Proofs, page 514.

Zirnbauer states that the factor $\frac{1}{2}$ and the reversed order of the annihilation operators are needed for the agreement on the two-particle subspace [AQM, p. 70]; we verify this. Applying Equation (7.29) twice gives the scalar $c_l c_k(\psi \textcircled{\zeta} \phi) = \langle k|\psi\rangle\langle l|\phi\rangle + \zeta\langle k|\phi\rangle\langle l|\psi\rangle$, and $c_i^\dagger c_j^\dagger 1 = |i\rangle \textcircled{\zeta} |j\rangle$. With $\sum_{k,l}\langle i,j|V|k,l\rangle\langle k|\psi\rangle\langle l|\phi\rangle = \langle |i\rangle \otimes |j\rangle, V(\psi\otimes\phi)\rangle$ we obtain

$$V^{2Q}(\psi \textcircled{\zeta} \phi) = \frac{1}{2}\sum_{i,j}\langle |i\rangle\otimes|j\rangle, V\,(\psi\otimes\phi + \zeta\phi\otimes\psi)\rangle\,|i\rangle \textcircled{\zeta} |j\rangle = \frac{1}{2}\sum_{i,j}\left\langle |i\rangle\otimes|j\rangle, V\imath(\psi \textcircled{\zeta} \phi)\right\rangle |i\rangle \textcircled{\zeta} |j\rangle.$$

Applying $\imath$, using $\imath(|i\rangle \textcircled{\zeta} |j\rangle) = (1+\zeta P)(|i\rangle\otimes|j\rangle)$ and the completeness $\sum_{i,j}\langle |i\rangle\otimes|j\rangle, x\rangle\,|i\rangle\otimes|j\rangle = x$ in $\mathcal{H}\otimes\mathcal{H}$, gives $\imath V^{2Q}(\psi \textcircled{\zeta} \phi) = \frac{1}{2}(1+\zeta P)V\imath(\psi \textcircled{\zeta} \phi)$. If $[V,P]=0$, then with $P\imath = \zeta\imath$ (exchange of the two factors in the definition of $\imath$) and $\zeta^2 = 1$,

$$\frac{1}{2}(1+\zeta P)V\imath = \frac{1}{2}V(1+\zeta P)\imath = \frac{1}{2}V(\imath + \zeta^2\imath) = V\imath.$$

Without the exchange symmetry, V^{2Q} realizes the (anti-)symmetrized operator $\frac{1}{2}(1+\zeta P)V$. Correspondingly, one may (anti-)symmetrize the matrix elements, $V^{2Q} = \frac{1}{4}\sum_{ijkl}\left(\langle i,j|V|k,l\rangle + \zeta\langle i,j|V|l,k\rangle\right) c_i^\dagger c_j^\dagger c_l c_k$, where the second term is the *exchange matrix element* [65, Eq. (3.50)].

Remark 7.45.1 This again implies, that the second-quantized-version of V is mathematically considered to be a so-called derivation.

Lemma 7.46 This is an hermitian operator on the Fock-space.

Proof 7.46 See Appendix, Proofs, page 514.

As for one-body operators, the statement is to be read as: if V is hermitian, then so is V^{2Q}. Reversing the order of the factors under the adjoint and using $(c^\dagger)^\dagger = c$ gives $(c_i^\dagger c_j^\dagger c_l c_k)^\dagger = c_k^\dagger c_l^\dagger c_j c_i$. With $\overline{\langle i,j|V|k,l\rangle} = \langle k,l|V^\dagger|i,j\rangle$ and the relabelling $(i,j,k,l)\to(k,l,i,j)$ we obtain

$$(V^{2Q})^\dagger = \frac{1}{2}\sum_{ijkl}\langle k,l|V^\dagger|i,j\rangle\, c_k^\dagger c_l^\dagger c_j c_i = \frac{1}{2}\sum_{ijkl}\langle i,j|V^\dagger|k,l\rangle\, c_i^\dagger c_j^\dagger c_l c_k = (V^\dagger)^{2Q},$$

which equals V^{2Q} for $V = V^\dagger$.

n-Body-Operators

Definition 7.47 TBD Extension to higher-order-cases, even if they are not so relevant, to give an interpretation for SC

Let $V \in \mathrm{End}(\mathcal{H}^{\otimes n})$ be an n-body-operator with matrix elements

$$\langle i_1,\dots,i_n|V|j_1,\dots,j_n\rangle := \langle |i_1\rangle\otimes\cdots\otimes|i_n\rangle, V(|j_1\rangle\otimes\cdots\otimes|j_n\rangle)\rangle\,.$$

Its *second quantized version* is

$$V^{2Q} \equiv \frac{1}{n!} \sum_{i_1,\dots,i_n,j_1,\dots,j_n} \langle i_1,\dots,i_n|V|j_1,\dots,j_n\rangle\, c^\dagger_{i_1}\cdots c^\dagger_{i_n} c_{j_n}\cdots c_{j_1} \quad \in \mathscr{A}_\zeta(\mathcal{H}\oplus\mathcal{H}^*, B_\zeta).$$

For $n = 1$ and $n = 2$ this reduces to Lemma 7.39 and to the Definition of two-body operators [65, Eqs. (3.42), (3.49)]. As in the proof of Corollary 7.45 one shows the following. Iterating Equation (7.29) gives (Laplace expansion)

$$c_{j_n}\cdots c_{j_1}(\psi_1 \textcircled{\zeta} \cdots \textcircled{\zeta} \psi_n) = \Big|\big(\langle j_a|\psi_b\rangle\big)_{a,b}\Big|_\zeta .$$

With $\iota_n(\psi_1 \textcircled{\zeta} \cdots \textcircled{\zeta} \psi_n) = \sum_\pi s_\zeta(\pi)\,\psi_{\pi(1)}\otimes\cdots\otimes\psi_{\pi(n)}$ (the coordinate representation (7.15), iterated by associativity) and the (anti-)symmetrizer $S_\zeta = \sum_\pi s_\zeta(\pi)P_\pi$ one then finds $\iota_n\circ V^{2Q} = \frac{1}{n!}S_\zeta V\circ\iota_n$ on $\mathscr{F}^n_\zeta$. Hence, by $S_\zeta\iota_n = n!\,\iota_n$, V^{2Q} acts as V on the n-particle subspace, if V commutes with all permutations of the tensor factors.

Theorem 7.48 An Hermitian n-body-operator on $\bigotimes_{j=1}^{n}\mathcal{H}$ will be also Hermitian in its second quantized form as an operator on $\mathscr{F}_\zeta(\mathcal{H})$.

Proof 7.48 See Appendix, Proofs, page 514.

With the Definition above, the adjoint reverses the order of the $2n$ factors, $(c^\dagger_{i_1}\cdots c^\dagger_{i_n}c_{j_n}\cdots c_{j_1})^\dagger = c^\dagger_{j_1}\cdots c^\dagger_{j_n}c_{i_n}\cdots c_{i_1}$. With $\overline{\langle i_1,\dots,i_n|V|j_1,\dots,j_n\rangle} = \langle j_1,\dots,j_n|V^\dagger|i_1,\dots,i_n\rangle$ and the relabelling $i\leftrightarrow j$ we obtain, exactly as for $n = 1, 2$ (Lemmas 7.38, 7.46),

$$(V^{2Q})^\dagger = \frac{1}{n!}\sum\langle j_1,\dots,j_n|V^\dagger|i_1,\dots,i_n\rangle\, c^\dagger_{j_1}\cdots c^\dagger_{j_n}c_{i_n}\cdots c_{i_1} = (V^\dagger)^{2Q},$$

which equals V^{2Q} if $V = V^\dagger$.

7.2.5. Useful Formulae

| ========== | Begin: To Be Updated / Corrected for n-body operators | ========== |

The template was the clean derivation of the Landauer-formula; Cf. also Zirnbauer p. 67, 68.

Probably this holds for Fermions *and* Bosons... One step needs to be filled.

Corollary 7.49 Let A and B be linear operators on $\mathcal{H}$. Denote by $[A, B] = AB - BA$ their commutator. Then

$$\begin{aligned} [A, B]^{2Q} &= [A^{2Q}, B^{2Q}] \\ e^{A^{2Q}} B^{2Q} e^{-A^{2Q}} &= \left(e^{A} B e^{-A}\right)^{2Q}, \end{aligned} \tag{7.53}$$

Proof 7.49 The first identity is easily proven using the anticommutation relations

$$\begin{aligned} [A^{2Q}, B^{2Q}] &= \sum_{k,j,m,n} \langle e_k, Ae_j\rangle\langle e_m, Be_n\rangle [a_k^\dagger a_j, a_m^\dagger a_n] \\ &= \sum_{k,j,m,n} \langle e_k, Ae_j\rangle\langle e_m, Be_n\rangle \left(a_k^\dagger a_m \delta_{j,n} - a_m^\dagger a_j \delta_{k,n}\right) \\ &= \text{TBD} \\ &= \sum_{k,j} \langle e_k, (AB - BA) e_j\rangle a_k^\dagger a_j = [A, B]^{2Q}, \end{aligned} \tag{7.54}$$

while the second one is implied by the first equality, the Baker–Campbell–Hausdorff formula

$$e^{A^{2Q}} B^{2Q} e^{-A^{2Q}} = B^{2Q} + [A^{2Q}, B^{2Q}] + \frac{1}{2}[B^{2Q}, [B^{2Q}, A^{2Q}]] + \cdots,$$

and the linearity of the scalar-product.

Correction note and missing step. This is the Problem in [65, Sect. 3.5, p. 68]: second quantization of one-body operators is a Lie algebra homomorphism, $\widehat{[L, M]} = [\widehat{L}, \widehat{M}]$. Here $\{e_k\}$ is an orthonormal basis, $a_k \equiv c_{\langle e_k|}$, and $A^{2Q} = \sum_{k,j} \langle e_k, Ae_j\rangle a_k^\dagger a_j$ (Lemma 7.39).

1. By Equation (7.51), $[a_k^\dagger a_j, a_m^\dagger a_n] = \delta_{jm} a_k^\dagger a_n - \delta_{kn} a_m^\dagger a_j$, i.e. in the second line above $a_k^\dagger a_m \delta_{j,n}$ has to be replaced by $a_k^\dagger a_n \delta_{j,m}$. The missing step then reads, with the completeness $\sum_j \langle e_k, Ae_j\rangle\langle e_j, Be_n\rangle = \langle e_k, ABe_n\rangle$,

$$\begin{aligned} [A^{2Q}, B^{2Q}] &= \sum_{k,n} \Big(\sum_j \langle e_k, Ae_j\rangle\langle e_j, Be_n\rangle \Big) a_k^\dagger a_n - \sum_{m,j} \Big(\sum_k \langle e_m, Be_k\rangle\langle e_k, Ae_j\rangle \Big) a_m^\dagger a_j \\ &= \sum_{k,n} \langle e_k, ABe_n\rangle a_k^\dagger a_n - \sum_{m,j} \langle e_m, BAe_j\rangle a_m^\dagger a_j = \sum_{k,j} \langle e_k, (AB - BA) e_j\rangle a_k^\dagger a_j. \end{aligned}$$

   Since Equation (7.51) holds for $\zeta = \pm 1$, the identity holds for fermions *and* bosons.

2. The second-order term of the Baker-Campbell-Hausdorff series reads

$$\frac{1}{2}[A^{2Q}, [A^{2Q}, B^{2Q}]] \qquad \left(\text{not } \frac{1}{2}[B^{2Q}, [B^{2Q}, A^{2Q}]]\right).$$

In general, $e^X Y e^{-X} = \sum_{m=0}^{\infty} \frac{1}{m!} \mathrm{ad}_X^m(Y)$ with $\mathrm{ad}_X(Y) = [X, Y]$. Iterating the first identity and using the linearity of $L \mapsto L^{2Q}$ gives $\mathrm{ad}_{A^{2Q}}^m(B^{2Q}) = (\mathrm{ad}_A^m(B))^{2Q}$, and hence

$$e^{A^{2Q}} B^{2Q} e^{-A^{2Q}} = \sum_{m=0}^{\infty} \frac{1}{m!} \left(\mathrm{ad}_A^m(B)\right)^{2Q} = \left(e^A B e^{-A}\right)^{2Q}.$$

By Equation (7.46), one-body operators preserve the particle number, so all identities may be considered on the finite-dimensional subspaces $\mathscr{F}_\xi^n$, where the series converge.

| ========== | End: To Be Updated / Corrected for n-body operators | ========== |

7.3. Examples of Operators on the Fock-Space

7.3.1. One-Body-Operators

Notation 7.50 We consider the Hilbert-space of a crystal $\mathcal{H} = L^2(\mathbb{R}^3/\sim)$. The most important operator on the single-particle Hilbert-space is a Schrödinger-Kohn-Sham-Bloch-Hamiltonian H, containing kinetic, potential, Hartree- and exchange-potential as

$$H \equiv -\hbar^2 \frac{\Delta}{2m} + V_{\text{ionic}} + V_{\text{Hartree}} + V_{\text{XC}} \tag{7.55}$$

with action on the single-particle Hilbert-space as

$$\left\langle \mathbf{r} \,\middle|\, H \,\middle|\, \psi \right\rangle \equiv -\frac{\hbar^2}{2m} (\Delta\psi)(\mathbf{r}) + \left(V_{\text{ionic}} + V_{\text{Hartree}} + V_{\text{XC}}\right)(\mathbf{r})\,\psi(\mathbf{r}) \tag{7.56}$$

Corollary 7.51 Using the basis in which the Schrödinger-Kohn-Sham-Bloch-Hamiltonian is diagonal, we obtain

$$H^{2\text{Q}} \equiv \sum_{\substack{\mathbf{k},\mathbf{k}' \in \text{Q} \\ n,n' \in \{1,2,3,\dots\}}} \left\langle n, \mathbf{k} \,\middle|\, H \,\middle|\, n', \mathbf{k}' \right\rangle c^\dagger_{n,\mathbf{k}} c_{n',\mathbf{k}'} \equiv \sum_{\substack{\mathbf{k} \in \text{Q} \\ n \in \{1,2,3,\dots\}}} \epsilon_n(\mathbf{k}) c^\dagger_{n,\mathbf{k}} c_{n,\mathbf{k}} \tag{7.57}$$

Remark 7.51.1 Later on, we will consider the sub-Hilbert-space that is spanned by the so-called Wannier-states of a selected band-subspace. Then we will also consider individual term-contributions of the Hamiltonian in the Wannier-basis.

7.3.2. Two-Body-Operators

Notation 7.52 We consider the Hilbert-space of a crystal $\mathcal{H} = L^2(\mathbb{R}^3/\sim)$. The most important operator on the single-particle Hilbert-space is the Coulomb-interaction energy between two particles with charge e

$$V_{\text{Coulomb}} \left(\psi \otimes \psi'\right)(\mathbf{x}, \mathbf{x}') = \frac{e^2}{4\pi\epsilon_0 |\mathbf{x} - \mathbf{x}'|} \psi(\mathbf{x}) \psi'(\mathbf{x}') \tag{7.58}$$

Fact 7.53 After choosing a basis of $\mathcal{H}$ (and therefore, by extension, of its tensor-product with itself) we obtain the Coulomb-interaction in second quantization as

$$V^{2\text{Q}}_{\text{Coulomb}} \equiv \frac{1}{2} \sum_{ijkl \in \mathscr{A}} \langle i, j \mid V_{\text{Coulomb}} \mid k, l \rangle\, c^\dagger_i c^\dagger_j c_l c_k \tag{7.59}$$

with matrix elements

$$\langle i, j \mid V_{\text{Coulomb}} \mid k, l \rangle = \iint_{\mathbb{R}^3/\sim} \overline{\psi_i(\mathbf{x}) \psi_j(\mathbf{x}')} V_{\text{Coulomb}} \left(\psi_k \otimes \psi_l\right)(\mathbf{x}, \mathbf{x}') \mathrm{d}^3\mathbf{x} \mathrm{d}^3\mathbf{x}' \tag{7.60}$$

7.3.3. n-Body-Operators

Fact 7.54 There are not so many n-body operators that appear "naturally" in physical systems. Most n-body operators (like the gravitational- or electrostatic- interaction between n-particles) can be traced back to sums of two-body operators. One of the only few "true" n-body operators that the author is aware of, is found after one integrates out the electronic system in a BCS-like theory and finds higher-order terms in the purely bosonic action. For more details on this, see Section 30.2 and more specifically Lemma 30.29.

8. Fundamentals II - Many-Particle Hilbert-Spaces, Time-Dependencies and Examples

8.1. Summary of the Many-Particle Hilbert-Spaces - Pure and Mixed Systems

Notation 8.1 When we speak about "Green-functions" (to be introduced later), we consider one of the following Hilbert-spaces:

$$(1)\quad \mathscr{H} \equiv \mathscr{H}_{m=0} = \mathrm{span}_{\mathbb{C}} \left\{ \prod_{j=1}^{\mathrm{d}} \frac{1}{\sqrt{n_j!}} \left(c_j^\dagger\right)^{n_j} \mid \mathrm{vac.}\rangle \equiv |n_1, n_2, \dots, n_{\mathrm{d}}\rangle \,\middle|\, n_1, n_2, \dots, n_{\mathrm{d}} \in \mathbb{N}_\zeta \right\} \quad \text{(massless particles)},$$

$$(2)\quad \mathscr{H} \equiv \mathscr{H}_{m>0} = \mathrm{span}_{\mathbb{C}} \left\{ \prod_{j=1}^{\mathrm{d}_{\mathscr{H}}} \frac{1}{\sqrt{n_j!}} \left(c_j^\dagger\right)^{n_j} \mid \mathrm{vac.}\rangle \equiv |n_1, n_2, \dots, n_{\mathrm{d}_{\mathscr{H}}}\rangle \,\middle|\, n_1, n_2, \dots, n_{\mathrm{d}_{\mathscr{H}}} \in \mathbb{N}_\zeta \right\} \quad \text{(massive particles)},$$

$$(3)\quad \mathscr{H} = \mathscr{H}_{m>0} \otimes \mathscr{H}_{m=0} \quad \text{(massive-massless-mixtures)},$$

$$(4)\quad \mathscr{H} = \mathscr{H}_{m_1>0} \otimes \mathscr{H}_{m_2=0} \otimes \mathscr{H}_{m_3=0} \quad \text{(massive-massless-massless-mixtures)},$$

$$(5)\quad \mathscr{H} = \mathscr{H}_{m_1>0} \otimes \mathscr{H}_{m_2>0} \otimes \mathscr{H}_{m_3=0} \quad \text{(massive-massive-massless-mixtures)},$$

$$\vdots$$

Remark 8.1.1 Notice that in every case except the first two cases, every Hilbert-space is composed of tensor-products of the particle-like or wave-like systems. In those cases, a basis of the total Hilbert-space is given by taking tensor-products of the respective occupation-number basis-elements. In turn, the basis of the total Hilbert-space is again given as an occupation-number basis (with a more tedious enumeration).

Remark 8.1.2 In the first two cases (i.e. in the case of exclusively massless or massive particles in the system), we will be speaking of a *pure system*.

Definition 8.2 Depending on the mass of the underlying particles in a system, we introduce a number η called *nature* as

$$\eta = \begin{cases} 0 & \text{for massless particles} \\ 1 & \text{for massive particles} \end{cases} \tag{8.1}$$

Remark 8.2.1 The table summarizes some examples of pure systems with their associated statistics ζ, nature η.

Particle / System (Example)	**Nature** η	**Statistics** ζ
Electron-Gas	1	-1
Phonon- & Photon-Gas	0	$+1$
Rubidium atoms / Bose-Einstein-Condensate	1	$+1$
XXZ-Model + Jordan-Wigner-Transformation (???)	0	-1

Definition 8.3 We introduce the so-called *ensemble Hamiltonian* Ξ as

$$\Xi = \begin{cases} H & \text{for } \eta = 0 \text{ (massless particles)}, \\ H - \mu N & \text{for } \eta = 1 \text{ (massive particles)}, \\ H_{m>0} - \mu N_{m>0} + H_{m=0} + V_{\text{int}} & \text{for massive-massless-mixtures}, \\ \quad \vdots & \end{cases} \tag{8.2}$$

whereas the role of the so-called "chemical potential" μ will become clear when we introduce the different ensembles that one uses.

Remark 8.3.1 Notice that one can rewrite the equation above in the concise form

$$\Xi = \begin{cases} H - \eta\mu N & \text{for a pure system with nature } \eta, \\ H_{m>0} - \mu N_{m>0} + H_{m=0} + V_{\text{int}} & \text{for massive-massless-mixtures.} \\ \quad \vdots & \end{cases} \tag{8.3}$$

Remark 8.3.2 For other cases, such as massive-massive-mixtures, one has to account for several chemical potentials.

Fact 8.4 The Hamiltonian of the system is usually expressed as a combination of a well-understood reference term, H_0, and a perturbation term, V, whereas the perturbation may represent a superposition of one-body interactions (such as external potentials or impurities in a crystal) and two-body interactions (such as Coulomb interactions)... Hence we concretely want to cover the cases ...

1. systems with massless particles

$$\begin{aligned} H &= \sum_{i,j=1}^{\mathrm{d}} H_{i,j} c_i^\dagger c_j \quad + \sum_{i,j,k=1}^{\mathrm{d}} \left(H_{i,j;k} c_i^\dagger c_j^\dagger c_k + H_{i;j,k} c_i^\dagger c_j c_k \right) + \dots, \\ &= H_0 \qquad\qquad + V \end{aligned} \tag{8.4}$$

2. systems with massive particles

$$\begin{aligned} H &= \sum_{i,j=1}^{\mathrm{d}} H_{i,j} c_i^\dagger c_j \quad + \frac{1}{2} \sum_{i,j,k,l=1}^{\mathrm{d}} H_{i,j;kl} c_i^\dagger c_j^\dagger c_l c_k + \dots, \\ &= H_0 \qquad\qquad + V \end{aligned} \tag{8.5}$$

whereas we emphasize the reversed order in the last two indices,

3. and for the interactions of, for example, massive-massless-systems

$$V_{\text{int}} = \sum_{i,j=1}^{d_{m>0}} \sum_{k=1}^{d_{m=0}} \left(V_{\underset{i,j;k}{\text{int}}} c_i^\dagger c_j c_k^\dagger + \widetilde{V}_{\underset{i,j;k}{\text{int}}} c_i^\dagger c_j c_k \right) + \dots , \tag{8.6}$$

with

$$H_0 \equiv H_{\underset{m=0}{0}} + H_{\underset{m>0}{0}} , \qquad V \equiv V_{m=0} + V_{m>0} + V_{\text{int}} \tag{8.7}$$

4. here and for the remaining cases, we consider similar Hamiltonians ...

Remark 8.4.1 Notice that for systems with massive particles the Hamiltonians are always particle-number conserving, as they emerge from a second quantization scheme.

8.2. Time-Dependencies in Many-Body Quantum Mechanics

8.2.1. Real Time

Notation 8.5 Let $\mathscr{H}$ a many-particle Hilbert-space of a quantum system with a (possibly spin-dependent) time-independent ensemble Hamiltonian Ξ (in the Schrödinger-picture) and consider the time-evolution in the Schrödinger- / Pauli-equation

$$\mathrm{i}\hbar\partial_t |\psi(t)\rangle = \Xi |\psi(t)\rangle .$$

Definition 8.6 For arbitrary times $t_\mathrm{i}, t_\mathrm{f} \in \mathbb{R}$ we define the *ensemble-time-evolution operator* $U_\Xi(t_\mathrm{f}, t_\mathrm{i})$ of the system as

$$U_\Xi(t_\mathrm{f}, t_\mathrm{i}) = \exp - \frac{\mathrm{i}}{\hbar} \left(t_\mathrm{f} - t_\mathrm{i} \right) \Xi .$$

Remark 8.6.1 Notice that one has the identity

$$U_\Xi(t_\mathrm{f}, t_\mathrm{i})^\dagger = U_\Xi(t_\mathrm{i}, t_\mathrm{f}) . \tag{8.8}$$

Remark 8.6.2 For notational convenience we will oftentimes drop the index in the time-evolution-operator as $U_\Xi \equiv U$.

Theorem 8.7 The time-evolution operator defined above gives a formal solution to a Schrödinger- / Pauli-equation (with ensemble-Hamiltonian) for a given initial-condition.

Proof 8.7 By taking the derivative, one sees that one indeeds obtains a solution for a given initial condition.

Definition 8.8 Let $X \equiv X_{\mathrm{S}} \equiv X_{\mathrm{S}}(t)$ be a possibly time-dependent operator in the [S]chrödinger-picture, then one defines the corresponding *ensemble-[H]eisenberg-representation* as

$$X_{\mathrm{H}}(t) := U(t,0)^{\dagger}\, X\, U(t,0).$$

Remark 8.8.1 If we want to emphasize from which ensemble-Hamiltonian the time-evolution originates from (this is, for example, important in Theorem 15.8) then we might also switch to the notation

$$X_{\mathrm{H}}(t) \equiv X_{\Xi}(t) \equiv X_{\mathrm{H}_{\Xi}} \tag{8.9}$$

etc.

Theorem 8.9 One immediately concludes the *ensemble-Heisenberg-"equation of motion"*

$$\frac{\mathrm{d}}{\mathrm{d}t} X_{\mathrm{H}}(t) = -\frac{\mathrm{i}}{\hbar}[X, \Xi]_{\mathrm{H}}(t) + \left(\frac{\partial X}{\partial t}\right)_{\mathrm{H}}(t) \tag{8.10}$$

Proof 8.9 See Appendix, Proofs, page 514.

Remark 8.9.1 Most of the operators we consider are creation- and annihilation-operators c, $c^{\dagger}$, which are time-independent in the Schrödinger-picture. But one oftentimes simply drops the index, even if they are written in the Heisenberg-picture. This doesn't lead to any confusion since they acquire a time-argument then $c_{\mathrm{H}}(t) \equiv c(t)$, etc.

Definition 8.10 We consider a monomial in fermionic ($\zeta_{\bullet} \equiv -1$) and / or bosonic ($\zeta_{\bullet} \equiv +1$) creation and annihilation-operators

$$X \equiv c^{\dagger}_{\alpha_1} \cdots c^{\dagger}_{\alpha_n} c_{\alpha'_1} \cdots c_{\alpha'_m}, \tag{8.11}$$

with statistics $\zeta_{\alpha_1}, \ldots, \zeta_{\alpha_n}, \zeta_{\alpha'_1}, \ldots, \zeta_{\alpha'_m} \in \{-1, +1\}$ then we define the *statistics of the operator* X as a sign

$$\mathrm{S}(X) := \prod_{i=1}^{n} \zeta_{\alpha_i} \cdot \prod_{j=1}^{m} \zeta_{\alpha'_j} \in \{-1, +1\}. \tag{8.12}$$

Remark 8.10.1 Analogous one defines the *statistics of a polynomial expression in creation- and annihilation-operators*, if every monomial has the same statistics. For a polynomial expression in creation- and annihilation-operators with monomials that differ (individually) in their statistics, there is no reasonable definition of the statistics.

Remark 8.10.2 Notice that one finds for creation- and annihilation-operators $\mathrm{S}(c_\bullet) = \mathrm{S}(c_\bullet^\dagger) = \zeta$.

Definition 8.11 For a pair of operators X, X', we define the *pair-statistics* $\mathrm{S} \equiv \mathrm{S}(X, X') \in \{-1, +1\}$ as

$$\mathrm{S}(X, X') \equiv \mathrm{S}_{X,X'} := \begin{cases} -1 & \text{if } \mathrm{S}(X) = \mathrm{S}(X') = -1, \\ +1 & \text{otherwise.} \end{cases} \tag{8.13}$$

Remark 8.11.1 Notice that the only case, in which the pair-statistics is equal to minus one, is if X and X' are (sums of) odd monomial expressions in fermionic operators.

Remark 8.11.2 Note further that $\mathrm{S}(c_\bullet, c_\bullet^\dagger) = \zeta$.

Definition 8.12 For a pair of operators X, X', we define the *pair-commutator* as

$$\left[X, X'\right]_{\mathrm{S}} \equiv XX' - \mathrm{S}_{X,X'}\, X'X. \tag{8.14}$$

Definition 8.13 We consider a pair of operators X, X'. Then we define the *time-ordered-pair-product* of their ensemble-Heisenberg-representation as

$$\mathrm{T}_t \left[X_{\mathrm{H}}(t)\, X'_{\mathrm{H}}\left(t'\right) \right] \equiv \theta(t - t')\, X_{\mathrm{H}}(t)\, X'_{\mathrm{H}}\left(t'\right) + \mathrm{S}_{X,X'}\, \theta(t' - t) X'_{\mathrm{H}}\left(t'\right) X_{\mathrm{H}}(t) \tag{8.15}$$

Remark 8.13.1 The definition of the pair-commutator and time-ordered-pair-product seem suspicious at first, but they will be integral in the formulation of Green-functions.

Remark 8.13.2 For X, X' being creation and annihilation-operators of the same statistics one has $\mathrm{S}_{X,X'} \equiv \zeta$ and it follows

$$\mathrm{T}_t\, c_\alpha(t)\, c^\dagger_{\alpha'}(t') \equiv \theta(t - t')\, c_\alpha(t)\, c^\dagger_{\alpha'}(t') + \zeta\, \theta(t' - t)\, c^\dagger_{\alpha'}(t')\, c_\alpha(t). \tag{8.16}$$

Remark 8.13.3 Analogously one also introduces an *anti-time-ordering-operator* $\overline{\mathrm{T}}_t$; For creation and annihilation-operators it follows

$$\overline{\mathrm{T}}_t \left[X_{\mathrm{H}}(t)\, X'_{\mathrm{H}}\left(t'\right) \right] \equiv \theta(t' - t)\, X_{\mathrm{H}}(t)\, X'_{\mathrm{H}}\left(t'\right) + \mathrm{S}_{X,X'}\, \theta(t - t')\, X'_{\mathrm{H}}\left(t'\right) X_{\mathrm{H}}(t)\,. \tag{8.17}$$

Note on the update. The original Definition and Lemma below contain the following errors:

1. The Koszul-sign χ_π is written as a *sum* instead of a *product*, so it is not a sign at all.
2. It uses the products $\mathrm{S}_\alpha \mathrm{S}_\beta$ of the individual statistics instead of the pair-statistics $\mathrm{S}(X_\alpha, X_\beta)$ (defined right before Definition 8.12). For one fermionic and one bosonic operator, $\mathrm{S}_\alpha \mathrm{S}_\beta = -1$, although their interchange produces no sign.
3. The sum over permutations counts several orderings at coinciding times.
4. The Remark is wrong: the time-ordering does not act „as a derivative“.

A corrected and extended version (with proofs) is given at the end of this block, starting with Definition 8.16.

Definition 8.14 We consider a family of statistical operators $\left\{X_\alpha\right\}_{\alpha\in\mathscr{A}}$ with statistics $\left\{\mathrm{S}_\alpha \equiv \mathrm{S}(X_\alpha)\right\}_{\alpha\in\mathscr{A}}$. Then we define the *time-ordered-product* of their ensemble-Heisenberg-representation as

$$\mathrm{T}_t\left[X_{\alpha_1}\left(t_1\right) X_{\alpha_2}\left(t_2\right)\cdots X_{\alpha_n}(t_n)\right] \equiv \sum_{\pi\in S_n} \chi_\pi\, \theta_\pi(t_1,t_2,\ldots,t_n)\, X_{\alpha_{\pi(1)}}\left(t_{\pi(1)}\right) X_{\alpha_{\pi(2)}}\left(t_{\pi(2)}\right)\cdots X_{\alpha_{\pi(n)}}\left(t_{\pi(n)}\right) \tag{8.18}$$

with a product of Heaviside-functions

$$\theta_\pi(t_1,t_2,\ldots,t_n) = \prod_{j=1}^{n-1} \theta(t_{\pi(j)} - t_{\pi(j+1)}) \tag{8.19}$$

enforcing the time-ordering $t_{\pi(1)} \geq t_{\pi(2)} \geq \ldots \geq t_{\pi(n)}$, and *Koszul-sign*

$$\chi_\pi = \sum_{\substack{1\leq i<j\leq n \\ \pi(i)>\pi(j)}} \mathrm{S}_{\alpha_{\pi(i)}}\, \mathrm{S}_{\alpha_{\pi(j)}} \tag{8.20}$$

counting the number of statistical transpositions required to bring the product into the order specified by the permutation π.

Lemma 8.15 If all operators have the same statistics $\mathrm{S} = \mathrm{S}_\alpha$ for all $\alpha \in \mathscr{A}$, then one obtains the simple formula

$$\mathrm{T}_t\left[X_{\alpha_1}\left(t_1\right) X_{\alpha_2}\left(t_2\right)\cdots X_{\alpha_n}(t_n)\right] \equiv \mathrm{sign}(\pi)^{1-\theta(\mathrm{S})} X_{\alpha_{\pi(1)}}\left(t_{\pi(1)}\right) X_{\alpha_{\pi(2)}}\left(t_{\pi(2)}\right)\cdots X_{\alpha_{\pi(n)}}\left(t_{\pi(n)}\right) \tag{8.21}$$

where

$$t_{\pi(1)} > t_{\pi(2)} > \ldots > t_{\pi(n)}. \tag{8.22}$$

Remark 8.15.1 When it cannot lead to any confusion, it is convenient to omit the brackets, with the notation that the time-ordering-operator acts (as a derivative) to everything that is „positioned right to it“

Updated version of this block. We follow the conventions of [38, Sect. 2.1, Eq. (2.8), p. 49], generalized to operators of mixed statistics.

Definition 8.16 Let $\{X_\alpha\}_{\alpha\in\mathscr{A}}$ be operators with well-defined statistics $\mathrm{S}(X_\alpha)$ (e.g. monomials in creation- and annihilation-operators, or polynomials whose monomials share their statistics), and write $X_\alpha(t) \equiv (X_\alpha)_{\mathrm{H}}(t)$ for their ensemble-Heisenberg-representation. For a list $X_{\alpha_1}(t_1), \dots, X_{\alpha_n}(t_n)$ and a permutation $\pi \in \mathrm{S}_n$ we define the *Koszul-sign*

$$\chi_\pi := \prod_{\substack{1\le i<j\le n \\ \pi(i)>\pi(j)}} \mathrm{S}\left(X_{\alpha_{\pi(i)}}, X_{\alpha_{\pi(j)}}\right) \quad \in \{-1,+1\}.$$

This is the product of the pair-statistics of all pairs of factors whose relative order is reversed when passing from $X_{\alpha_1}\cdots X_{\alpha_n}$ to $X_{\alpha_{\pi(1)}}\cdots X_{\alpha_{\pi(n)}}$. For pairwise distinct times $t_1, \dots, t_n$ we define the *time-ordered product*

$$\mathrm{T}_t\left[X_{\alpha_1}(t_1)X_{\alpha_2}(t_2)\cdots X_{\alpha_n}(t_n)\right] := \chi_\pi\, X_{\alpha_{\pi(1)}}(t_{\pi(1)})X_{\alpha_{\pi(2)}}(t_{\pi(2)})\cdots X_{\alpha_{\pi(n)}}(t_{\pi(n)}), \tag{8.23}$$

where π is the unique permutation with $t_{\pi(1)} > t_{\pi(2)} > \ldots > t_{\pi(n)}$ (latest time to the left).

Remark 8.16.1 The Koszul-sign χ_π is the sign one picks up when reordering the product by successive interchanges of neighbouring factors, if each interchange of X_α and X_β is weighted by their pair-statistics $\mathrm{S}(X_\alpha, X_\beta)$, i.e. by -1 exactly for two fermionically odd operators. Indeed, each interchange reverses the order of exactly one pair. A pair whose order is reversed in total is interchanged an odd number of times, all other pairs an even number of times, and $\mathrm{S}^2 = 1$. In particular, χ_π does not depend on the chosen sequence of interchanges.

Remark 8.16.2 For coinciding times the definition has to be supplemented by a convention. Negele and Orland put creation operators to the left of annihilation operators (normal order) at equal times [38, p. 49]; another common choice is to keep the original order of the factors with equal time arguments. In integrals over the times the choice is irrelevant (coinciding times form a set of measure zero), but for equal-time quantities such as a Green-function at $t = t'$ it has to be stated explicitly, e.g. by $t' = t + 0^+$.

Lemma 8.17 For pairwise distinct times one has, with θ_π as in Definition 8.14,

$$\mathrm{T}_t\left[X_{\alpha_1}(t_1)\cdots X_{\alpha_n}(t_n)\right] = \sum_{\pi\in\mathrm{S}_n} \chi_\pi\, \theta_\pi(t_1,\dots,t_n)\, X_{\alpha_{\pi(1)}}(t_{\pi(1)})\cdots X_{\alpha_{\pi(n)}}(t_{\pi(n)}).$$

For $n = 2$ this is Definition 8.13.

Proof 8.17 For pairwise distinct times, $\theta_\pi = 1$ for the unique permutation of Definition 8.16, and $\theta_\pi = 0$ for all others. For $n = 2$, the identity contributes $\theta(t_1 - t_2)X_{\alpha_1}(t_1)X_{\alpha_2}(t_2)$, and the transposition reverses the single pair, such that $\chi_{(12)} = \mathrm{S}(X_{\alpha_1}, X_{\alpha_2})$ and it contributes $\mathrm{S}(X_{\alpha_1}, X_{\alpha_2})\,\theta(t_2 - t_1)X_{\alpha_2}(t_2)X_{\alpha_1}(t_1)$. At coinciding times (and with $\theta(0) = 1$) several θ_π would equal one, which is why the sum formula cannot serve as a definition there.

Lemma 8.18 For pairwise distinct times and every $\sigma \in \mathrm{S}_n$ one has

$$\mathrm{T}_t\left[X_{\alpha_1}(t_1)\cdots X_{\alpha_n}(t_n)\right] = \chi_\sigma\ \mathrm{T}_t\left[X_{\alpha_{\sigma(1)}}(t_{\sigma(1)})\cdots X_{\alpha_{\sigma(n)}}(t_{\sigma(n)})\right],$$

i.e. inside the time-ordering the factors may be rearranged as if they (anti-)commuted according to their pair-statistics.

Proof 8.18 Let π be the time-ordering permutation of the original list. The rearranged list $Y_i = X_{\alpha_{\sigma(i)}}(t_{\sigma(i)})$ is time-ordered by $\rho = \sigma^{-1}\circ\pi$, since $Y_{\rho(k)} = X_{\alpha_{\pi(k)}}(t_{\pi(k)})$. Hence both sides contain the same operator product $X_{\alpha_{\pi(1)}}(t_{\pi(1)})\cdots X_{\alpha_{\pi(n)}}(t_{\pi(n)})$, with the prefactors χ_π on the left and $\chi_\sigma\chi_\rho^{(Y)}$ on the right, where $\chi_\rho^{(Y)}$ is computed relative to the order of the Y_i. A pair of factors is reversed between the original order and the π-order if and only if it is reversed in exactly one of the two steps „original order → σ-order → π-order“. Pairs that are reversed in both steps contribute $\mathrm{S}^2 = 1$, so $\chi_\pi = \chi_\sigma\chi_\rho^{(Y)}$.

Lemma 8.19 (Corrected version of the Lemma above.) If all operators have the same statistics, $\mathrm{S}(X_\alpha) = \mathrm{S}$ for all $\alpha \in \mathscr{A}$, then

$$\mathrm{T}_t\left[X_{\alpha_1}(t_1)\cdots X_{\alpha_n}(t_n)\right] = \mathrm{sign}(\pi)^{1-\theta(\mathrm{S})}\, X_{\alpha_{\pi(1)}}(t_{\pi(1)})\cdots X_{\alpha_{\pi(n)}}(t_{\pi(n)}),$$

where π is the permutation with $t_{\pi(1)} > \ldots > t_{\pi(n)}$. For creation- and annihilation-operators this is ζ^P in the notation of [38, Eq. (2.8)].

Proof 8.19 By the definition of the pair-statistics, $\mathrm{S}(X_\alpha, X_\beta) = \mathrm{S}$ for all pairs: it is -1 if both statistics are -1, and $+1$ if both are $+1$. Hence $\chi_\pi = \mathrm{S}^{N(\pi)}$, where $N(\pi)$ is the number of inversions of π. Since $\mathrm{sign}(\pi) = (-1)^{N(\pi)}$, this is $\mathrm{sign}(\pi) = \mathrm{sign}(\pi)^{1-\theta(-1)}$ for $\mathrm{S} = -1$ and $1 = \mathrm{sign}(\pi)^{1-\theta(+1)}$ for $\mathrm{S} = +1$.

Corollary 8.20 If $\mathrm{S}(X_\alpha, X_\beta) = +1$ for all α, β, then $\mathrm{T}_t[\ldots]$ is symmetric under all permutations of the factors. This holds in particular if all X_α are even, $\mathrm{S}(X_\alpha) = +1$, as Hamiltonians, interaction terms or fermion bilinears. Even operators may also be moved freely past odd ones inside the time-ordering. Consequently, for an even operator V and $t \geq t_0$,

$$\int_{t_0}^{t} \mathrm{d}t_1 \cdots \int_{t_0}^{t} \mathrm{d}t_n\ \mathrm{T}_t\left[V(t_1)\cdots V(t_n)\right] = n!\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\cdots\int_{t_0}^{t_{n-1}}\mathrm{d}t_n\, V(t_1)V(t_2)\cdots V(t_n),$$

which is the origin of the factor $1/n!$ in time-ordered exponentials and Dyson-series (cf. Corollary 15.8).

Proof 8.20 The symmetry is Lemma 8.18 with all $\chi_\sigma = 1$; and $\mathrm{S}(X, X') = +1$ whenever one of the two operators is even. For the integral, the cube $[t_0, t]^n$ is, up to the set of measure zero with coinciding times, the disjoint union of the $n!$ simplices $\Delta_\pi = \{t_{\pi(1)} > \ldots > t_{\pi(n)}\}$. On Δ_π the integrand equals $V(t_{\pi(1)})\cdots V(t_{\pi(n)})$. Renaming the integration variables, $s_k = t_{\pi(k)}$, maps the integral over Δ_π onto the integral over Δ_{id}, which is the right-hand side divided by $n!$.

Lemma 8.21 Assume that the ensemble-Hamiltonian Ξ is even, such that $\dot{X}(t) \equiv \frac{\mathrm{d}}{\mathrm{d}t}X_{\mathrm{H}}(t)$ (Theorem 8.9) has the same statistics as X. Then, in the sense of distributions,

$$\partial_t\,\mathrm{T}_t\left[X(t)X'(t')\right] = \mathrm{T}_t\left[\dot{X}(t)X'(t')\right] + \delta(t-t')\left[X, X'\right]_{\mathrm{S}}(t),$$

with the equal-time pair-commutator (Definition 8.12)

$$[X, X']_{\mathrm{S}}(t) := X(t)X'(t) - \mathrm{S}_{X,X'}\, X'(t)X(t) = \left([X, X']_{\mathrm{S}}\right)_{\mathrm{H}}(t).$$

More generally, $\partial_{t_k} \mathrm{T}_t[X_{\alpha_1}(t_1)\cdots X_{\alpha_n}(t_n)]$ equals $\mathrm{T}_t[\cdots \dot{X}_{\alpha_k}(t_k)\cdots]$ plus terms proportional to $\delta(t_k - t_l)$, $l \neq k$. Each of these terms contains the equal-time pair-commutator $[X_{\alpha_k}, X_{\alpha_l}]_{\mathrm{S}}(t_k)$ as a factor. In particular, no δ-terms arise if X_{α_k} has vanishing equal-time pair-commutators with all other factors.

Proof 8.21 Distributional derivatives only depend on the values almost everywhere, so we may use Lemma 8.17. For $n = 2$, the product rule with $\partial_t \theta(t - t') = \delta(t - t') = -\partial_t \theta(t' - t)$ gives

$$\partial_t \mathrm{T}_t\left[X(t)X'(t')\right] = \theta(t - t')\dot{X}(t)X'(t') + \mathrm{S}_{X,X'}\,\theta(t' - t)X'(t')\dot{X}(t) + \delta(t - t')\left(X(t)X'(t') - \mathrm{S}_{X,X'}\, X'(t')X(t)\right).$$

The first two terms form $\mathrm{T}_t[\dot{X}(t)X'(t')]$, since $\mathrm{S}_{\dot{X},X'} = \mathrm{S}_{X,X'}$, and the δ-function sets $t' = t$ in the last bracket. Finally, $U^\dagger XUU^\dagger X'U = U^\dagger XX'U$ shows that the equal-time pair-commutator of Heisenberg operators is the Heisenberg-representation of the pair-commutator.

For general n, the derivative of θ_π w.r.t. t_k acts on the (at most two) factors $\theta(t_{\pi(j)} - t_{\pi(j+1)})$ that contain t_k, producing $\delta(t_k - t_l)$ with l the time-neighbour of k in the ordering π. The terms of π and of $\pi' = \pi \circ (j, j+1)$, in which the neighbours k, l are interchanged, carry opposite δ-functions and the Koszul-signs $\chi_{\pi'} = \mathrm{S}(X_{\alpha_k}, X_{\alpha_l})\chi_\pi$, while their remaining θ-factors coincide at $t_k = t_l$. Hence their sum contains (up to an overall sign) the factor

$$X_{\alpha_k}(t_k)X_{\alpha_l}(t_k) - \mathrm{S}(X_{\alpha_k}, X_{\alpha_l})X_{\alpha_l}(t_k)X_{\alpha_k}(t_k) = [X_{\alpha_k}, X_{\alpha_l}]_{\mathrm{S}}(t_k).$$

Remark 8.21.1 Two typical applications:

- For $X = c_\alpha$, $X' = c^\dagger_{\alpha'}$, one has $[c_\alpha, c^\dagger_{\alpha'}]_\zeta = \delta_{\alpha\alpha'}$, and Lemma 8.21 gives $\partial_t \mathrm{T}_t[c_\alpha(t)c^\dagger_{\alpha'}(t')] = \mathrm{T}_t[\dot{c}_\alpha(t)c^\dagger_{\alpha'}(t')] + \delta(t - t')\delta_{\alpha\alpha'}$. This is the origin of the inhomogeneity in the equations of motion of Green-functions.
- Phonon operators $b, b^\dagger$ and electron operators $c, c^\dagger$ act on different tensor factors and commute at equal times, $[b(t), c(t)] = U^\dagger[b, c]U = 0$, even in an interacting system. Therefore, differentiating a time-ordered product w.r.t. the time argument of a phonon operator produces no δ-terms with electron operators. In contrast, a factorization $\mathrm{T}_t[B\,F] = \mathrm{T}_t[B]\ \mathrm{T}_t[F]$ into a bosonic and a fermionic part does *not* hold in general for interacting Heisenberg operators, since $b(t)$ and $c(t')$ need not commute for $t \neq t'$.

Remark 8.21.2 (Correction of the Remark above.) The time-ordering acts on the entire product to its right, but not „as a derivative“: it satisfies no Leibniz rule. Strictly speaking, it is not even a map on operators, but on formal products of time-labelled operators. For example, $\mathrm{T}_t[A(t_1)B(t_2)]$ depends on the individual factors and their time arguments, not only on the operator $A(t_1)B(t_2)$, which can be factorized in many ways. It is linear in each factor.

Remark 8.21.3 Analogously, one defines the *anti-time-ordered product* $\overline{\mathrm{T}}_t[\ldots] := \chi_\pi X_{\alpha_{\pi(1)}}(t_{\pi(1)})\cdots X_{\alpha_{\pi(n)}}(t_{\pi(n)})$ with $t_{\pi(1)} < \ldots < t_{\pi(n)}$ (earliest time to the left), which reduces to the anti-time-ordering above for $n = 2$. All statements of this block hold verbatim in imaginary time, with $\tau \in (-\hbar\beta, \hbar\beta)$, the imaginary-time Heisenberg-representation of the next subsection, and T_τ in place of T_t.

8.2.2. „Imaginary“ Time

For reasons that are difficult to motivate several chapters in advance, we introduce another kind of time-evolution-operator.

Definition 8.22 For arbitrary values $\tau_{\mathrm{i}}, \tau_{\mathrm{f}} \in (-\hbar\beta, +\hbar\beta)$ we define the *ensemble-imaginary-time-evolution operator* $U_{\Xi}(\tau_{\mathrm{f}}, \tau_{\mathrm{i}})$ of the system as

$$U_{\Xi}(\tau_{\mathrm{f}}, \tau_{\mathrm{i}}) = \exp -\frac{1}{\hbar}\left(\tau_{\mathrm{f}} - \tau_{\mathrm{i}}\right)\Xi.$$

Remark 8.22.1 Notice that the phraseology „imaginary“ time is a little bit misleading: τ defines a real variable. The thing that changed w.r.t. the previous subsection is the evolution-operator, not the nature of the variables.

Remark 8.22.2 Notice further that we have, in contrast to the real-time case

$$U_{\Xi}(\tau_{\mathrm{f}}, \tau_{\mathrm{i}}) \neq U_{\Xi}(\tau_{\mathrm{i}}, \tau_{\mathrm{f}})^{\dagger}. \tag{8.24}$$

Remark 8.22.3 Just as in the real-time case, we usually drop the index $U_{\Xi} \equiv U$.

Definition 8.23 Let $X \equiv X_{\mathrm{S}} \equiv X_{\mathrm{S}}(\tau)$ be the Wick-rotated version of a possibly time-dependent operator. Then one defines the corresponding *ensemble-Heisenberg-representation in imaginary time* as

$$X_{\mathrm{H}}(\tau) := U(0,\tau)\, X\, U(\tau, 0).$$

Theorem 8.24 One immediately concludes the *ensemble-Heisenberg-"equation of motion" in imaginary time*

$$\frac{\mathrm{d}}{\mathrm{d}\tau} X_{\mathrm{H}}(\tau) = -\frac{1}{\hbar}[X, \Xi]_{\mathrm{H}}(\tau) + \left(\frac{\partial X}{\partial \tau}\right)_{\mathrm{H}}(\tau) \tag{8.25}$$

Proof 8.24 See Appendix, Proofs, page 515.

Remark 8.24.1 Accordingly one introduces also the *imaginary-time-ordering operator* T_{τ}, analog to Definition 8.13.

8.3. Examples - Pure Systems

To remain as general as possible (and simultaneously reasonable) we specifiy neither the statistics nor the nature of the systems in this section.

8.3.1. Non-Interacting Cases

Example: A Quantum-Dot with Nature η and Statistics ζ

Definition 8.25 A *quantum-dot* is a system described by the Hamiltonian

$$H_0 = \epsilon c^\dagger c$$

and Fock-space

$$\mathscr{F}_\zeta \equiv \mathrm{span}_{\mathbb{C}} \left\{ |n\rangle \,\middle|\, n \in \mathbb{N}_\zeta \right\}.$$

Remark 8.25.1 One finds for the Heisenberg-time-evolution in the grand canonical ensemble as a special case of Lemma 8.28.

Example: A Two-Level-System with Nature η and Statistics ζ

Definition 8.26 A *two-level-system* is a system described by the Hamiltonian

$$H_0 \equiv \begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix}^\dagger \begin{pmatrix} \epsilon_0 + \epsilon_z & -\mathrm{i}\epsilon_y + \epsilon_x \\ +\mathrm{i}\epsilon_y + \epsilon_x & \epsilon_0 - \epsilon_z \end{pmatrix} \begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix}$$

Remark 8.26.1 Notice that a *spin-$\frac{1}{2}$-particle*, described through the Zeeman-contribution to the Pauli-equation leads (after going over to the second quantized formalism) to a two-level-system.

Remark 8.26.2 Computing the Heisenberg-time-evolution for the creation- and annihilation-operators analogously to Lemma 8.28 requires in this case a basis-change. This is done in Lemma TBReferenced.

Example: A Diagonalized, Non-Interacting Gas with Nature η and Statistics ζ

Definition 8.27 A *diagonalized, non-interacting "gas"*[1] is a system described by the Hamiltonian

$$H_0 = \sum_\alpha \epsilon_\alpha c_\alpha^\dagger c_\alpha$$

and Fock-space $\mathscr{F}_\zeta$ spanned by occupation-number-states as usual

$$\mathscr{F}_\zeta = \mathrm{span}_{\mathbb{C}} \left\{ |n_{\alpha_1}, n_{\alpha_2}, \dots, n_{\alpha_{\mathrm{d}_\mathcal{H}}}\rangle \,\middle|\, n_{\alpha_1}, n_{\alpha_2}, \dots, n_{\alpha_{\mathrm{d}_\mathcal{H}}} \in \mathbb{N}_\zeta \right\} \tag{8.26}$$

whereas the state with $n_{\alpha_1} = n_{\alpha_2} = \dots = n_{\alpha_{\mathrm{d}_\mathcal{H}}} = 0$ represents the *vacuum-state* a.k.a *the empty state*.

Lemma 8.28 One finds for the ensemble-Heisenberg-time-evolutions the identities

$$\begin{aligned} c_\bullet(t) &= \mathrm{e}^{-\mathrm{i}t(\epsilon_\bullet - \eta\mu)/\hbar} c_\bullet, & c_\bullet^\dagger(t) &= \mathrm{e}^{\mathrm{i}t(\epsilon_\bullet - \eta\mu)/\hbar} c_\bullet^\dagger \\ c_\bullet(\tau) &= \mathrm{e}^{-\tau(\epsilon_\bullet - \eta\mu)/\hbar} c_\bullet, & c_\bullet^\dagger(\tau) &= \mathrm{e}^{\tau(\epsilon_\bullet - \eta\mu)/\hbar} c_\bullet^\dagger \end{aligned} \tag{8.27}$$

Proof 8.28 See Appendix, Proofs, page 515.

Remark 8.28.1 A fermionic, particle-like example of this Hamiltonian is the *free electron gas in the LDA-approximation* in a crystal

$$H_0 = \sum_{\substack{\mathbf{k}\in \mathrm{Q} \\ \sigma \in \{\downarrow,\uparrow\} \\ n \in \{1,\dots,\infty\}}} \epsilon_{n\sigma}(\mathbf{k})\, c_{n\sigma}^\dagger(\mathbf{k}) c_{n\sigma}(\mathbf{k}).$$

The states in the Fock-space $\mathscr{F}$ are then written as

$$\mathscr{F} = \mathrm{span}_{\mathbb{C}} \left\{ |n_{\alpha_1}, n_{\alpha_2}, \dots, n_{\alpha_{\mathrm{d}_\mathcal{H}}}\rangle \,\middle|\, n_{\alpha_\bullet} \in \{0,1\},\ \alpha_i \equiv (m_i, \sigma_i, \mathbf{k}_i) \in \{1,\dots,\infty\} \times \{\downarrow,\uparrow\} \times \mathrm{Q} \right\} \tag{8.28}$$

Notice that the dimension $\mathrm{d}_\mathcal{H}$ of the single-particle Hilbert-space is given as

$$\mathrm{d}_\mathcal{H} = \dim \mathcal{H} = \left| \{1,\dots,\infty\} \times \{\downarrow,\uparrow\} \times \mathrm{Q} \right| = \infty \tag{8.29}$$

Usually one introduces a cutoff for the bands, and one considers crystals that are „large“, but finite size, such that one can work with a finite-dimensional basis.

Remark 8.28.2 Without proof, we remark that ...

[1] Note that this unfortunately a poor convention regarding the phraseology. Systems that one describes with this formalism are not neccessarily gases in the traditional sense of having a gas-*phase* (like steam). One treats electrons and phonons in solid materials with this formalism.

- for a crystal with time-reversal-symmetry one obtains $\epsilon_{m,\uparrow}(+\mathbf{k}) = \epsilon_{m,\downarrow}(-\mathbf{k})$, which is also called a *two-fold Kramers-degeneracy of the bands*.
- for a crystal with inversion-symmetry one obtains $\epsilon_{m,\sigma}(+\mathbf{k}) = \epsilon_{m,\sigma}(-\mathbf{k})$.

Remark 8.28.3 In the derivation of the Eliashberg-equations, it is explicitly used that one has a *two-fold Kramers-degeneracy of the bands*, i.e. $\epsilon_m(\mathbf{k}) \equiv \epsilon_{m,\uparrow}(\mathbf{k}) = \epsilon_{m,\downarrow}(\mathbf{k})$, which holds for systems that are time-reversal symmetric *and* inversion-symmetric[2].

Remark 8.28.4 A bosonic example of this Hamiltonian is the *free phonon gas* in a $d_{\mathbf{x}}$-dimensional crystal (within the harmonic approximation)

$$H_0 = \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ \nu \in \{1,\dots,rd_{\mathbf{x}}\}}} \hbar\omega_\nu(\mathbf{q})\, c_\nu^\dagger(\mathbf{q}) c_\nu(\mathbf{q}) \tag{8.30}$$

The Hilbert-space $\mathscr{H}$ of the system reads

$$\mathscr{H} = \mathrm{span}_{\mathbb{C}} \left\{ |n_{\alpha_1}, n_{\alpha_2}, \dots, n_{\alpha_{d_{\mathcal{H}}}}\rangle \,\middle|\, n_{\alpha_\bullet} \in \{0,1,2,\dots\},\ \alpha_i \equiv (\nu_i, \mathbf{q}_i) \in \{1,\dots,rd_{\mathbf{x}}\} \times \mathrm{Q} \right\} \tag{8.31}$$

Remark 8.28.5 Usually one denotes the phononic creation- and annihilation operators with the symbol b instead of c.

Remark 8.28.6 Notice that the have proven in the earlier chapters that the time-reversal-symmetry of the crystal implies for the dispersions $\omega_\nu(+\mathbf{q}) = \omega_\nu(-\mathbf{q})$.

Example: A Non-Interacting Gas with Nature η and Statistics ζ

Definition 8.29 A *quadratic, non-interacting gas* is a system described by the Hamiltonian

$$H_0 = \sum_{\alpha,\beta} H_{0\,\alpha,\beta} c_\alpha^\dagger c_\beta \equiv \mathbf{c}^\dagger \cdot \mathbf{H}_0 \cdot \mathbf{c} \tag{8.32}$$

and Fock-space $\mathscr{F}_\zeta$ spanned by occupation-number-states as usual

$$\mathscr{F}_\zeta = \mathrm{span}_{\mathbb{C}} \left\{ |n_{\alpha_1}, n_{\alpha_2}, \dots, n_{\alpha_{d_{\mathcal{H}}}}\rangle \,\middle|\, n_{\alpha_1}, n_{\alpha_2}, \dots, n_{\alpha_{d_{\mathcal{H}}}} \in \mathbb{N}_\zeta \right\} \tag{8.33}$$

whereas the state with $n_{\alpha_1} = n_{\alpha_2} = \dots = n_{\alpha_{d_{\mathcal{H}}}} = 0$ represents the vacuum-state.

Remark 8.29.1 Computing the Heisenberg-time-evolution for the creation- and annihilation-operators analogously to Lemma 8.28 requires in this case a basis-change. We will not elaborate on this.

[2] Cf. Waste-Folder 1 book reference; Cf. also Lemmas 26.19, 26.22 where we used $\omega(+\mathbf{q}) = \omega(-\mathbf{q})$ and also `https://claude.ai/share/90eda456-0a78-475d-a118-289c0021d85e`.

8.3.2. Interacting Cases

Definition 8.30 The Hamiltonian of *a diagonal gas with quadratic interactions* reads

$$\begin{aligned} H \equiv & \quad H_0 \quad + \quad V \\ \equiv & \sum_{\alpha \in \mathscr{A}} \epsilon_\alpha c_\alpha^\dagger c_\alpha + \sum_{\alpha_1, \alpha_2 \in \mathscr{A}} V_{\alpha_1 \alpha_2} c_{\alpha_1}^\dagger c_{\alpha_2}. \end{aligned}$$

Remark 8.30.1 A typical example of this model is a free electron gas in the LDA-approximation with non-local potentials (e.g. defects in the crystal).

Definition 8.31 The Hamiltonian of *a diagonal gas with cubic interactions* reads

$$\begin{aligned} H \equiv & \quad H_0 \quad + \quad V \\ \equiv & \sum_{\alpha \in \mathscr{A}} \epsilon_\alpha c_\alpha^\dagger c_\alpha + \sum_{\substack{n_1, n_2, n_3 \in \mathbb{N}_\zeta \\ \overline{n_1}, \overline{n_2}, \overline{n_3} \in \mathbb{N}_\zeta}} \delta_{n_1+n_2+n_3+\overline{n_1}+\overline{n_2}+\overline{n_3}=3} \sum_{\alpha_1, \alpha_2, \alpha_3 \in \mathscr{A}} V^{\alpha_1 \alpha_2 \alpha_3}_{n_1 n_2 n_3} \left(c_{\alpha_1}^\dagger\right)^{\overline{n_1}} \left(c_{\alpha_2}^\dagger\right)^{\overline{n_2}} \left(c_{\alpha_3}^\dagger\right)^{\overline{n_3}} c_{\alpha_3}^{n_3} c_{\alpha_2}^{n_2} c_{\alpha_1}^{n_1}. \end{aligned}$$

Remark 8.31.1 Recall from the scheme of second quantization that cubic interactions are relevant only for systems with nature $\eta = 1$, since the Hamiltonian of a system with nature $\eta = 0$ must be even in the creation- and annihilation-operators (i.e. particle number conserving).

Remark 8.31.2 A typical example of this model is a free phonon gas in a crystal with anharmonic interactions, i.e. the *phono3py-model*[3]

$$\begin{aligned} & \quad H_0 \quad + \quad V \\ = & \sum_{\substack{\mathbf{q} \in \mathrm{Q} \\ \nu \in \{1, \ldots, r d_{\mathbf{x}}\}}} \hbar \omega_\nu(\mathbf{q})\, b_\nu^\dagger(\mathbf{q}) b_\nu(\mathbf{q}) \quad + \quad \sum_{\substack{\mathbf{q}, \mathbf{q}', \mathbf{q}'' \in \mathrm{Q} \\ \nu, \nu', \nu'' \in \{1, \ldots, r d_{\mathbf{x}}\}}} \Phi_{\nu\nu'\nu''}(\mathbf{q}, \mathbf{q}', \mathbf{q}'') \left(b_\nu(\mathbf{q}) + b_\nu^\dagger(-\mathbf{q})\right) \left(b_{\nu'}(\mathbf{q}') + b_{\nu'}^\dagger(-\mathbf{q}')\right) \left(b_{\nu''}(\mathbf{q}'') + b_{\nu''}^\dagger(-\mathbf{q}'')\right). \end{aligned} \tag{8.34}$$

whereas we relabeled the creation- and annihilation-operators with the "usual" symbol b instead of c.

Remark 8.31.3 For future reference we abbreviate the matrix-elements as

$$\Phi_{\nu\nu'\nu''}(\mathbf{q}, \mathbf{q}', \mathbf{q}'') \equiv \Phi_{\lambda_1 \lambda_2 \lambda_3} \tag{8.35}$$

and emphasize that they obey the symmetries

[3] Cf. phono3py-paper.

$$\forall \pi \in \mathrm{S}_3 : \Phi_{\lambda_1\lambda_2\lambda_3} = \Phi_{\lambda_{\pi(1)}\lambda_{\pi(2)}\lambda_{\pi(3)}} \tag{8.36}$$

and

$$\Phi_{\nu\nu'\nu''}(\mathbf{q},\mathbf{q}',\mathbf{q}'') = \Phi^*_{\nu\nu'\nu''}(-\mathbf{q},-\mathbf{q}',-\mathbf{q}'') \tag{8.37}$$

Lemma 8.32 One finds that $\Phi_{\nu\nu''\nu''}(0,\mathbf{q}'',-\mathbf{q}'') \in \mathbb{R}$.

Proof 8.32 Using the complex-conjugation symmetry and permutation symmetry, we obtain

$$\begin{aligned} \Phi_{\nu\nu''\nu''}(0,\mathbf{q}'',-\mathbf{q}'') &= \Phi^*_{\nu\nu''\nu''}(0,-\mathbf{q}'',\mathbf{q}'') && (8.38)\\ &= \Phi^*_{\nu\nu''\nu''}(0,\mathbf{q}'',-\mathbf{q}''). && (8.39) \end{aligned}$$

Hence, $\Phi_{\nu\nu''\nu''}(0,\mathbf{q}'',-\mathbf{q}'')$ is real-valued.

Definition 8.33 The Hamiltonian of *a diagonal gas in a crystal with quartic interactions* reads

$$\begin{aligned} H \equiv \quad & H_0 \quad + \quad V \\ \equiv & \sum_{\alpha\in\mathscr{A}} \epsilon_\alpha c^\dagger_\alpha c_\alpha + \frac{1}{2} \sum_{\alpha_1,\alpha_2,\alpha_3,\alpha_4\in\mathscr{A}} V_{\alpha_1\alpha_2\alpha_3\alpha_4} c^\dagger_{\alpha_1} c^\dagger_{\alpha_2} c_{\alpha_4} c_{\alpha_3} \end{aligned}$$

with the additional property

$$V_{\alpha_1\alpha_2\alpha_3\alpha_4} = V_{\alpha_2\alpha_1\alpha_4\alpha_3} \quad \text{for all } \alpha_1,\alpha_2,\alpha_3,\alpha_4 \in \mathscr{A}. \tag{8.40}$$

Remark 8.33.1 A typical example of this model is the "GW-system"[4] for electrons in a crystal with screened Coulomb-interactions.

Definition 8.34 The Hamiltonian of *a non-diagonal gas in a crystal with quartic interactions* reads

$$\begin{aligned} H \equiv \quad & H_0 \quad + \quad V \\ \equiv & \sum_{\alpha,\beta\in\mathscr{A}} H_{0\,\alpha,\beta} c^\dagger_\alpha c_\beta + \frac{1}{2} \sum_{\alpha_1,\alpha_2,\alpha_3,\alpha_4\in\mathscr{A}} V_{\alpha_1\alpha_2\alpha_3\alpha_4} c^\dagger_{\alpha_1} c^\dagger_{\alpha_2} c_{\alpha_4} c_{\alpha_3} \end{aligned}$$

with the additional property

[4] Cf. TBReferenced

$$V_{\alpha_1\alpha_2\alpha_3\alpha_4} = V_{\alpha_2\alpha_1\alpha_4\alpha_3} \quad \text{for all } \alpha_1, \alpha_2, \alpha_3, \alpha_4 \in \mathscr{A}. \tag{8.41}$$

Remark 8.34.1 A typical example of this model is a tight-binding model for electrons in a crystal with Hubbard-interactions.

8.4. Examples - Mixed Systems

8.4.1. Non-Interacting Cases

Definition 8.35 We consider a spin unpolarized, diagonal electron-gas and a diagonal phonon-gas that do not interact with each other

$$\begin{aligned} H &= && H_0 \\ &= H_{0,\mathrm{el}} && + H_{0,\mathrm{ph}} \\ &= \sum_{\substack{\mathbf{k}\in Q \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\dots,\infty\}}} \epsilon_{m\mathbf{k}\sigma} c^\dagger_{m\mathbf{k}\sigma} c_{m\mathbf{k}\sigma} && + \sum_{\substack{\mathbf{q}\in Q \\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} \Omega_{\mathbf{q},\nu} b^\dagger_{\mathbf{q}\nu} b_{\mathbf{q}\nu} \end{aligned} \tag{8.42}$$

with $\epsilon_{m\mathbf{k}\uparrow} = \epsilon_{m\mathbf{k}\downarrow}$.

8.4.2. Interacting Cases

Definition 8.36 We consider the *EPW-system*, i.e. a spin unpolarized, diagonal electron-gas and a diagonal phonon-gas interacting with each other over a spin-independent-interaction as

$$\begin{aligned} H &= && H_0 && + && V \\ &= \sum_{\substack{\mathbf{k}\in Q \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\dots,\infty\}}} \epsilon_{m\mathbf{k}\sigma} c^\dagger_{m\mathbf{k}\sigma} c_{m\mathbf{k}\sigma} && + \sum_{\substack{\mathbf{q}\in Q \\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} \hbar\omega_{\mathbf{q},\nu} b^\dagger_{\mathbf{q}\nu} b_{\mathbf{q}\nu} && + \sum_{\substack{\mathbf{k},\mathbf{q}\in Q \\ \sigma\in\{\uparrow,\downarrow\} \\ \nu\in\{1,\dots,rd_{\mathbf{x}}\} \\ m,n\in\{1,\dots,\infty\}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\sqrt{N_p}} c^\dagger_{\mathbf{k}+\mathbf{q}m\sigma} c_{\mathbf{k}n\sigma} \left(b_{\mathbf{q}\nu} + b^\dagger_{-\mathbf{q}\nu} \right) \end{aligned} \tag{8.43}$$

with $\epsilon_{m\mathbf{k}\uparrow} = \epsilon_{m\mathbf{k}\downarrow}$.

Lemma 8.37 The hermiticity of the Hamiltonian implies for the coupling

$$g_{mn\nu}(\mathbf{k},\mathbf{q}) = g^*_{nm\nu}(\mathbf{k}+\mathbf{q},-\mathbf{q}). \tag{8.44}$$

Proof 8.37 See Appendix, Proofs, page 516.

Remark 8.37.1 Notice that this property implies that $g_{nn\nu}(\mathbf{k},0) = g^*_{nn\nu}(\mathbf{k},0) \in \mathbb{R}$, i.e. the diagonal coupling at zero phonon-momentum is real-valued.

Lemma 8.38 Notice that for inversion-symmetric crystals one has the additional symmetry

$$g_{mn\nu}(\mathbf{k},\mathbf{q}) = g^*_{mn\nu}(-\mathbf{k},-\mathbf{q}). \tag{8.45}$$

Proof 8.38 This can[5] be concluded from the expressions that appear in [19].

Definition 8.39 We consider the *EPy3W-system*, i.e. a spin unpolarized, diagonal electron-gas and an interacting phonon-gas interacting with each other over a spin-independent-interaction as

$$\begin{aligned} H &= H_0 + V \\ &= \sum_{\substack{\mathbf{k}\in \mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\dots,\infty\}}} \epsilon_{m\mathbf{k}\sigma} c^\dagger_{m\mathbf{k}\sigma} c_{m\mathbf{k}\sigma} + \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} \hbar\omega_{\mathbf{q},\nu} b^\dagger_{\mathbf{q}\nu} b_{\mathbf{q}\nu} + V_{\text{el-ph}} + V_{\text{ph-ph}} \end{aligned}$$

with $\epsilon_{m\mathbf{k}\uparrow} = \epsilon_{m\mathbf{k}\downarrow}$ and

$$\begin{aligned} V_{\text{el-ph}} &= \sum_{\substack{\mathbf{k},\mathbf{q}\in \mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ \nu\in\{1,\dots,rd_{\mathbf{x}}\} \\ m,n\in\{1,\dots,\infty\}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\sqrt{N_p}} c^\dagger_{\mathbf{k}+\mathbf{q}m\sigma} c_{\mathbf{k}n\sigma} \left(b_{\mathbf{q}\nu} + b^\dagger_{-\mathbf{q}\nu} \right) \\ V_{\text{ph-ph}} &= \sum_{\substack{\mathbf{q},\mathbf{q}',\mathbf{q}''\in \mathrm{Q} \\ \nu,\nu',\nu''\in\{1,\dots,rd_{\mathbf{x}}\}}} \Phi_{\nu\nu'\nu''}(\mathbf{q},\mathbf{q}',\mathbf{q}'') \left(b_\nu(\mathbf{q}) + b^\dagger_\nu(-\mathbf{q}) \right) \left(b_{\nu'}(\mathbf{q}') + b^\dagger_{\nu'}(-\mathbf{q}') \right) \left(b_{\nu''}(\mathbf{q}'') + b^\dagger_{\nu''}(-\mathbf{q}'') \right). \end{aligned} \tag{8.46}$$

Remark 8.39.1 For notational symmetry, we also introduce

$$\phi_{\nu\nu'\nu''}(\mathbf{q},\mathbf{q}',\mathbf{q}'') \equiv \frac{\Phi_{\nu\nu'\nu''}(\mathbf{q},\mathbf{q}',\mathbf{q}'')}{\sqrt{N_p}} \tag{8.47}$$

Definition 8.40 We consider the *CEPy3W-system*, i.e. a spin unpolarized, diagonal *[C]oulomb-interacting* electron-gas and an interacting phonon-gas interacting with each other over a spin-independent-interaction as

[5] For the details: See Waste-Folder 1, Topic 6.

$$\begin{aligned} H &= H_0 + V \\ &= \sum_{\substack{\mathbf{k}\in \mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\}}} \epsilon_{m\mathbf{k}\sigma} c^\dagger_{m\mathbf{k}\sigma} c_{m\mathbf{k}\sigma} + \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\}}} \hbar\omega_{\mathbf{q},\nu} b^\dagger_{\mathbf{q}\nu} b_{\mathbf{q}\nu} + V_{\text{el-el}} + V_{\text{el-ph}} + V_{\text{ph-ph}} \end{aligned}$$

with $\epsilon_{m\mathbf{k}\uparrow} = \epsilon_{m\mathbf{k}\downarrow}$ and the precise form of the Coulomb-interaction from second quantization.

Definition 8.41 We consider the *EPy3W++-system*, i.e. a spin unpolarized, diagonal electron-gas and an interacting phonon-gas interacting with each other over a spin-independent-interaction as

$$\begin{aligned} H &= H_0 + V \\ &= \sum_{\substack{\mathbf{k}\in \mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\}}} \epsilon_{m\mathbf{k}\sigma} c^\dagger_{m\mathbf{k}\sigma} c_{m\mathbf{k}\sigma} + \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\}}} \hbar\omega_{\mathbf{q},\nu} b^\dagger_{\mathbf{q}\nu} b_{\mathbf{q}\nu} + V^{++}_{\text{el-ph}} + V_{\text{ph-ph}} \end{aligned}$$

with $\epsilon_{m\mathbf{k}\uparrow} = \epsilon_{m\mathbf{k}\downarrow}$ and

$$V^{++}_{\text{el-ph}} - V_{\text{el-ph}} \equiv V^{\text{DW}}_{\text{el-ph}} = \sum_{\substack{\mathbf{k},\mathbf{q},\mathbf{q}'\in \mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ \nu,\nu'\in\{1,\ldots,rd_{\mathbf{x}}\} \\ m,n\in\{1,\ldots,\infty\}}} \frac{g^{\text{DW}}_{mn\nu\nu'}(\mathbf{k},\mathbf{q},\mathbf{q}')}{N_p} c^\dagger_{\mathbf{k}+\mathbf{q}+\mathbf{q}',m,\sigma} c_{\mathbf{k},n,\sigma} \left(b_{\mathbf{q}\nu} + b^\dagger_{-\mathbf{q}\nu}\right)\left(b_{\mathbf{q}'\nu'} + b^\dagger_{-\mathbf{q}'\nu'}\right) \tag{8.48}$$

Lemma 8.42 The hermiticity conditions yields

$$g^{\text{DW}}_{mn\nu\nu'}(\mathbf{k},\mathbf{q},\mathbf{q}') = \left(g^{\text{DW}}_{nm\nu'\nu}(\mathbf{k}+\mathbf{q}+\mathbf{q}',-\mathbf{q},-\mathbf{q}')\right)^* \tag{8.49}$$

Proof 8.42 TBD

Remark 8.42.1 Another symmetry ("exchange symmetry of the two phonon legs") reads

$$g^{\text{DW}}_{mn\nu\nu'}(\mathbf{k},\mathbf{q},\mathbf{q}') = g^{\text{DW}}_{nm\nu'\nu}(\mathbf{k},\mathbf{q}',\mathbf{q}) \tag{8.50}$$

Remark 8.42.2 Another symmetry ("time reversal symmetry") (for a system with a real phonon-mode convention) reads

$$g^{\text{DW}}_{mn\nu\nu'}(\mathbf{k},\mathbf{q},\mathbf{q}') = g^{\text{DW}}_{mn\nu\nu'}(-\mathbf{k},-\mathbf{q},-\mathbf{q}') \tag{8.51}$$

Definition 8.43 We consider the *CEPy3W++-system*, i.e. a spin unpolarized, diagonal *[C]oulomb-interacting* electron-gas and an interacting phonon-gas interacting with each other over a spin-independent-interaction as

$$\begin{aligned} H &= H_0 + V \\ &= \sum_{\substack{\mathbf{k}\in \mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\}}} \epsilon_{m\mathbf{k}\sigma} c^\dagger_{m\mathbf{k}\sigma} c_{m\mathbf{k}\sigma} + \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\}}} \hbar\omega_{\mathbf{q},\nu} b^\dagger_{\mathbf{q}\nu} b_{\mathbf{q}\nu} + V_{\text{el-el}} + V^{++}_{\text{el-ph}} + V_{\text{ph-ph}} \end{aligned}$$

with $\epsilon_{m\mathbf{k}\uparrow} = \epsilon_{m\mathbf{k}\downarrow}$ and the precise form of the Coulomb-interaction from second quantization.

9. Fundamentals III - Quantum Statistical Mechanics - Pure Systems

Quoting from [38, p. 47]:

> *In quantum statistical mechanics, the thermodynamic properties of a system in equilibrium are specified by the assumption of the equal occupation of accessible states. The physical problem is idealized by considering an appropriate ensemble of identical systems, and the probability of observing a particular state is given by the ratio of the number of systems in the ensemble in that state to the total number of systems in the ensemble. Three ensembles are commonly used. The microcanonical ensemble describes an isolated system, which has fixed energy E and fixed particle number. The probability of obsenring a state of energy $E' \neq E$ is zero and that of observing a state of energy $E' = E$ is constant, equal to the inverse of the total number of states of energy E. The canonical ensemble describes a system of fixed particle number in equilibrium with a thermal reservoir with which it may exchange energy at a specified temperature. By enumerating the number of states in which the system and the reservoir combined have a fixed total energy, it follows that the probability of observing this system alone with energy E is proportional to $\mathrm{e}^{-E/k_B T} \equiv \mathrm{e}^{-\beta E}$ where k_B is Boltzmann's constant. The average energy of the system is fixed and is, controlled by the temperature T. The grand canonical ensemble describes a system in equilibrium with a particle reservoir, with which it may change particles, as well as a thermal reservoir. Enumeration of the states in which the system and reservoir have fixed total energy and particle number leads to the result that the probability of observing the system alone with energy E and particle number N is proportional to $\mathrm{e}^{-\beta(E-\mu N)}$. In addition to the average energy of the system, the average particle number is now fixed and is controlled by the chemical potential. The thermodynamic limit for a physical system of N particles contained in a volume V is defined by taking the limit as N and V go to infinity such that the ratio $\rho = N/V$ remains constant. An essential result of thermodynamics is that the three ensembles are equivalent for describing the macroscopic properties of most systems in the thermodynamic limit. One is then free to select the ensemble on the basis of formal convenience, and as in the case of classical statistical mechanics, the grand canonical ensemble offers the greatest formal simplicity.*

9.1. Linear Mappings

In this section, we will carefully explain how expressions of the type "ket-bra" are to be understood.

Definition 9.1 Let V,W denote vector-spaces over a field $\mathbb{K}$. Let us write further $\mathrm{Hom}(V,W)$ for the $\mathbb{K}$-vector space of linear mappings from V to W, and V^* for the dual vector space of V.

Theorem 9.2 The mapping

$$\begin{aligned} I:\ W\otimes V^\star &\longrightarrow \mathrm{Hom}(V,W)\\ w\otimes f\ &\mapsto I(w\otimes f)\end{aligned}$$

with

$$\forall v\in V\ :\ I(w\otimes f)(v) := f(v)w \tag{9.1}$$

and linear extension over the remaining tensor-product, is an isomorphism.

Proof 9.2 The linearity is given by construction:

$$I(w_1\otimes f_1+w_2\otimes f_2)=I(w_1\otimes f_1)+I(w_2\otimes f_2) \tag{9.2}$$

For the linearity w.r.t. $\mathbb{K}$-multiplication one finds for $\lambda\in\mathbb{K}$

$$I((\lambda w)\otimes f)(v)=f(v)\cdot\lambda\cdot w=I(w\otimes(\lambda f))(v)=(\lambda\cdot f)(v)\cdot w=\lambda\cdot f(v)\cdot w \tag{9.3}$$

For the injectivity, let us assume that $I(w\otimes f)=0$, meaning that

$$\forall v\in V\ :\ I(w\otimes f)(v)=f(v)w=0. \tag{9.4}$$

There is two solutions for this: Either $\forall v\in V\ :\ f(v)=0$ or $w=0$. Since f is a linear map, both cases imply that $w\otimes f=0$, that only the zero gets mapped to zero.

For the surjectivity, we take $A\in\mathrm{Hom}(V,W)$ and prove that there is a decomposition, such that

$$\forall v\in V\ :\ Av=I\left(\sum_i w_i\otimes f_i\right)(v) \tag{9.5}$$

For this, we choose a basis $e_1,\dots,e_n$ of V with dual basis $e^1,\dots,e^n$ of V^*, such that $e^i(e_j)=\delta_{i,j}$. Next, we decompose v w.r.t. this basis, i.e.

$$v=\sum_{i=1}^n e^i(v)e_i\quad\left(\equiv\sum_{i=1}^n v_i e_i\right) \tag{9.6}$$

This yields, using the linearity of A,

$$Av = \sum_{i=1}^{n} e^i(v) Ae_i = \dots \tag{9.7}$$

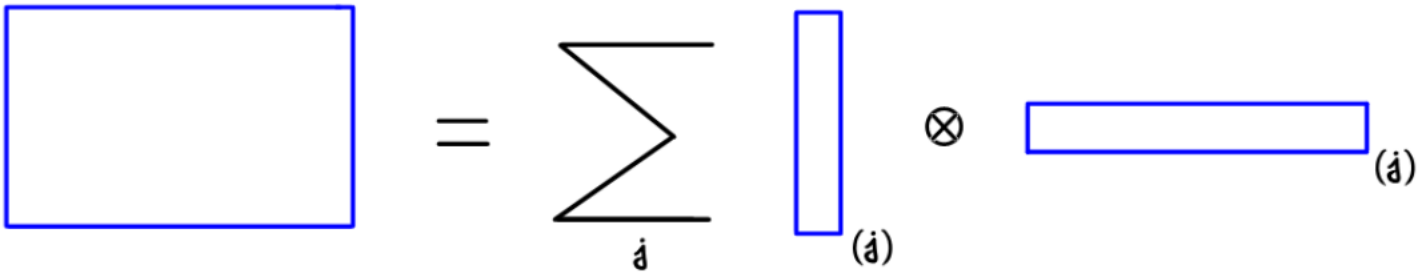
Since $Ae_i \in W$, and $e^i \in V^*$ we can rewrite this expression as

$$\dots = \sum_{i=1}^{n} I\left(Ae_i \otimes e^i\right)(v) = I\left(\sum_{i=1}^{n} Ae_i \otimes e^i\right)(v) \tag{9.8}$$

proving the surjectivity.

Remark 9.2.1 Since, after referring to a basis, vectors are usually interpreted as standing vectors, and dual-vectors are usually interpreted as lyings-vectors, one sees that each matrix of size $m \times n$ can be decomposed uniquely (up to an ambiguity due to scalar factors moving in the tensor product) as a sum of terms each of which is the tensor product (sometimes called a 'dyadic' product in physics textbooks) of an m-component column vector with an n-component row vector.

Remark 9.2.2 The figure elucidates the isomorphism.



Notation 9.3 Switching to the physics-conventions, we realize that in the case of $V = W \equiv \mathscr{H}$ for some (single- or many-particle) Hilbert-space, $V^* \equiv \mathscr{H}^*$ its dual space, and End($\mathscr{H}$) the set of all endomorphisms on the Hilbert-space, one can, for arbitrary $\psi, \chi \in \mathscr{H}$, interprete expressions of the type

$$|\psi\rangle\langle\chi| \tag{9.9}$$

as linear mappings, and by referring to a basis, their underlying matrix can be determined from a dyadic-product.

9.2. Density Matrices

Motivation: The need for a new Technique

Consider a Hilbert-space $\mathscr{H}$ with scalar-product $\langle\ ,\ \rangle$. So far, we have only considered state-vectors in this Hilbert-space, so called *pure states*. But with this idea, one can not tackle all physically relevant situations:

Let us assume that $\{|\psi_i\rangle\}_{i=1,\dots,N} \subset \mathscr{H}$ is an arbitrary series of pure states, and let us assume a situation, in which a pure state $|\psi_i\rangle$ is created with probability $q_i \in [0,1]$, s.t. $\sum_i q_i = 1$. Then, common-sense tells us, that we have for the expectation-value of an observable A the following equation

$$\langle A\rangle = \sum_i q_i \langle\psi_i|A|\psi_i\rangle. \tag{9.10}$$

Now let's rewrite the r.h.s.:

$$\langle A\rangle = \sum_i q_i \langle\psi_i|A|\psi_i\rangle = \sum_i q_i \operatorname{Tr}\left(|\psi_i\rangle\langle\psi_i|A\right) = \operatorname{Tr}\left(\sum_i q_i |\psi_i\rangle\langle\psi_i|A\right) =: \operatorname{Tr}(\rho A) \tag{9.11}$$

Remark 9.3.1 In this example it immediately follows that $\operatorname{Tr}\rho = 1$.

Remark 9.3.2 One calls such an operator ρ, that describes the systems state, a *density(-operator)*. We will introduce them now more carefully.

The Formalism of Density Matrices

Quantum mechanics distinguishes between two types of states that physical systems can be in: "pure" and "mixed states". In this section we will introduce both.

Definition 9.4 A **pure state** is a state that can be described by a ket vector $|\psi\rangle$ in a Hilbert-space $\mathscr{H}$.

Remark 9.4.1 Notice that this Hilbert-space can be either a single-particle Hilbert-space or a many-particle Hilbert-space.

Definition 9.5 We assume that the system is with probabilities

$$p_i \in [0,1) \quad \text{and} \quad \sum_{i=1}^{n} p_i = 1 \tag{9.12}$$

in orthonormalized pure states

$$|\psi_i\rangle \quad \text{with} \quad \langle\psi_i|\psi_j\rangle = \delta_{ij}. \tag{9.13}$$

The system is then described by the *density matrix*, or *density* for short,

$$\begin{aligned} \rho : \mathscr{H} &\to \mathscr{H} \\ |\chi\rangle &\mapsto \rho|\chi\rangle \end{aligned}$$

which is defined as a sum of *projectors*

$$\hat{\rho} = \sum_{i=1}^{n} p_i |\psi_i\rangle\langle\psi_i|. \tag{9.14}$$

Remark 9.5.1 For $n = 1$, the density matrix still represents a pure state, for $n > 1$, we shall refer to it as describing a *mixed state*.

Remark 9.5.2 One can also introduce densities for states that are not orthonormalized. We will however not do so, since we are not interested in these cases.

Lemma 9.6 We have the following properties for the density matrix $\hat{\rho}$:

1. $\hat{\rho}$ is hermitian, i.e. $\hat{\rho} = \hat{\rho}^\dagger$.
2. $\hat{\rho}$ has the eigenvalues p_i with eigenstates $|\psi_i\rangle$.
3. $\hat{\rho}$ is positive, i.e. $\langle\chi|\hat{\rho}|\chi\rangle \geq 0$ for all $|\chi\rangle$.
4. $\hat{\rho}$ is *normalized*, i.e. $\mathrm{Tr}(\hat{\rho}) = 1$.

Proof 9.6 TBDigitalized from Nolting p. 106 f.

We follow [40, Sect. 2.1.1, p. 106 f.]. Throughout, $\{|\varphi_k\rangle\}_k$ denotes an arbitrary orthonormal basis of $\mathscr{H}$, i.e. $\sum_k |\varphi_k\rangle\langle\varphi_k| = \mathbb{1}$, and $\hat{\rho} = \sum_{i=1}^n p_i|\psi_i\rangle\langle\psi_i|$ as in Definition 9.5.

1. *Hermiticity.* Every projector $|\psi_i\rangle\langle\psi_i|$ is hermitian, since for all $|\chi\rangle, |\phi\rangle \in \mathscr{H}$

$$\langle\chi|\left(|\psi_i\rangle\langle\psi_i|\right)|\phi\rangle = \langle\chi|\psi_i\rangle\langle\psi_i|\phi\rangle = \left(\langle\phi|\psi_i\rangle\langle\psi_i|\chi\rangle\right)^* = \langle\phi|\left(|\psi_i\rangle\langle\psi_i|\right)|\chi\rangle^*,$$

   and the p_i are real. Hence $\hat{\rho}^\dagger = \sum_i p_i^* \left(|\psi_i\rangle\langle\psi_i|\right)^\dagger = \hat{\rho}$.

2. *Eigenvalues.* By the orthonormality $\langle\psi_i|\psi_j\rangle = \delta_{ij}$ one finds

$$\hat{\rho}|\psi_j\rangle = \sum_{i=1}^{n} p_i |\psi_i\rangle\langle\psi_i|\psi_j\rangle = p_j|\psi_j\rangle.$$

   (If $n < \dim\mathscr{H}$, every $|\chi\rangle \perp \mathrm{span}\{|\psi_1\rangle, \ldots, |\psi_n\rangle\}$ satisfies $\hat{\rho}|\chi\rangle = 0$, i.e. the only further eigenvalue is 0.) As Nolting remarks, this statement is no longer true if the $|\psi_i\rangle$ are normalized, but not orthogonal.

3. *Positivity.* Since $p_i \geq 0$,

$$\langle\chi|\hat{\rho}|\chi\rangle = \sum_{i=1}^{n} p_i \langle\chi|\psi_i\rangle\langle\psi_i|\chi\rangle = \sum_{i=1}^{n} p_i \left|\langle\chi|\psi_i\rangle\right|^2 \geq 0.$$

For normalized $|\chi\rangle$, this can be interpreted as the probability to find the system described by $\hat{\rho}$ in the state $|\chi\rangle$.

4. *Normalization.* Using the completeness of $\{|\varphi_k\rangle\}_k$,

$$\mathrm{Tr}(\hat{\rho}) = \sum_k \langle\varphi_k|\hat{\rho}|\varphi_k\rangle = \sum_{i=1}^{n} p_i \sum_k \langle\psi_i|\varphi_k\rangle\langle\varphi_k|\psi_i\rangle = \sum_{i=1}^{n} p_i \langle\psi_i|\psi_i\rangle = \sum_{i=1}^{n} p_i = 1.$$

Theorem 9.7 For time-dependent states $|\psi_i\rangle \equiv |\psi_i(t)\rangle$ that obey the Schrödinger-equation

$$\mathrm{i}\hbar \frac{d}{dt}|\psi_i(t)\rangle = \hat{H}|\psi_i(t)\rangle \tag{9.15}$$

we find that $\hat{\rho} \equiv |\psi_i\rangle\langle\psi_i|$ obeys the von Neumann-equation

$$\frac{d}{dt}\hat{\rho} = -\frac{\mathrm{i}}{\hbar}[\hat{H}, \hat{\rho}]. \tag{9.16}$$

Proof 9.7 TBDigitalized from Nolting p. 108

Nolting [40, p. 108, Eq. (2.11)] only quotes this result from his Volume 5/1, Eq. (3.167), which is not contained in the literature folder. We therefore follow [47, Sect. 1.4.2, Eq. (1.4.8)] and prove the statement directly for a general density $\hat{\rho}(t) = \sum_{i=1}^{n} p_i |\psi_i(t)\rangle\langle\psi_i(t)|$ with time-independent probabilities p_i. The case of a single projector $\hat{\rho} = |\psi_i\rangle\langle\psi_i|$ corresponds to $n = 1$ and $p_1 = 1$.

Since $\hat{H}$ is hermitian, the Schrödinger-equation and its adjoint read

$$\frac{d}{dt}|\psi_i(t)\rangle = -\frac{\mathrm{i}}{\hbar}\hat{H}|\psi_i(t)\rangle, \qquad \frac{d}{dt}\langle\psi_i(t)| = +\frac{\mathrm{i}}{\hbar}\langle\psi_i(t)|\hat{H}.$$

With the product rule we obtain

$$\begin{aligned}\frac{d}{dt}\hat{\rho} &= \sum_{i=1}^{n} p_i \left(\left(\frac{d}{dt}|\psi_i\rangle\right)\langle\psi_i| + |\psi_i\rangle\left(\frac{d}{dt}\langle\psi_i|\right)\right) = -\frac{\mathrm{i}}{\hbar}\sum_{i=1}^{n} p_i \left(\hat{H}|\psi_i\rangle\langle\psi_i| - |\psi_i\rangle\langle\psi_i|\hat{H}\right) \\ &= -\frac{\mathrm{i}}{\hbar}\left(\hat{H}\hat{\rho} - \hat{\rho}\hat{H}\right) = -\frac{\mathrm{i}}{\hbar}[\hat{H}, \hat{\rho}].\end{aligned}$$

Following [47, p. 16] we add three remarks: (i) the derivation also holds for time-dependent $\hat{H}$; (ii) the sign differs from the one in the Heisenberg equation of motion $\frac{d}{dt}\hat{A}_{\mathrm{H}} = +\frac{\mathrm{i}}{\hbar}[\hat{H}, \hat{A}_{\mathrm{H}}]$, since $\hat{\rho}$ is an operator in the Schrödinger-picture; (iii) with the unitary time-evolution operator $U(t, t_0)$ one has $\hat{\rho}(t) = U(t, t_0)\hat{\rho}(t_0)U(t, t_0)^\dagger$ [47, Eq. (1.4.11)]. In particular $\langle\psi_i(t)|\psi_j(t)\rangle = \langle\psi_i(t_0)|U^\dagger U|\psi_j(t_0)\rangle = \delta_{ij}$, such that $\hat{\rho}(t)$ remains a density matrix in the sense of Definition 9.5 for all times.

Remark 9.7.1 We call a solution a *stationary state* if $\hat{\rho}$ is time-independent.

Definition 9.8 We define the expectation value of an operator $\hat{A}$ in the state $\hat{\rho}$ as

$$\langle \hat{A} \rangle := \mathrm{Tr}(\hat{\rho}\hat{A}). \tag{9.17}$$

Lemma 9.9 It follows that

$$\langle \hat{A} \rangle^* = \langle \hat{A}^\dagger \rangle \tag{9.18}$$

Proof 9.9 Follows from the hermiticity of the density matrix.

Theorem 9.10 The expectation value of an operator $\hat{A}$ in the state $\hat{\rho}$ is given by

$$\langle \hat{A} \rangle = \sum_{i=1}^{n} p_i \langle \psi_i | \hat{A} | \psi_i \rangle. \tag{9.19}$$

Proof 9.10 TBDigitalized from Nolting p. 109

The computation is given in [40, p. 106], where it is read from right to left. Let $\{|\varphi_k\rangle\}_k$ be an arbitrary orthonormal basis of $\mathscr{H}$ with $\sum_k |\varphi_k\rangle\langle\varphi_k| = \mathbb{1}$ (the trace does not depend on this choice). Inserting Definition 9.5 yields

$$\begin{aligned}\langle \hat{A} \rangle = \mathrm{Tr}(\hat{\rho}\hat{A}) &= \sum_k \langle \varphi_k | \hat{\rho}\hat{A} | \varphi_k \rangle = \sum_k \sum_{i=1}^{n} p_i \langle \varphi_k | \psi_i \rangle \langle \psi_i | \hat{A} | \varphi_k \rangle \\ &= \sum_{i=1}^{n} p_i \langle \psi_i | \hat{A} \left(\sum_k |\varphi_k\rangle\langle\varphi_k| \right) |\psi_i\rangle = \sum_{i=1}^{n} p_i \langle \psi_i | \hat{A} | \psi_i \rangle.\end{aligned}$$

Equivalently, in matrix notation with $\rho_{kj} = \langle \varphi_k | \hat{\rho} | \varphi_j \rangle$ and $A_{jk} = \langle \varphi_j | \hat{A} | \varphi_k \rangle$, this reads $\langle \hat{A} \rangle = \sum_{j,k} \rho_{kj} A_{jk} = \sum_k (\rho A)_{kk}$ [40, p. 106].

Remark 9.10.1 Notice that this expression is completely intuitive, given the situation from Definition 9.5.

Definition 9.11 Given a state ρ, we define the *entropy* as

$$S(\hat{\rho}) = -k_\mathrm{B} \,\mathrm{Tr}(\hat{\rho} \ln \hat{\rho}). \tag{9.20}$$

Remark 9.11.1 Notice that in the template[1] it is also proven that this identity holds for all ensembles.

Proof 9.11.1 We follow [40, Sect. 2.5.1, Eqs. (2.88)–(2.97)] and show

$$S = -k_{\mathrm{B}} \operatorname{Tr}(\hat{\rho} \ln \hat{\rho}) = -k_{\mathrm{B}} \langle \ln \hat{\rho} \rangle$$

separately for the three ensembles, anticipating the densities of the subsequent sections. In each case $\hat{\rho}$ is diagonal in an orthonormal basis of eigenstates of $\hat{H}$ (and $\hat{N}$), and $\ln \hat{\rho}$ is defined via the eigenvalues of $\hat{\rho}$ (with the convention $0 \ln 0 := 0$).

Microcanonical ensemble. The postulated density $\hat{\rho}_{\mathrm{MCE}}$ has the eigenvalue $\Omega(E, V, N)^{-1}$ on the states $|E_m\rangle$ with $E_m \in \mathscr{E}$, and 0 otherwise. Thus

$$\operatorname{Tr}(\hat{\rho}_{\mathrm{MCE}} \ln \hat{\rho}_{\mathrm{MCE}}) = \sum_m \langle E_m | \hat{\rho}_{\mathrm{MCE}} \ln \hat{\rho}_{\mathrm{MCE}} | E_m \rangle = \sum_{E_m \in \mathscr{E}} \frac{1}{\Omega} \ln \frac{1}{\Omega} = -\ln \Omega,$$

and hence $-k_{\mathrm{B}} \operatorname{Tr}(\hat{\rho}_{\mathrm{MCE}} \ln \hat{\rho}_{\mathrm{MCE}}) = k_{\mathrm{B}} \ln \Omega = S_{\mathrm{MCE}}$ (Definition 9.18).

Canonical ensemble. With $\hat{\rho}_{\mathrm{CE}} = Z^{-1} \mathrm{e}^{-\beta \hat{H}}$ (Theorem 9.27) and the free energy $F = -k_{\mathrm{B}} T \ln Z$, i.e. $Z = \mathrm{e}^{-\beta F}$ [40, Eq. (2.93)], one has $\hat{\rho}_{\mathrm{CE}} = \mathrm{e}^{\beta(F - \hat{H})}$ and thus, with $U = \langle \hat{H} \rangle$,

$$-k_{\mathrm{B}} \langle \ln \hat{\rho}_{\mathrm{CE}} \rangle = -k_{\mathrm{B}} \beta \left(F - \langle \hat{H} \rangle \right) = -\frac{1}{T} (F - U) = S,$$

where the thermodynamic relation $F = U - TS$ was used in the last step.

Grand canonical ensemble. With $\hat{\rho}_{\mathrm{GCE}} = \Xi^{-1} \mathrm{e}^{-\beta(\hat{H} - \mu \hat{N})}$ and $\Xi = \operatorname{Tr} \mathrm{e}^{-\beta(\hat{H} - \mu \hat{N})} = \mathrm{e}^{-\beta \Omega}$, where here $\Omega = F - \mu \langle \hat{N} \rangle$ denotes the grand canonical potential (not the number of microstates) [40, Eqs. (2.95)–(2.97)], one has $\hat{\rho}_{\mathrm{GCE}} = \mathrm{e}^{\beta(\Omega - \hat{H} + \mu \hat{N})}$ and thus

$$-k_{\mathrm{B}} \langle \ln \hat{\rho}_{\mathrm{GCE}} \rangle = -\frac{1}{T} \left(\Omega - \langle \hat{H} \rangle + \mu \langle \hat{N} \rangle \right) = -\frac{1}{T} (F - U) = S.$$

Read from right to left, the canonical computation shows conversely that $F = -k_{\mathrm{B}} T \ln Z$ satisfies $F = U - TS$ if the entropy is *defined* as $S = -k_{\mathrm{B}} \operatorname{Tr}(\hat{\rho}_{\mathrm{CE}} \ln \hat{\rho}_{\mathrm{CE}})$, which is the route taken in [47, Eqs. (2.6.18), (2.6.44), (2.6.48)].

The subsequent sections will become a bit messy with notation, so we believe that it is appropriate to end this section with the following quote (again).

> *"Zudem ist es ein Irrtum zu glauben, dass die Strenge in der Beweisführung die Feindin der Einfachheit wäre."*
>
> David Hilbert in a lecture given at the International Congress of Mathematicians in Paris 1900

[1] Cf. TBDigitalized from Nolting p. 151. Digitalized in the proof below, following [40, Sect. 2.5.1, p. 151 ff.].

9.3. The Microcanonical Ensemble

Fact 9.12 For macroscopically large systems, it is impossible to determine the exact state of the system by solving the time-dependent Schrödinger-equation for some given initial value. In statistical physics, it is then common to "guess" / postulate the state of the system, by considering a more or less reasonable density matrix $\hat{\rho}$.

Definition 9.13 We define the *natural variables of the microcanonical ensemble* as the triplet $(E, V, N) \in (-\infty, +\infty) \times (0, +\infty) \times \mathbb{N}_0$, whereas ...

- $E \in (-\infty, +\infty)$ is the energy (relative to some reference-energy) of the system,
- $V \in (0, +\infty)$ is the volume of the system, and
- $N \in \mathbb{N}_0 = \{0, 1, 2, \dots, \infty\}$ is the number of particles.

Notation 9.14 For a fixed particle number N and a fixed volume V we enumerate the set of eigen-energies $\{E_1, E_2, \dots\}$ and orthonormal eigenstates $\{|E_1\rangle, |E_2\rangle, \dots\}$ of the Hamilton-operator of the system

$$\hat{H}|E_i\rangle = E_i|E_i\rangle \quad \text{with} \quad \langle E_i|E_j\rangle = \delta_{ij} \quad \text{and} \quad \mathscr{H}_N = \text{span}_{\mathbb{C}} \{|E_1\rangle, |E_2\rangle, \dots\}, \tag{9.21}$$

whereas $\mathscr{H}_N$ represents the underlying N-particle Hilbert-space.

Remark 9.14.1 Notice that the volume influences the eigen-energies, and that the eigen-states above are such that they correspond to N-particle states

$$\langle E_i|\hat{N}|E_i\rangle = N. \tag{9.22}$$

with the particle-number operator $\hat{N}$ from Definition 7.40. Thus, the eigenenergies actually depend on the volume V and the particle number N as

$$E_i \equiv E_i(V, N). \tag{9.23}$$

However, we will suppress this dependence for notational convenience.

Definition 9.15 For an uncertainty Δ, that corresponds to the energy-uncertainty in the measuring-process, we define the subset

$$\mathscr{E} = \left\{ E_\bullet \in \{E_1, E_2, \dots\} \,\middle|\, E_\bullet \in [E - \Delta, E] \right\}. \tag{9.24}$$

The corresponding states $\left\{ |E_\bullet\rangle \,\middle|\, E_\bullet \in \mathscr{E} \right\}$ is called *the set of microstates corresponding to the triplet* (E, V, N). Further we introduce the *total number of accessible microstates in the microcanonical ensemble* $\Omega_\Delta(E, V, N)$ as the cardinal number of $\mathscr{E}$, i.e.

$$\Omega_\Delta(E, V, N) = \sum_{E_\bullet \in \mathscr{E}} 1 = |\mathscr{E}|. \tag{9.25}$$

Remark 9.15.1 When one explicitly computes the total number of microstates for some simple toy-models, one finds that Ω depends only lightly on Δ. One usually then *postulates* that this is also the case for more complicated systems and drops the index $\Omega_\Delta(E,V,N) \equiv \Omega(E,V,N)$.

Hypothesis 9.16 We *postulate* that the system is in a state that is described by the density matrix

$$\hat{\rho}_{\mathrm{MCE}} = \sum_{m=1,2,\ldots} p_m^{\mathrm{MCE}} |E_m\rangle\langle E_m| \tag{9.26}$$

with the probabilities

$$p_m^{\mathrm{MCE}} = \begin{cases} \Omega(E,V,N)^{-1} & \text{for} \quad E_m \in \mathscr{E}. \\ 0 \quad \text{otherwise.} \end{cases} \tag{9.27}$$

Remark 9.16.1 This assumption is sometimes referred to as the *principle of equal a priori probabilities* or *the fundamental postulate of statistical mechanics*. It is oftentimes formulated in prose as

> *A closed system in equilibrium is equally probable in each of its accessible microstates.*

We further say, that the system is in the *thermal state* if the system is properly described by the density above.

Remark 9.16.2 The fact that this is the correct state to describe the system is proven a posteriori by the fact that it leads to the correct experimental results. Thinking about it longer, it is a rather unreasonable assumption.

Corollary 9.17 The following statements are immediate

- $\hat{\rho}$ is a density matrix in the sense of Definition TBReferenced. [Definition 9.5]
- $\hat{\rho}$ solves the stationary von Neumann equation (TBReferenced). [Theorem 9.7 with $\frac{d}{dt}\hat{\rho} = 0$, i.e. $[\hat{H}, \hat{\rho}] = 0$]
- $\hat{\rho}$ is describes a system with energy E, i.e. $\langle \hat{H} \rangle \approx E$

Proof 9.17 TBDigitalized from Nolting p. 113 The only non-trivial thing is the normalization, i.e. $\mathrm{Tr}(\hat{\rho}) = 1$. For this we ...

...evaluate the trace in the orthonormal eigenbasis $\{|E_m\rangle\}$ of $\hat{H}$, see [40, Sect. 2.2.1, Eqs. (2.16) to (2.19)]. Since $\hat{\rho}_{\mathrm{MCE}}|E_m\rangle = p_m^{\mathrm{MCE}}|E_m\rangle$,

$$\mathrm{Tr}(\hat{\rho}_{\mathrm{MCE}}) = \sum_m \langle E_m|\hat{\rho}_{\mathrm{MCE}}|E_m\rangle = \sum_{E_m \in \mathscr{E}} \frac{1}{\Omega(E,V,N)} = \frac{|\mathscr{E}|}{\Omega(E,V,N)} = 1.$$

Notice that the sum runs over *states*, not over energies, i.e. in case of degeneracies every eigenstate has to be counted separately [40, p. 113]. This is consistent with Ω counting microstates. In particular $\Omega \geq 1$ (for $\mathscr{E} \neq \emptyset$), such that $p_m^{\mathrm{MCE}} \in [0,1]$. The remaining statements follow from:

- The $|E_m\rangle$ are orthonormal, $p_m^{\mathrm{MCE}} \geq 0$ and $\sum_m p_m^{\mathrm{MCE}} = \mathrm{Tr}(\hat{\rho}_{\mathrm{MCE}}) = 1$. Hence $\hat{\rho}_{\mathrm{MCE}}$ is of the form of Definition 9.5.

- Since $\hat{H}|E_m\rangle\langle E_m| = E_m|E_m\rangle\langle E_m| = |E_m\rangle\langle E_m|\hat{H}$, one finds

$$[\hat{H}, \hat{\rho}_{\mathrm{MCE}}] = \sum_m p_m^{\mathrm{MCE}} \left(E_m - E_m\right) |E_m\rangle\langle E_m| = 0,$$

  such that $\frac{d}{dt}\hat{\rho}_{\mathrm{MCE}} = 0$ by Theorem 9.7. (Nolting argues the other way round: an equilibrium ensemble must be stationary, hence $\hat{\rho}$ must commute with $\hat{H}$ and be diagonal in the energy representation, which motivates the ansatz for $\hat{\rho}_{\mathrm{MCE}}$ [40, p. 112].)

- By Theorem 9.10 [40, Eq. (2.19)],

$$\langle \hat{H} \rangle = \sum_m p_m^{\mathrm{MCE}} \langle E_m|\hat{H}|E_m\rangle = \frac{1}{\Omega(E,V,N)} \sum_{E_m \in \mathscr{E}} E_m.$$

  This is the arithmetic mean of numbers in $[E-\Delta, E]$, hence $E - \Delta \leq \langle \hat{H} \rangle \leq E$, i.e. $\langle \hat{H} \rangle \approx E$ for a small energy uncertainty Δ.

Definition 9.18 We define the *Boltzmann-entropy* in the microcanonical ensemble as

$$S_{\mathrm{MCE}}(E,V,N) = k_{\mathrm{B}} \ln \Omega(E,V,N). \tag{9.28}$$

and the *temperature* $T \equiv T(E,V,N)$ as

$$\frac{1}{T(E,V,N)} = \left(\frac{\partial S_{\mathrm{MCE}}}{\partial E}\right)_{V,N} (E,V,N), \tag{9.29}$$

and the *pressure* $P \equiv P(E,V,N)$ as

$$P(E,V,N) = T(E,V,N) \cdot \left(\frac{\partial S_{\mathrm{MCE}}}{\partial V}\right)_{E,N} (E,V,N), \tag{9.30}$$

and the *chemical potential* $\mu \equiv \mu(E,V,N)$ as

$$\mu(E,V,N) = -T(E,V,N) \cdot \left(\frac{\partial S_{\mathrm{MCE}}}{\partial N}\right)_{E,V} (E,V,N). \tag{9.31}$$

Remark 9.18.1 The entropy is one of several so-called *state functions* or *thermodynamic potentials*. The temperature, pressure and chemical potential are then the corresponding *conjugate variables* to the energy, volume and particle number.

Remark 9.18.2 The appearance of the temperature in the definition of the pressure and chemical potential might seem to complicate matters at first glance. This will however turn out to be a very neat definition, as one can attribute physical interpretations to the pressure and the chemical potential, as we will see in the examples and in the following sections.

Remark 9.18.3 The chemical potential has, in physical terms, the meaning of the energy increase when one particle is added (at constant entropy and constant volume). This will become clear in Corollary 9.49.

Remark 9.18.4 Notice that one can rewrite the partial derivatives as

$$\left(\frac{\partial S_{\mathrm{MCE}}}{\partial V}\right)_{E,N}(E,V,N) = \frac{P(E,V,N)}{T(E,V,N)}, \qquad \left(\frac{\partial S_{\mathrm{MCE}}}{\partial N}\right)_{E,V}(E,V,N) = -\frac{\mu(E,V,N)}{T(E,V,N)}, \tag{9.32}$$

such that we can write for the differential of the entropy

$$\mathrm{d}S_{\mathrm{MCE}} = \frac{1}{T}\mathrm{d}E + \frac{P}{T}\mathrm{d}V - \frac{\mu}{T}\mathrm{d}N \quad \Longleftrightarrow \quad \mathrm{d}E = T\mathrm{d}S_{\mathrm{MCE}} - P\mathrm{d}V + \mu\mathrm{d}N \tag{9.33}$$

Definition 9.19 Definition of two systems being in thermal equilibrium.

Let Σ_A and Σ_B be two systems with numbers of accessible microstates $\Omega_A(E_A, V_A, N_A)$ and $\Omega_B(E_B, V_B, N_B)$, which are in *thermal contact*, i.e. they can exchange energy (heat) via a weak interaction, but neither volume nor particles, and which together form an isolated system with fixed total energy $E = E_A + E_B$. We say that Σ_A and Σ_B are in *thermal equilibrium* with each other, if the energy is partitioned such that the number of accessible microstates of the total system, or equivalently the total entropy

$$S(E_A) = k_{\mathrm{B}} \ln\left(\Omega_A(E_A)\,\Omega_B(E - E_A)\right) = S_A(E_A) + S_B(E - E_A), \tag{9.34}$$

is maximal w.r.t. E_A [15, Chapter 9, Eqs. (9.12), (9.16)].

Remark 9.19.1 We collect some consequences, following [15, pp. 69 to 71] and [47, Sect. 2.7.1].

- The necessary condition $\partial S/\partial E_A = 0$ for the maximum in Equation (9.34) reads $\partial S_A/\partial E_A - \partial S_B/\partial E_B = 0$, i.e. with Definition 9.18

  $$T_A = T_B$$

  [15, Eq. (9.17)]. Two systems in thermal equilibrium thus have the same temperature.
- For macroscopic systems the maximum is extremely sharp, i.e. (almost) all of the $\Omega_A\Omega_B$ microstates of the total system lie at the most probable partition of the energy [15, Eq. (9.11) and p. 69]. This is why the equilibrium is found by maximizing the entropy.
- If, initially, Σ_A and Σ_B are separately in equilibrium with $T_A \neq T_B$, the total system is not in equilibrium; there is no temperature of the total system, but its entropy is still given by $S = S_A + S_B$. After the energy exchange has been allowed, a global equilibrium with $T = T_A = T_B$ and $S = S_A + S_B =$ maximal is established [15, p. 70 f.].
- If, in addition, the systems can exchange volume and particles, maximizing the total entropy w.r.t. E_A, V_A and N_A yields with Definition 9.18 the equality of temperature, pressure and chemical potential [47, Eq. (2.7.4)]

  $$T_A = T_B, \qquad P_A = P_B, \qquad \mu_A = \mu_B.$$

Theorem 9.20 Zustandssumme des idealen Gases: Fließbach, Gleichung (6.20).

Consider an ideal (i.e. non-interacting), monatomic gas of $N \gg 1$ indistinguishable particles of mass m without internal degrees of freedom, enclosed in a cubic box of volume $V = L^3$ with impenetrable walls. In the classical limit (see the proof), the total number of accessible microstates is given by

$$\ln \Omega(E, V, N) = \frac{3N}{2} \ln\left(\frac{E}{N}\right) + N \ln\left(\frac{V}{N}\right) + N \ln c, \tag{9.35}$$

with a constant c that does not depend on E, V and N.

Proof 9.20 TBDigitalized.

We follow [15, Chapter 6, Eqs. (6.2)–(6.20)].

Step 1 (Spectrum). The Hamilton-operator reads

$$\hat{H} = \sum_{\nu=1}^{N} \left(-\frac{\hbar^2}{2m} \Delta_\nu + U(\mathbf{r}_\nu) \right),$$

where the wall potential U vanishes inside the box and is infinite outside. Each particle is thus a particle in an infinitely deep potential well, and the $3N$ Cartesian momentum components take the values

$$p_k = \frac{\pi \hbar}{L} n_k, \qquad n_k \in \{1, 2, \dots\}, \qquad k = 1, \dots, 3N.$$

A microstate is labelled by $r = (n_1, \dots, n_{3N})$ and has the energy

$$E_r(V, N) = \sum_{k=1}^{3N} \frac{p_k^2}{2m} = \sum_{k=1}^{3N} \frac{\pi^2 \hbar^2}{2mL^2} n_k^2.$$

Step 2 (Counting). Let $\Phi(E, V, N) = \sum_{r\,:\,E_r \le E} 1$ denote the number of microstates with energy smaller than or equal to E, such that $\Phi(E) - \Phi(E - \Delta) \le \Omega_\Delta(E, V, N) \le \Phi(E)$. In the classical limit $\overline{p_k} \gg \hbar/L$, i.e. if the relevant n_k are large [15, Eq. (6.8)], the sum can be replaced by an integral, where the restriction $n_k > 0$ is accounted for by a factor $1/2$ per dimension. Substituting $p_k = (\pi\hbar/L) n_k$ and using $V = L^3$ we find

$$\Phi(E, V, N) \approx \frac{1}{2^{3N}} \int_{\sum_k n_k^2 \le 2mEL^2/(\pi\hbar)^2} \mathrm{d}n_1 \cdots \mathrm{d}n_{3N} = \frac{V^N}{(2\pi\hbar)^{3N}} \int_{\sum_k p_k^2 \le 2mE} \mathrm{d}p_1 \cdots \mathrm{d}p_{3N} = \frac{V^N}{(2\pi\hbar)^{3N}} V_{3N}\left(\sqrt{2mE}\right),$$

where $V_{3N}(R)$ denotes the volume of a $3N$-dimensional ball of radius R. This is the classical phase-space volume divided by $(2\pi\hbar)^{3N}$ [15, Eq. (6.11)]. Since $V_{3N}(R) \propto R^{3N}$, one has $\Phi \propto E^{3N/2}$ and hence [15, Eq. (6.14)]

$$\frac{\Phi(E - \Delta)}{\Phi(E)} = \left(1 - \frac{\Delta}{E}\right)^{3N/2} \le \exp\left(-\frac{3N}{2}\frac{\Delta}{E}\right),$$

which is of the order $\mathrm{e}^{-10^{19}}$ for, e.g., $3N/2 = 10^{24}$ and $\Delta/E = 10^{-5}$. Thus $\Omega(E, V, N) \approx \Phi(E, V, N)$ to excellent accuracy, and in particular Ω is practically independent of Δ [15, Eq. (6.15)]. Notice that $\ln \Omega$, in contrast to Ω itself, depends only moderately on E and V.

Step 3 (Volume of the ball). The volume of the $3N$-dimensional ball is [15, Eq. (6.17)]

$$V_{3N}(R) = \frac{\pi^{3N/2}}{(3N/2)!} R^{3N} \approx \left(\frac{2\pi \mathrm{e}}{3}\frac{R^2}{N}\right)^{3N/2},$$

where Stirling's approximation $n! \approx (n/\mathrm{e})^n$ was used.

Step 4 (Indistinguishability). The particles are indistinguishable, such that an interchange $\mathbf{p}_\nu \leftrightarrow \mathbf{p}_{\nu'}$ of two particles does not yield a new state. Since Step 2 counted the (in general) $N!$ permutations of a state separately, we have to divide by $N! \approx (N/\mathrm{e})^N$ [15, Eq. (6.19)]. Strictly, this requires that multiply occupied one-particle states are rare, i.e. the stronger condition $\overline{p} \gg N^{1/3}\hbar/L$ [15, p. 44].

Step 5 (Result). Combining Steps 2 to 4 with $R^2 = 2mE$ yields

$$\begin{aligned}\ln \Omega(E, V, N) &\approx \ln\left(\frac{1}{N!}\frac{V^N}{(2\pi\hbar)^{3N}} V_{3N}\left(\sqrt{2mE}\right)\right) \approx N \ln V - N \ln\frac{N}{\mathrm{e}} - \frac{3N}{2}\ln\left(4\pi^2\hbar^2\right) + \frac{3N}{2}\ln\left(\frac{4\pi \mathrm{e}\, m}{3}\frac{E}{N}\right) \\ &= \frac{3N}{2}\ln\left(\frac{E}{N}\right) + N\ln\left(\frac{V}{N}\right) + N\ln c, \qquad c = \mathrm{e}^{5/2}\left(\frac{m}{3\pi\hbar^2}\right)^{3/2},\end{aligned}$$

which proves Equation (9.35). Fließbach [15, Eq. (6.20)] leaves c unspecified; the explicit value above reproduces the Sackur-Tetrode entropy $S_{\mathrm{MCE}} = k_{\mathrm{B}} \ln \Omega$. The resulting N-dependence states that the number of states per atom is proportional to V/N and $(E/N)^{3/2}$, i.e. energy and volume have to be related to the particle number [15, p. 46].

9.4. The Canonical Ensemble

To introduce the canonical ensemble, we start from a description that uses the microcanonical ensemble.

Notation 9.21 We consider a isolated system $\Sigma_{I\cup II} \equiv \Sigma_I \cup \Sigma_{II}$ that consists of two parts Σ_I and Σ_{II}.

Here are some further assumptions and notations:

1. The Hilbert-space of the total system is given as a tensor-product $\mathscr{H}_{N_{I\cup II}} = \mathscr{H}_{N_I} \otimes \mathscr{H}_{N_{II}}$.
2. The Hamilton-operator of the total system is given by

$$H_{I\cup II} = H_I + H_{II} + H_{I\cap II}, \tag{9.36}$$

   where H_I and H_{II} are the Hamilton-operators of Σ_I and Σ_{II} and $H_{I\cap II}$ is the interaction[2] Hamilton-operator.
3. The total system has an energy, volume and particle-number $E_{I\cup II}$, $V_{I\cup II}$ and $N_{I\cup II}$, respectively.
4. The subsystems Σ_I and Σ_{II} have energies E_1 and E_2 and volumes V_1 and V_2 and particle-numbers N_1 and N_2, such that

$$\begin{aligned}E_I + E_{II} &= E_{I\cup II}, \\ V_I + V_{II} &= V_{I\cup II}, \\ N_I + N_{II} &= N_{I\cup II}.\end{aligned}$$

[2] Notice that this interaction in the Hamiltonian is neccessary for the two systems to reach thermal equilibrium.

5. This total system $\Sigma_{I\cup II}$ is assumed to be properly described in the microcanonical ensemble, such that entropy $S_{I\cup II}$ and a temperature $T_{I\cup II}$ can be defined.
6. We further assume that Σ_I and Σ_{II} are in thermal equilibrium with each other *and* have the same temperature T as the total system $T \equiv T_{I\cup II} \equiv T_I \equiv T_{II}$.
7. For reasons that will become clear later, we call the second subsystem Σ_{II} the *reservoir* or *heat bath*.

The first subsystem $\Sigma_I \equiv \Sigma$ with Hilbert-space $\mathscr{H}_{N_I} \equiv \mathscr{H}_N$ and Hamilton-operator $H_I \equiv H$ is the system of interest, which we ultimately seek to describe. Thus we write for its volume $V_I \equiv V$ and particle number $N_1 \equiv N$. The system Σ is considered to be a "very small", yet "macroscopic", part of the "very large" system $\Sigma_{1\cup 2}$.

Hypothesis 9.22 We assume that the interaction between Σ_I and Σ_{II} is so weak that the energy exchange between the two systems is negligible $H_{I\cap II} \approx 0$ in the following discussions.

Definition 9.23 We define the *natural variables of the canonical ensemble* as the triplet (T, V, N), where T is the temperature (of a so-called "reservoir", see below), V is the volume and N is the number of particles.

Notation 9.24 Just as in Notation 9.14: For a fixed particle number N and a fixed volume V we enumerate the set of eigen-energies $\{E_1, E_2, \dots\}$ and orthonormal eigenstates $\{|E_1\rangle, |E_2\rangle, \dots\}$ of the Hamilton-operator H of the system Σ as

$$\hat{H}|E_i\rangle = E_i|E_i\rangle \quad \text{with} \quad \langle E_i|E_j\rangle = \delta_{ij} \quad \text{and} \quad \mathscr{H}_N = \operatorname{span}_{\mathbb{C}}\{|E_1\rangle, |E_2\rangle, \dots\}, \tag{9.37}$$

whereas $\mathscr{H}_N$ represents the underlying N-particle Hilbert-space.

Hypothesis 9.25 We assume, that the energies $E_\bullet$ of the system are so small, such that the following approximation is valid

TBDone. (9.38)

More precisely, we assume that $E_\bullet \ll E$ and that the logarithm of the number of states of the reservoir can be expanded to first order in $E_\bullet$ [47, Eq. (2.6.3)], i.e.

$$\ln \Omega_{II}(E - E_\bullet) \approx \ln \Omega_{II}(E) - E_\bullet \left(\frac{\partial \ln \Omega_{II}}{\partial E}\right)(E). \tag{9.39}$$

The expansion is performed for $\ln \Omega_{II}$ rather than for Ω_{II} itself, since Ω_{II} varies extremely rapidly with the energy, whereas $\ln \Omega_{II}$ depends only moderately on it (cf. [15, Eqs. (6.14)–(6.16)]). A justification for dropping the higher orders is given in Step 4 of the proof of Theorem 9.27.

Fact 9.26 The number of states of the total system at energy $E \approx E_{II} \gg E_\bullet$, surpressing the volumes and particle-numbers for notational convenience, is given by

$$\Omega_{I\cup II}(E) = \sum_{E_\bullet \in \{E_1, E_2, \dots\}} \Omega_I(E_\bullet)\Omega_{II}(E - E_\bullet) \tag{9.40}$$

whereas we identify

$\Omega_I(E_\bullet)\Omega_{II}(E - E_\bullet)$ = "number of ways to configure the system + reservoir with the system in microstate $|E_\bullet\rangle$".

Thus we obtain in the expansion of the density matrix in the canonical ensemble

$$\hat{\rho}_{\mathrm{CE}} = \sum_{\bullet=1,2,\ldots} p_\bullet^{\mathrm{CE}} |E_\bullet\rangle\langle E_\bullet|. \tag{9.41}$$

the ansatz

$$p_\bullet^{\mathrm{CE}} = \frac{\Omega_I(E_\bullet)\Omega_{II}(E - E_\bullet)}{\Omega_{I\cup II}(E)} \propto \Omega_{II}(E - E_\bullet). \tag{9.42}$$

Theorem 9.27 One finds for the density $\rho \equiv \rho(T, V, N)$ in the canonical ensemble

$$\hat{\rho}_{\mathrm{CE}} = \frac{1}{Z} \sum_{\bullet=1,2,\ldots} \mathrm{e}^{-\beta E_\bullet} |E_\bullet\rangle\langle E_\bullet| \tag{9.43}$$

with

$$Z = \sum_{\bullet=1,2,\ldots} \mathrm{e}^{-\beta E_\bullet} \tag{9.44}$$

where $\beta = 1/k_{\mathrm{B}}T$ is the inverse temperature.

Proof 9.27 TBDigitalized.

We follow [47, Sect. 2.6.1, Eqs. (2.6.2)–(2.6.6)] in the notation of the Fact above.

Step 1 (Temperature of the reservoir). Applying Definition 9.18 to the reservoir Σ_{II}, with $S_{II} = k_{\mathrm{B}} \ln \Omega_{II}$, and using that the reservoir has the temperature T (item 6 of the Notation above), we find

$$\left(\frac{\partial \ln \Omega_{II}}{\partial E}\right)(E) = \frac{1}{k_{\mathrm{B}}} \left(\frac{\partial S_{II}}{\partial E}\right)(E) = \frac{1}{k_{\mathrm{B}}T} = \beta,$$

where the derivative is evaluated at $E \approx E_{II}$, since $E_\bullet \ll E$.

Step 2 (Boltzmann factor). Exponentiating Equation (9.39) of Hypothesis 9.25 and using Step 1 gives $\Omega_{II}(E - E_\bullet) \approx \Omega_{II}(E)\,\mathrm{e}^{-\beta E_\bullet}$. Inserted into the ansatz of the Fact above, this yields

$$p_\bullet^{\mathrm{CE}} \propto \Omega_{II}(E - E_\bullet) \approx \Omega_{II}(E)\,\mathrm{e}^{-\beta E_\bullet} \qquad \Rightarrow \qquad p_\bullet^{\mathrm{CE}} = C\,\mathrm{e}^{-\beta E_\bullet},$$

with a constant C that does not depend on the microstate $|E_\bullet\rangle$ of the system.

Step 3 (Normalization). The constant C is fixed by $\sum_\bullet p_\bullet^{\mathrm{CE}} = \mathrm{Tr}(\hat{\rho}_{\mathrm{CE}}) = 1$ (Lemma 9.6), which yields $C^{-1} = \sum_\bullet \mathrm{e}^{-\beta E_\bullet} = Z$ [47, Eqs. (2.6.4), (2.6.5)]. Notice that Z is determined by properties of the system Σ alone. Hence

$$\hat{\rho}_{\mathrm{CE}} = \sum_{\bullet} p_{\bullet}^{\mathrm{CE}} |E_\bullet\rangle\langle E_\bullet| = \frac{1}{Z}\sum_{\bullet} \mathrm{e}^{-\beta E_\bullet} |E_\bullet\rangle\langle E_\bullet|.$$

Step 4 (Justification of the first-order truncation). Following [47, p. 52 f., remark (iv)], the second-order term of the expansion in Hypothesis 9.25 is

$$\frac{1}{2}\left(\frac{\partial^2 \ln \Omega_{II}}{\partial E^2}\right) E_\bullet^2 = \frac{1}{2k_{\mathrm{B}}}\frac{\partial}{\partial E}\left(\frac{1}{T}\right) E_\bullet^2 = -\frac{1}{2k_{\mathrm{B}}T^2}\frac{\partial T}{\partial E} E_\bullet^2 = -\frac{E_\bullet^2}{2k_{\mathrm{B}}T^2 C_{II}},$$

where $C_{II} = \partial E/\partial T$ is the heat capacity of the reservoir. Relative to the first-order term $-\beta E_\bullet$, it is suppressed by the factor $E_\bullet/(2TC_{II})$. Since the heat capacity is extensive, C_{II} is huge for a large reservoir, such that $E_\bullet \ll TC_{II}$ and the higher orders are negligible.

Remark 9.27.1 Notice that we can rewrite the density as

$$\hat{\rho}_{\mathrm{CE}} = \frac{1}{Z}\sum_{\bullet=1,2,\ldots} \mathrm{e}^{-\beta E_\bullet} |E_\bullet\rangle\langle E_\bullet| = \frac{1}{Z}\mathrm{e}^{-\beta \hat{H}} \tag{9.45}$$

Corollary 9.28 The following statements are immediate

- $\hat{\rho}$ is a density matrix in the sense of Definition TBReferenced. [Definition 9.5]
- $\hat{\rho}$ solves the stationary von Neumann equation (TBReferenced). [Theorem 9.7 with $\frac{d}{dt}\hat{\rho} = 0$, i.e. $[\hat{H}, \hat{\rho}] = 0$]

Proof 9.28 The normalization is trivial. The fact that it solves the von Neumann equation as well.

Theorem 9.29 The (Helmholtz) free energy is minimal in the canonical ensemble.

Proof 9.29 03 page 28 for minimality of (Helmholtz) free energy in the canonical ensemble.

We follow [40, Sects. 2.5.2 and 2.5.4, Eqs. (2.98)–(2.107)].

Precise statement. Fix (T, V, N) and let $\hat{\rho} \equiv \hat{\rho}_{\mathrm{CE}}$ be the canonical density of Theorem 9.27 with free energy $F = -k_{\mathrm{B}}T \ln Z$. For an arbitrary density $\hat{\rho}'$ on $\mathscr{H}_N$ (e.g. describing a non-equilibrium state) we define

$$U' = \mathrm{Tr}(\hat{\rho}'\hat{H}), \qquad S' = -k_{\mathrm{B}}\,\mathrm{Tr}(\hat{\rho}'\ln\hat{\rho}'), \qquad F' = U' - TS'.$$

Then $F \le F'$. For $\hat{\rho}' = \hat{\rho}$ one recovers $F' = F$ (cf. Remark 9.11.1 and its proof).

Step 1 (Boltzmann's $\mathcal{H}$-function). Let $\hat{\rho}|\rho_n\rangle = \rho_n|\rho_n\rangle$ and $\hat{\rho}'|\rho'_m\rangle = \rho'_m|\rho'_m\rangle$ with orthonormal eigenbases (Lemma 9.6). We show

$$\mathcal{H} := \mathrm{Tr}\left[\hat{\rho}'\left(\ln\hat{\rho} - \ln\hat{\rho}'\right)\right] \le 0.$$

Using the hermiticity of $\hat{\rho}'$ and the completeness of $\{|\rho_n\rangle\}$ one finds

$$\mathcal{H} = \sum_m \rho'_m \left(\langle \rho'_m | \ln \hat{\rho} | \rho'_m \rangle - \ln \rho'_m \right) = \sum_{m,n} \rho'_m \ln \frac{\rho_n}{\rho'_m} \left| \langle \rho'_m | \rho_n \rangle \right|^2 ,$$

where terms with $\rho'_m = 0$ do not contribute, and $\rho_n = \mathrm{e}^{-\beta E_n}/Z > 0$. The function $f(x) = x - 1 - \ln x$ has its minimum $f(1) = 0$ on $x > 0$, such that $\ln x \leq x - 1$. Hence

$$\mathcal{H} \leq \sum_{m\,:\,\rho'_m > 0} \sum_n \rho'_m \left(\frac{\rho_n}{\rho'_m} - 1 \right) \left| \langle \rho'_m | \rho_n \rangle \right|^2 \leq \sum_n \rho_n - \sum_m \rho'_m = \mathrm{Tr}(\hat{\rho}) - \mathrm{Tr}(\hat{\rho}') = 0,$$

where we used $\sum_n |\langle \rho'_m | \rho_n \rangle|^2 = 1$ and $\sum_m |\langle \rho'_m | \rho_n \rangle|^2 = 1$ (extending the sum to all m can only increase the first term) [40, Eq. (2.101)].

Step 2 (Application to the canonical ensemble). The eigenstates of $\hat{\rho}$ are the $|E_n\rangle$ with $\ln \rho_n = -\ln Z - \beta E_n$. Therefore

$$k_\mathrm{B} \,\mathrm{Tr}(\hat{\rho}' \ln \hat{\rho}) = k_\mathrm{B} \sum_n \left(-\ln Z - \beta E_n \right) \langle E_n | \hat{\rho}' | E_n \rangle = -k_\mathrm{B} \ln Z \,\mathrm{Tr}(\hat{\rho}') - \frac{1}{T} \mathrm{Tr}(\hat{\rho}' \hat{H}) = \frac{1}{T} \left(F - U' \right),$$

and thus, with Step 1,

$$k_\mathrm{B} \mathcal{H} = S' + k_\mathrm{B} \,\mathrm{Tr}(\hat{\rho}' \ln \hat{\rho}) = S' - \frac{1}{T} U' + \frac{1}{T} F = \frac{1}{T} \left(F - F' \right) \leq 0,$$

i.e. $F \leq F'$. In words: in all processes that can still occur in a system with $T, V, N = \text{const}$, the free energy does not increase; it is minimal in equilibrium [40, Eq. (2.107)].

9.5. The Grand Canonical Ensemble

TBD

See also 03 page 35 for a derivation.

Minimality of the grand canonical potential a.k.a. Landau-potential : Nolting page 157.

Ehrenfest Categorization of Phase Transitions: Some book page 314.

We generalize the canonical ensemble by additionally allowing for the exchange of particles between the system and the reservoir, following [47, Sect. 2.7] and [40, Sects. 1.5 and 2.5.5].

Notation 9.30 As in the canonical ensemble, we consider an isolated system $\Sigma_{I\cup II}$ consisting of the system of interest $\Sigma_I \equiv \Sigma$ and a reservoir Σ_{II}, which now can exchange energy *and* particles, such that [47, Eq. (2.7.1)]

$$E = E_I + E_{II}, \qquad N = N_I + N_{II}, \qquad V = V_I + V_{II}.$$

Since the particle number of Σ is not fixed, its states live in the Fock-space $\mathscr{F} = \bigoplus_{N_I=0}^{\infty} \mathscr{H}_{N_I}$. We assume that the Hamilton-operator conserves the particle number, $[\hat{H}, \hat{N}] = 0$, and denote the orthonormal eigenstates of $\hat{H}$ in $\mathscr{H}_{N_I}$ by $|E_n(N_I)\rangle$ with eigen-energies $E_n(N_I)$, which are thus also eigenstates of $\hat{N}$ with eigenvalue N_I. We further assume that the system Σ is in equilibrium with the reservoir, i.e. (Remark 9.19.1) both have the same temperature T and the same chemical potential μ.

Definition 9.31 We define the *natural variables of the grand canonical ensemble* as the triplet (T, V, μ), where T and μ are the temperature and chemical potential of the reservoir, and V is the volume of the system.

Theorem 9.32 One finds for the density $\hat{\rho}_{\mathrm{GCE}} \equiv \hat{\rho}_{\mathrm{GCE}}(T, V, \mu)$ in the grand canonical ensemble

$$\hat{\rho}_{\mathrm{GCE}} = \frac{1}{\Xi} \sum_{N_I=0}^{\infty} \sum_{n} \mathrm{e}^{-\beta(E_n(N_I)-\mu N_I)} |E_n(N_I)\rangle\langle E_n(N_I)| = \frac{1}{\Xi} \mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}$$

with the *grand canonical partition function* [47, Eq. (2.7.8)]

$$\Xi(T, V, \mu) = \mathrm{Tr}_{\mathscr{F}}\, \mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})} = \sum_{N_I=0}^{\infty} \mathrm{e}^{\beta\mu N_I} Z_{N_I}(T, V),$$

where Z_{N_I} denotes the canonical partition function of Theorem 9.27 for N_I particles. Schwabl denotes Ξ by Z_G.

Proof 9.32 We follow [47, Sect. 2.7.2]. The probability that Σ contains N_I particles and is in the microstate $|E_n(N_I)\rangle$ is, by the microcanonical postulate for the total system and in analogy to the Fact of the canonical ensemble, given by [47, Eq. (2.7.5)]

$$p\left(N_I, E_n(N_I)\right) = \frac{\Omega_{II}\left(E - E_n(N_I), N - N_I\right)}{\Omega_{I\cup II}(E, N)}.$$

In analogy to Hypothesis 9.25, we assume that Σ is much smaller than the reservoir and expand the logarithm to first order in $E_n(N_I)$ and N_I:

$$\begin{aligned}\ln \Omega_{II}\left(E - E_n(N_I), N - N_I\right) &\approx \ln \Omega_{II}(E,N) - E_n(N_I)\frac{\partial \ln \Omega_{II}}{\partial E} - N_I \frac{\partial \ln \Omega_{II}}{\partial N} \\ &= \ln \Omega_{II}(E,N) - \beta E_n(N_I) + \beta\mu N_I,\end{aligned}$$

where we used Definition 9.18 for the reservoir, i.e. $\partial_E \ln \Omega_{II} = \frac{1}{k_B}\partial_E S_{II} = \frac{1}{k_B T} = \beta$ and $\partial_N \ln \Omega_{II} = \frac{1}{k_B}\partial_N S_{II} = -\frac{\mu}{k_B T} = -\beta\mu$ [47, Eq. (2.7.3)]. Hence $p(N_I, E_n(N_I)) = \Xi^{-1} \mathrm{e}^{-\beta(E_n(N_I) - \mu N_I)}$ with a constant Ξ that is fixed by the normalization $\sum_{N_I}\sum_n p(N_I, E_n(N_I)) = 1$ [47, Eqs. (2.7.6)–(2.7.8)]. Since $\hat{H}$ and $\hat{N}$ are diagonal in the basis $\{|E_n(N_I)\rangle\}$, the sum equals $\Xi^{-1}\mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}$. Notice that the trace in Ξ runs over the whole Fock-space, i.e. it includes the sum over all particle numbers [47, p. 65].

Definition 9.33 We define the *grand canonical potential* (or *Landau-potential*) as [47, Eq. (2.7.13)], [40, Eq. (1.178)]

$$\Omega(T,V,\mu) = -k_B T \ln \Xi(T,V,\mu).$$

Despite the identical symbol, it should not be confused with the number of microstates $\Omega(E,V,N)$; the arguments tell them apart. Schwabl denotes it by Φ.

Corollary 9.34 With $U = \langle \hat{H}\rangle$, $\langle \hat{N}\rangle$ and $S = -k_B \operatorname{Tr}(\hat{\rho}_{GCE} \ln \hat{\rho}_{GCE})$ one has [47, Eqs. (2.7.14)–(2.7.18)]

$$\Omega = U - TS - \mu\langle \hat{N}\rangle, \qquad \mathrm{d}\Omega = -S\,\mathrm{d}T - P\,\mathrm{d}V - \langle \hat{N}\rangle\,\mathrm{d}\mu, \qquad \mathrm{d}U = T\,\mathrm{d}S - P\,\mathrm{d}V + \mu\,\mathrm{d}\langle \hat{N}\rangle,$$

i.e. $S = -(\partial\Omega/\partial T)_{V,\mu}$, $P = -(\partial\Omega/\partial V)_{T,\mu}$ and $\langle \hat{N}\rangle = -(\partial\Omega/\partial\mu)_{T,V}$, where the pressure is defined mechanically as $P = -\langle \partial \hat{H}/\partial V\rangle$ [47, Eq. (2.6.47)], [40, Eq. (1.172)].

Proof 9.34 Since $\ln \hat{\rho}_{GCE} = -\beta(\hat{H} - \mu\hat{N}) - \ln\Xi$, one finds $S = \frac{1}{T}(U - \mu\langle \hat{N}\rangle) + k_B \ln\Xi = \frac{1}{T}(U - \mu\langle \hat{N}\rangle - \Omega)$ [47, Eq. (2.7.10)], which is the first identity. For the partial derivatives we use $[\hat{H}, \hat{N}] = 0$ and the cyclicity of the trace:

$$\begin{aligned}\left(\frac{\partial\Omega}{\partial T}\right)_{V,\mu} &= -k_B \ln\Xi - k_B T \frac{1}{k_B T^2}\langle \hat{H} - \mu\hat{N}\rangle = \frac{1}{T}\left(\Omega - U + \mu\langle \hat{N}\rangle\right) = -S, \\ \left(\frac{\partial\Omega}{\partial V}\right)_{T,\mu} &= -k_B T \frac{1}{\Xi}\operatorname{Tr}\left(-\beta\frac{\partial \hat{H}}{\partial V}\mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}\right) = \left\langle \frac{\partial \hat{H}}{\partial V}\right\rangle = -P, \\ \left(\frac{\partial\Omega}{\partial\mu}\right)_{T,V} &= -k_B T \frac{1}{\Xi}\operatorname{Tr}\left(\beta\hat{N}\mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}\right) = -\langle \hat{N}\rangle.\end{aligned}$$

Finally, $\mathrm{d}U = \mathrm{d}(\Omega + TS + \mu\langle \hat{N}\rangle) = T\,\mathrm{d}S - P\,\mathrm{d}V + \mu\,\mathrm{d}\langle \hat{N}\rangle$, which is the first law of thermodynamics (cf. Equation (9.48)).

Theorem 9.35 The grand canonical potential is minimal in the grand canonical ensemble. Precisely: fix (T,V,μ) and let $\hat{\rho}'$ be an arbitrary density on $\mathscr{F}$ with $U' = \operatorname{Tr}(\hat{\rho}'\hat{H})$, $\langle \hat{N}\rangle' = \operatorname{Tr}(\hat{\rho}'\hat{N})$, $S' = -k_B \operatorname{Tr}(\hat{\rho}'\ln\hat{\rho}')$ and $\Omega' = U' - TS' - \mu\langle \hat{N}\rangle'$. Then $\Omega \le \Omega'$.

Proof 9.35 We follow [40, Sect. 2.5.5, p. 156 f.]. Step 1 of the proof of Theorem 9.29 (Boltzmann's $\mathcal{H}$-function) applies verbatim to $\hat{\rho} = \hat{\rho}_{\mathrm{GCE}}$, whose eigenvalues $\rho_n(N_I) = \Xi^{-1} \mathrm{e}^{-\beta(E_n(N_I)-\mu N_I)}$ are positive [40, Eq. (2.108)]. With $\ln \rho_n(N_I) = -\ln \Xi - \beta(E_n(N_I) - \mu N_I)$ we find

$$k_{\mathrm{B}} \operatorname{Tr}(\hat{\rho}' \ln \hat{\rho}_{\mathrm{GCE}}) = -k_{\mathrm{B}} \ln \Xi - \frac{1}{T} \operatorname{Tr}\left(\hat{\rho}'(\hat{H} - \mu \hat{N})\right) = \frac{1}{T}\left(\Omega - U' + \mu \langle \hat{N} \rangle'\right),$$

and therefore

$$k_{\mathrm{B}} \mathcal{H} = S' + k_{\mathrm{B}} \operatorname{Tr}(\hat{\rho}' \ln \hat{\rho}_{\mathrm{GCE}}) = \frac{1}{T}\left(\Omega - \Omega'\right) \leq 0.$$

Thus $\Omega \leq \Omega'$: in all processes that can still occur in a system with $T, V, \mu = \text{const}$, the grand canonical potential does not increase; it is minimal in equilibrium [40, Eq. (2.109)].

Definition 9.36 (*Ehrenfest classification of phase transitions* [15, Chapter 35, pp. 312–315].) Consider two phases A and B of a substance with chemical potentials $\mu_A(T, P)$ and $\mu_B(T, P)$ (i.e. Gibbs free energy per particle). In equilibrium, the system is in the phase with the lower chemical potential, and at a transition point one has $\mu_A = \mu_B$. The transition is called a *phase transition of n-th order*, if the n-th derivative is the first one that jumps, i.e. [15, Eq. (35.5)]

$$\left(\frac{\partial^m}{\partial T^m}\left(\mu_A - \mu_B\right)\right)_P \begin{cases} = 0 & \text{for } m < n, \\ \neq 0 & \text{for } m = n, \end{cases}$$

at the transition temperature, and analogously for the derivatives w.r.t. the pressure P.

Remark 9.36.1 For a transition of first order, the entropy per particle $s = -(\partial\mu/\partial T)_P$ and the volume per particle $v = (\partial\mu/\partial P)_T$ jump, which implies a latent heat (transition enthalpy) and a δ-like behaviour of the specific heat c_P. For a transition of second order, s and v are continuous, while e.g. c_P jumps. Nowadays, phase transitions are usually classified by the behaviour of an *order parameter* ψ at the transition: a discontinuous ψ corresponds to a transition of first order, a continuous one to a transition of second order [15, Eq. (35.6)]. Since all thermodynamic quantities follow from the partition function, phase transitions must show up as non-analyticities of $F = -k_{\mathrm{B}} T \ln Z$, which can only arise in the thermodynamic limit: every finite sum of the analytic terms $\mathrm{e}^{-\beta E_r}$ is analytic, whereas an infinite sum of analytic functions can be singular [15, p. 315 f.].

Theorem 9.37 For fixed (T, V), the function

$$\mu \mapsto N(\mu) \equiv -\left(\frac{\partial \Omega}{\partial \mu}\right)(\mu, T, V) \tag{9.46}$$

is monotonically increasing.

Proof 9.37 See [Salmhofer, page 118]. [46, p. 118]

We follow [46, Sect. 4.2.2, Lemma 4.1 and Corollary 4.2, Eqs. (4.22)–(4.30)]. We assume that the Hamilton-operator conserves the particle number, $[\hat{H}, \hat{N}] = 0$, and that $\Xi = \operatorname{Tr} \mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}$ is finite (Salmhofer works on a

finite lattice, i.e. on a finite-dimensional Fock-space). The grand canonical potential is $\Omega(\mu,T,V) = -k_B T \ln \Xi$ (Definition 9.33; Salmhofer writes Z_Λ for Ξ), and expectation values are given by $\langle \hat{O} \rangle = \Xi^{-1} \operatorname{Tr}\left(\mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}\hat{O}\right)$.

Step 1 ($N(\mu)$ is the mean particle number). Since $[\hat{H},\hat{N}] = 0$, we have $\mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})} = \mathrm{e}^{-\beta\hat{H}}\mathrm{e}^{\beta\mu\hat{N}}$, such that $\partial_\mu \mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})} = \beta\hat{N}\mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}$, and therefore [46, Eq. (4.24)]

$$N(\mu) = -\frac{\partial\Omega}{\partial\mu} = \frac{1}{\beta}\frac{\partial}{\partial\mu}\ln\Xi = \frac{1}{\beta\Xi}\operatorname{Tr}\left(\beta\hat{N}\mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}\right) = \langle\hat{N}\rangle.$$

Step 2 (Derivative). With $\partial_\mu^2\Xi = \beta^2 \operatorname{Tr}\left(\hat{N}^2\mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}\right)$, differentiating once more yields [46, Eq. (4.30)]

$$\frac{\partial N}{\partial\mu} = \frac{1}{\beta}\frac{\partial^2}{\partial\mu^2}\ln\Xi = \frac{1}{\beta}\left(\frac{\partial_\mu^2\Xi}{\Xi} - \left(\frac{\partial_\mu\Xi}{\Xi}\right)^2\right) = \beta\left(\langle\hat{N}^2\rangle - \langle\hat{N}\rangle^2\right) = \beta\left\langle\left(\hat{N}-\langle\hat{N}\rangle\right)^\dagger\left(\hat{N}-\langle\hat{N}\rangle\right)\right\rangle.$$

Step 3 (Positivity). Let $\{\eta_\alpha\}_\alpha$ be an orthonormal eigenbasis of the self-adjoint operator $\hat{H}-\mu\hat{N}$ with real eigenvalues ϵ_α. Then $\Xi = \sum_\alpha \mathrm{e}^{-\beta\epsilon_\alpha} > 0$, and for every linear operator $\hat{B}$ [46, Lemma 4.1, Eq. (4.29)]

$$\Xi\langle\hat{B}^\dagger\hat{B}\rangle = \sum_\alpha \mathrm{e}^{-\beta\epsilon_\alpha}\langle\eta_\alpha|\hat{B}^\dagger\hat{B}|\eta_\alpha\rangle = \sum_\alpha \mathrm{e}^{-\beta\epsilon_\alpha}\left\|\hat{B}\eta_\alpha\right\|^2 \geq 0.$$

Applying this to $\hat{B} = \hat{N} - \langle\hat{N}\rangle$ in Step 2 gives $\partial N/\partial\mu \geq 0$, i.e. $\mu \mapsto N(\mu)$ is monotonically increasing. This is not unexpected, since μ contributes to the energy via the term $-\mu\hat{N}$ [46, p. 119].

9.6. Equivalence of Ensembles

9.6.1. Equivalence of the Microcanonical and Canonical Ensemble

TBDigitalized from Nolting p. 74.

We follow [40, Sect. 1.4.4, pp. 74–77]. Nolting works classically; the quantum version is literally the same, once the classical phase-space density of states is replaced by the quantum mechanical one [40, Eqs. (2.21), (2.22)].

Notation 9.38 For fixed (V,N) we write $D(E) = \sum_n \delta(E-E_n)$ for the *density of states* of $\hat{H}$, such that $\Omega_\Delta(E) \approx D(E)\,\Delta$. For macroscopic systems $S_{\mathrm{MCE}}(E) = k_B \ln\Omega(E) = k_B \ln D(E)$, up to the additive constant $k_B \ln\Delta$, which is negligible compared to the extensive quantity S_{MCE} [40, Eqs. (2.21), (2.22)]. The canonical partition function then reads [40, Eq. (1.140)], [47, Eq. (2.6.12)]

$$Z(T,V,N) = \sum_n \mathrm{e}^{-\beta E_n} = \int \mathrm{d}E\, D(E)\,\mathrm{e}^{-\beta E}.$$

Definition 9.39 We call the canonical ensemble at temperature T and the microcanonical ensemble at energy E *equivalent*, if for $E = U = \langle\hat{H}\rangle_{\mathrm{CE}}$ temperature and entropy coincide [40, Eq. (1.150)], i.e.

$$T_{\mathrm{MCE}}(E=U) = T, \qquad S_{\mathrm{MCE}}(E=U,V,N) = S_{\mathrm{CE}}(T,V,N).$$

Theorem 9.40 For macroscopic (asymptotically large) systems, the canonical and the microcanonical ensemble are equivalent. Moreover [40, Eqs. (1.152), (1.153)]

$$Z(T,V,N) \approx D(U)\,\mathrm{e}^{-\beta U}\sqrt{2\pi k_\mathrm{B}T^2 C_V}, \qquad F(T,V,N) = U - TS_\mathrm{MCE}(E=U,V,N),$$

where the second identity holds up to terms of order $\ln N$.

Proof 9.40 *Step 1 (Sharp maximum).* The integrand $D(E)\mathrm{e}^{-\beta E}$ is proportional to the probability that the system has an energy in $[E, E+\mathrm{d}E]$. By Lemma 9.54, the relative width of this distribution is [40, Eq. (1.149)]

$$\frac{\sqrt{\langle \hat{H}^2\rangle - \langle \hat{H}\rangle^2}}{\langle \hat{H}\rangle} = \frac{\sqrt{C_V k_\mathrm{B}T^2}}{U} \sim \frac{1}{\sqrt{N}} \xrightarrow{N\to\infty} 0,$$

since $C_V \sim N$ and $U \sim N$. Hence the integrand has an extremely sharp maximum at $E = U$, and so has its logarithm.

Step 2 (Temperatures). The extremum condition reads

$$0 = \frac{\partial}{\partial E}\ln\left(D(E)\,\mathrm{e}^{-\beta E}\right)\Big|_{E=U} = -\beta + \frac{1}{k_\mathrm{B}}\left(\frac{\partial S_\mathrm{MCE}}{\partial E}\right)_{V,N}(E=U),$$

i.e. with Definition 9.18 $1/T_\mathrm{MCE}(E=U) = 1/T$ [40, Eq. (1.151)]. This is the first equivalence condition: the temperature T of the canonical ensemble is exactly the temperature of the microcanonical ensemble at the energy $E = U$, which almost all members of the canonical ensemble have.

Step 3 (Gaussian approximation). We expand around the maximum:

$$\ln\left(D(E)\,\mathrm{e}^{-\beta E}\right) = \ln\left(D(U)\,\mathrm{e}^{-\beta U}\right) + \frac{1}{2}(E-U)^2\left(\frac{\partial^2}{\partial E^2}\ln D(E)\right)_{V,N}(E=U) + \ldots$$

With $\partial_E \ln D = 1/(k_\mathrm{B}T_\mathrm{MCE})$, Step 2, and $(\partial T/\partial U)_{V,N} = 1/C_V$ one finds

$$\left(\frac{\partial^2}{\partial E^2}\ln D(E)\right)_{V,N}(E=U) = -\frac{1}{k_\mathrm{B}T_\mathrm{MCE}^2}\left(\frac{\partial T_\mathrm{MCE}}{\partial E}\right)_{V,N}(E=U) = -\frac{1}{k_\mathrm{B}T^2C_V}.$$

Hence $D(E)\,\mathrm{e}^{-\beta E} \approx D(U)\,\mathrm{e}^{-\beta U}\exp\left[-(E-U)^2/(2k_\mathrm{B}T^2C_V)\right]$, and the Gaussian integral (the limits may be extended to $\pm\infty$ due to the rapid decay) yields the claimed expression for Z [40, Eq. (1.152)].

Step 4 (Entropies). With $F = -k_\mathrm{B}T\ln Z$ we obtain

$$F(T,V,N) = U - k_\mathrm{B}T\ln D(U) - \frac{k_\mathrm{B}T}{2}\ln\left(2\pi k_\mathrm{B}T^2C_V\right) = U - TS_\mathrm{MCE}(E=U,V,N) - \frac{k_\mathrm{B}T}{2}\ln\left(2\pi k_\mathrm{B}T^2C_V\right).$$

For asymptotically large systems, the last term ($\ln C_V \sim \ln N$) is negligible compared to the others ($U \sim N$, $S_\mathrm{MCE} \sim N$). Comparing with $F = U - TS_\mathrm{CE}$ (Remark 9.11.1 and its proof) yields $S_\mathrm{CE}(T,V,N) = S_\mathrm{MCE}(E=U,V,N)$, which is the second equivalence condition [40, Eq. (1.153)].

Remark 9.40.1 It cannot be stressed often enough that this equivalence holds only for asymptotically large systems, since terms of order $\ln N$ were neglected compared to terms of order N. Although in principle all energies occur in the canonical ensemble, there is *de facto* a unique relation between the temperature T and the energy, such that one can choose the ensemble according to convenience; in most cases the canonical ensemble is the mathematically more convenient one [40, p. 76 f.].

9.6.2. Equivalence of the Microcanonical and Canonical Ensemble

TBDigitalized from Nolting p. 88 f. (partly).

Note: Judging from the cited pages, this subsection is meant to treat the equivalence of the canonical and the grand canonical ensemble, which is what the following content does.

We follow [40, Sect. 1.5.2, pp. 87–91] (classical there, the quantum version is identical with the partition functions of Theorems 9.27 and 9.32). We write $Z_N(T,V)$ for the canonical and $\Xi(T,V,\mu) = \sum_N \mathrm{e}^{\beta\mu N} Z_N(T,V)$ for the grand canonical partition function.

Lemma 9.41 The probability [40, Eq. (1.167)] to find the system of the grand canonical ensemble with N particles is

$$w_N(T,V) = \frac{\mathrm{e}^{\beta\mu N} Z_N(T,V)}{\Xi(T,V,\mu)},$$

and the mean particle number and its fluctuations are given by

$$\langle \hat{N} \rangle = \sum_N N w_N = \frac{1}{\beta}\left(\frac{\partial}{\partial\mu}\ln\Xi\right)_{T,V}, \qquad \langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2 = k_\mathrm{B} T \left(\frac{\partial \langle \hat{N} \rangle}{\partial \mu}\right)_{T,V}.$$

Proof 9.41 Summing $\Xi^{-1}\mathrm{e}^{-\beta(E_n(N)-\mu N)}$ (Theorem 9.32) over all n at fixed N gives w_N. The other two identities are Steps 1 and 2 of the proof of Theorem 9.37 [40, Eq. (1.168)], [46, Eq. (4.30)].

Remark 9.41.1 By Theorem 9.37, $\mu \mapsto \langle \hat{N} \rangle$ is monotonically increasing (strictly, if the particle number fluctuates), such that the relation can be inverted to $\mu = \mu(T,V,\langle \hat{N} \rangle)$ [40, Eq. (1.169)]. Since $\langle \hat{N} \rangle$ and $\partial\langle \hat{N} \rangle/\partial\mu$ are extensive, the relative fluctuations $\sqrt{\langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2}/\langle \hat{N} \rangle \sim 1/\sqrt{\langle \hat{N} \rangle}$ vanish for macroscopic systems, i.e. w_N has an extremely sharp maximum at $N = \langle \hat{N} \rangle$.

Theorem 9.42 For macroscopic systems, the canonical ensemble with particle number $N = \langle \hat{N} \rangle$ and the grand canonical ensemble with chemical potential $\mu = \mu(T,V,\langle \hat{N} \rangle)$ yield the same internal energy, free energy, pressure and entropy, i.e. [40, Eqs. (1.176), (1.182), (1.187), (1.188)]

$$
\begin{aligned}
U(T,V,\langle\hat{N}\rangle) &\approx -\left(\frac{\partial}{\partial\beta}\ln Z_{\langle\hat{N}\rangle}(T,V)\right)_{V,\langle\hat{N}\rangle},\\
F(T,V,\langle\hat{N}\rangle) &= \mu\langle\hat{N}\rangle + \Omega(T,V,\mu) \approx -k_{\mathrm{B}}T\ln Z_{\langle\hat{N}\rangle}(T,V),\\
P(T,V,\langle\hat{N}\rangle) &\approx k_{\mathrm{B}}T\left(\frac{\partial}{\partial V}\ln Z_{\langle\hat{N}\rangle}(T,V)\right)_{T,\langle\hat{N}\rangle},\\
S(T,V,\langle\hat{N}\rangle) &\approx k_{\mathrm{B}}\left(\frac{\partial}{\partial T}\left(T\ln Z_{\langle\hat{N}\rangle}(T,V)\right)\right)_{V,\langle\hat{N}\rangle}.
\end{aligned}
$$

Proof 9.42 Since almost all systems of the grand canonical ensemble have the particle number $\langle\hat{N}\rangle$, the sum over N in Ξ is dominated by its maximal term [40, Eq. (1.175)]:

$$\Xi(T,V,\mu) \approx \mathrm{e}^{\beta\mu\langle\hat{N}\rangle} Z_{\langle\hat{N}\rangle}(T,V).$$

Internal energy. With the fugacity $z = \mathrm{e}^{\beta\mu}$ as independent variable instead of μ, one has $U = \langle\hat{H}\rangle = -(\partial_\beta \ln\Xi)_{z,V}$ [40, Eq. (1.174)], and inserting the approximation for Ξ (the factor $z^{\langle\hat{N}\rangle}$ does not depend on β at fixed z) yields the canonical result [40, Eq. (1.176)].

Free energy. By Corollary 9.34, $F = U - TS = \Omega + \mu\langle\hat{N}\rangle$ [40, Eq. (1.181)], where $\mu = \mu(T,V,\langle\hat{N}\rangle)$ has to be inserted. With the approximation for Ξ,

$$F = \mu\langle\hat{N}\rangle - k_{\mathrm{B}}T\ln\Xi \approx \mu\langle\hat{N}\rangle - \mu\langle\hat{N}\rangle - k_{\mathrm{B}}T\ln Z_{\langle\hat{N}\rangle} = -k_{\mathrm{B}}T\ln Z_{\langle\hat{N}\rangle}$$

which is the canonical expression [40, Eq. (1.182)]. Conversely, the grand canonical potential Ω is the Legendre transform of the free energy F w.r.t. the particle number (Section 9.7) [40, Eq. (1.183)].

Pressure and entropy. Since F and Ω are related by a Legendre transformation w.r.t. $(\langle\hat{N}\rangle,\mu)$, their derivatives w.r.t. the passive variables T and V coincide [40, Eqs. (1.184), (1.185)]:

$$P = -\left(\frac{\partial\Omega}{\partial V}\right)_{T,\mu} = -\left(\frac{\partial F}{\partial V}\right)_{T,\langle\hat{N}\rangle}, \qquad S = -\left(\frac{\partial\Omega}{\partial T}\right)_{V,\mu} = -\left(\frac{\partial F}{\partial T}\right)_{V,\langle\hat{N}\rangle},$$

where $\mu = \mu(T,V,\langle\hat{N}\rangle)$ is inserted on the left-hand sides. With $F \approx -k_{\mathrm{B}}T\ln Z_{\langle\hat{N}\rangle}$ this yields the claimed canonical expressions [40, Eqs. (1.186)–(1.188)].

Remark 9.42.1 Thus, canonical and grand canonical ensemble are equivalent, if the grand canonical mean value $\langle\hat{N}\rangle$ is identified with the canonical particle number N. This is justified, if almost all systems of the grand canonical ensemble have the same particle number $\langle\hat{N}\rangle$, which, again, is only the case for macroscopic, asymptotically large systems [40, p. 91].

9.7. Legendre Transformations

TBCopied from... Was it Schwabl that did a great job on this?

We follow [47, Sects. 3.1.1 and 3.1.2, pp. 75–80].

Definition 9.43 Let $Y = Y(x_1, x_2, \ldots)$ be a function with partial derivatives [47, Eq. (3.1.20a)]

$$a_i(x_1, x_2, \ldots) = \left(\frac{\partial Y}{\partial x_i}\right)_{\{x_j, j\neq i\}},$$

and assume that $x_1 \mapsto a_1$ is invertible (e.g. Y strictly convex or concave in x_1), such that $x_1 = x_1(a_1, x_2, \ldots)$. The *Legendre transform* of Y w.r.t. x_1 is the function [47, Eq. (3.1.22)]

$$Y_1(a_1, x_2, \ldots) = Y - a_1 x_1,$$

regarded as a function of its *natural variables* $a_1, x_2, \ldots$, i.e. with $x_1 = x_1(a_1, x_2, \ldots)$ inserted.

Theorem 9.44 The Legendre transform Y_1 has the differential [47, Eqs. (3.1.21'a), (3.1.21'b)]

$$\mathrm{d}Y_1 = -x_1\,\mathrm{d}a_1 + a_2\,\mathrm{d}x_2 + \ldots, \qquad \text{i.e.} \qquad \left(\frac{\partial Y_1}{\partial a_1}\right)_{x_2,\ldots} = -x_1, \qquad \left(\frac{\partial Y_1}{\partial x_2}\right)_{a_1,\ldots} = a_2, \quad \ldots$$

Moreover, the Legendre transformation is an involution: transforming Y_1 w.r.t. a_1 yields Y again.

Proof 9.44 The total differential of Y is $\mathrm{d}Y = a_1\,\mathrm{d}x_1 + a_2\,\mathrm{d}x_2 + \ldots$ [47, Eq. (3.1.20b)]. With $a_1\,\mathrm{d}x_1 = \mathrm{d}(a_1x_1) - x_1\,\mathrm{d}a_1$ it follows that [47, Eq. (3.1.21)]

$$\mathrm{d}(Y - a_1x_1) = -x_1\,\mathrm{d}a_1 + a_2\,\mathrm{d}x_2 + \ldots,$$

which is the claimed differential, and the partial derivatives can be read off. For the involution, notice that the derivative of Y_1 w.r.t. a_1 is $-x_1$, such that the Legendre transform of Y_1 w.r.t. a_1 is $Y_1 - a_1 \cdot (-x_1) = Y$.

Remark 9.44.1 The geometric meaning [47, p. 79, footnote 1]: a curve $x_1 \mapsto Y(x_1)$ can either be described by its points, or as the envelope of its tangents. For the latter, one needs the intercept of the tangents with the ordinate as a function of their slope a_1, which is exactly $Y_1(a_1) = Y - a_1x_1$. If one simply eliminated x_1 in favour of a_1 in $Y(x_1)$, one would obtain Y as a function of a_1, but one could no longer reconstruct $Y(x_1)$ from it.

Corollary 9.45 Starting from the internal energy $E(S, V, N)$ with $\mathrm{d}E = T\,\mathrm{d}S - P\,\mathrm{d}V + \mu\,\mathrm{d}N$ (Equation (9.48)), Legendre transformations yield the *thermodynamic potentials* [47, Eqs. (3.1.6)–(3.1.18) and Table 3.1]

Potential	Definition	Natural variables	Differential
Internal energy	E	S, V, N	$\mathrm{d}E = T\,\mathrm{d}S - P\,\mathrm{d}V + \mu\,\mathrm{d}N$
Free energy	$F = E - TS$	T, V, N	$\mathrm{d}F = -S\,\mathrm{d}T - P\,\mathrm{d}V + \mu\,\mathrm{d}N$
Enthalpy	$\mathrm{H} = E + PV$	S, P, N	$\mathrm{d}\,\mathrm{H} = T\,\mathrm{d}S + V\,\mathrm{d}P + \mu\,\mathrm{d}N$
Free enthalpy	$G = E - TS + PV$	T, P, N	$\mathrm{d}G = -S\,\mathrm{d}T + V\,\mathrm{d}P + \mu\,\mathrm{d}N$
Grand canonical potential	$\Omega = E - TS - \mu N$	T, V, μ	$\mathrm{d}\Omega = -S\,\mathrm{d}T - P\,\mathrm{d}V - N\,\mathrm{d}\mu$

In terms of the partition functions, $F = -k_B T \ln Z$ and $\Omega = -k_B T \ln \Xi$. Here the enthalpy is denoted by an upright H to distinguish it from the Hamilton-operator. With three pairs of conjugate variables one obtains eight potentials in total; the table lists the most important ones. From each potential, the conjugate variables follow by differentiation w.r.t. its natural variables, e.g. $S = -(\partial F/\partial T)_{V,N}$, $P = -(\partial F/\partial V)_{T,N}$, $\mu = (\partial F/\partial N)_{T,V}$, analogous to forces in mechanics, which explains the name *potentials* [47, p. 80].

Proof 9.45 Each line follows from Theorem 9.44 applied to $\mathrm{d}E$: F is the transform w.r.t. (S,T), H the transform w.r.t. $(V,-P)$, G the transform of F w.r.t. $(V,-P)$, and Ω the transform of F w.r.t. (N,μ). E.g. $\mathrm{d}F = \mathrm{d}E - T\,\mathrm{d}S - S\,\mathrm{d}T = -S\,\mathrm{d}T - P\,\mathrm{d}V + \mu\,\mathrm{d}N$. The relations to the partition functions are Equations (2.6.44) and (2.7.13) in [47], cf. Definition 9.33.

9.8. Thermodynamics

9.8.1. Deductions in the Microcanonical Ensemble

Notation 9.46 We consider a system that is properly described in the microcanonical ensemble by the natural variables (E, V, N), with entropy-function S_{MCE} as in Definition 9.18.

Remark 9.46.1 For notational convenience, we will in the following suppress the index "MCE" in $S_{\mathrm{MCE}} \equiv S$.

Corollary 9.47 Inverting the entropy S w.r.t. the energy E we can conclude that there exists an energy-function E such that

$$(S, V, N) \mapsto E(S, V, N) \in \mathbb{R} \tag{9.47}$$

with differential as in Equation (9.33) as

$$\mathrm{d}E = T\mathrm{d}S - P\mathrm{d}V + \mu\mathrm{d}N \tag{9.48}$$

Proof 9.47 Follows from the theorem of local invertibility.

Hypothesis 9.48 We keep in mind all possible ways of supplying energy to a system. This can occur through ...

1. through contact with other bodies from which heat is transferred,
2. the performance of work,
3. through the addition of material (i.e. increasing the particle number).

The total change in energy therefore takes the form

$$\mathrm{d}E = \delta\mathrm{Q} + \delta W + \delta E_N \tag{9.49}$$

with ...

1. *heat supply* δQ,
2. *mechanical work* δW,
3. *energy increase due to material supply* δE_N.

Remark 9.48.1 It is Equation (9.49), that is usually referred to as the *first law of thermodynamics*. Notice however that Equation (9.48) is equivalent to it.

Remark 9.48.2 One usually says that the energy of a system changes according to Equation (9.49) when passing from one equilibrium state to another, infinitesimally close one.

Corollary 9.49 By comparing these two expressions for $\mathrm{d}E$ we find the identifications ...

1. $\delta\mathrm{Q} = T\,\mathrm{d}S$ (the change of energy due to heat supply),
2. $\delta W = -P\,\mathrm{d}V$ (the work performed on the system),
3. $\delta E_N = \mu\,\mathrm{d}N$ (the change of the energy when the particle number increases).

Proof 9.49 We interpret the individual terms in Equation (9.48) as in Equation (9.49).

Remark 9.49.1 The relationship

$$\delta\mathrm{Q} = T\mathrm{d}S \tag{9.50}$$

is called *the second law of thermodynamics for reversible changes*. Later, we shall formulate the second law in its general form.

9.8.2. Transitioning from Microcanonical to Canonical Ensemble

Legendretransformation to the free energy etc...

We follow [47, Sects. 2.6.5 and 3.1.1] and use Section 9.7.

Definition 9.50 We define the *(Helmholtz) free energy* $F(T, V, N)$ as the Legendre transform of the energy $E(S, V, N)$ w.r.t. the entropy [47, Eq. (3.1.6)],

$$F = E - TS, \qquad T = \left(\frac{\partial E}{\partial S}\right)_{V,N},$$

where $S = S(T, V, N)$ is obtained by inverting $T = T(S, V, N)$. This inversion is possible if $(\partial T/\partial S)_{V,N} = T/C_{V,N} > 0$, i.e. for positive heat capacity (Lemma 9.54).

Corollary 9.51 One has [47, Eqs. (3.1.7)–(3.1.9)]

$$\mathrm{d}F = -S\,\mathrm{d}T - P\,\mathrm{d}V + \mu\,\mathrm{d}N, \qquad \left(\frac{\partial F}{\partial T}\right)_{V,N} = -S, \quad \left(\frac{\partial F}{\partial V}\right)_{T,N} = -P, \quad \left(\frac{\partial F}{\partial N}\right)_{T,V} = \mu,$$

and the energy can be recovered from F as

$$E = F - T\left(\frac{\partial F}{\partial T}\right)_{V,N} = -T^2\left(\frac{\partial}{\partial T}\frac{F}{T}\right)_{V,N}.$$

Proof 9.51 The differential follows from Theorem 9.44 and Equation (9.48). The last identity follows from $-T^2\partial_T(F/T) = -T\partial_T F + F = F + TS = E$.

Remark 9.51.1 By the differential, $(\mathrm{d}F)_{T,N} = -P\,\mathrm{d}V = \delta W$: the free energy is the part of the energy that is available as work in an isothermal process, whereas $(\mathrm{d}E)_{T,N} \neq \delta W$, since heat has to be exchanged to keep the temperature constant [47, p. 77].

Theorem 9.52 In the canonical ensemble, the free energy is given by [47, Eqs. (2.6.44)–(2.6.53)]

$$F(T,V,N) = -k_\mathrm{B}T\ln Z(T,V,N),$$

in the sense that with $U = \langle\hat{H}\rangle$, $S = -k_\mathrm{B}\,\mathrm{Tr}(\hat{\rho}_\mathrm{CE}\ln\hat{\rho}_\mathrm{CE})$ and the mechanical pressure $P = -\langle\partial\hat{H}/\partial V\rangle$ one has $F = U - TS$ and $\mathrm{d}F = -S\,\mathrm{d}T - P\,\mathrm{d}V + (\partial F/\partial N)_{T,V}\,\mathrm{d}N$, where $(\partial F/\partial N)_{T,V} = \mu$ in the thermodynamic limit. Further, $F = U - TS_\mathrm{MCE}(E = U, V, N)$ for macroscopic systems (Theorem 9.40).

Proof 9.52 $F = U - TS$ is shown in the proof of Remark 9.11.1, and $(\partial F/\partial T)_{V,N} = -S$ in the proof of Lemma 9.54. For the volume derivative, $\partial_V \ln Z = Z^{-1}\,\mathrm{Tr}(-\beta\,\partial_V\hat{H}\,\mathrm{e}^{-\beta\hat{H}})$ gives $(\partial F/\partial V)_{T,N} = \langle\partial\hat{H}/\partial V\rangle = -P$ [47, p. 59]. Considering Z as a function of the particle number as well, the total differential acquires the term $(\partial F/\partial N)_{T,V}\,\mathrm{d}N$; comparing $\mathrm{d}U = \mathrm{d}(F + TS) = T\,\mathrm{d}S - P\,\mathrm{d}V + (\partial F/\partial N)_{T,V}\,\mathrm{d}N$ with the microcanonical differential (9.48) in the thermodynamic limit yields $(\partial F/\partial N)_{T,V} = \mu$ [47, Eqs. (2.6.51)–(2.6.53)].

Definition 9.53 We define the *heat capacity* of a system in the canonical ensemble as derivative

$$C_{V,N}(T) = T\left(\frac{\partial S}{\partial T}\right)_{V,N}(T) \tag{9.51}$$

Lemma 9.54 The following identities are immediate

$$\begin{aligned}
&\bullet \quad C_{V,N}(T) = \partial_T\langle H\rangle_{V,N}(T)\\
&\bullet \quad C_{V,N}(T) = -T\left(\partial_T^2 F\right)(N,T,V)\\
&\bullet \quad C_{V,N}(T) = k_\mathrm{B}\beta^2\left(\langle H^2\rangle_{N,V}(T) - \langle H\rangle_{N,V}^2(T)\right) = k_\mathrm{B}\beta^2\left\langle(H - \langle H\rangle)^2\right\rangle_{N,V,T} \geq 0
\end{aligned} \tag{9.52}$$

Proof 9.54 TBD; Schwabl for the first two, Nolting page 73 for the third one.

Exception for positivity of the heat capacity: Black holes. Cf. Tong Lecture notes, under Equation (1.11).

We work in the canonical ensemble with $\hat{\rho} = Z^{-1}\mathrm{e}^{-\beta H}$, $Z = \operatorname{Tr}\,\mathrm{e}^{-\beta H}$, $\beta = 1/(k_{\mathrm{B}}T)$, free energy $F = -k_{\mathrm{B}}T\ln Z$ [47, Eq. (2.6.44)] and entropy $S = -k_{\mathrm{B}}\operatorname{Tr}(\hat{\rho}\ln\hat{\rho})$ (Remark 9.11.1), and we abbreviate $\langle\,\cdot\,\rangle \equiv \langle\,\cdot\,\rangle_{N,V}(T)$. All derivatives are taken at fixed (V, N), i.e. for a fixed Hamilton-operator H.

Step 0 (Auxiliary identities). From $\partial_\beta Z = -\operatorname{Tr}(H\mathrm{e}^{-\beta H})$ and $\partial_\beta^2 Z = \operatorname{Tr}(H^2\mathrm{e}^{-\beta H})$ one obtains the relations [47, Eq. (2.6.46)]

$$\langle H\rangle = -\frac{\partial}{\partial\beta}\ln Z, \qquad \langle H^2\rangle = \frac{1}{Z}\frac{\partial^2 Z}{\partial\beta^2}, \qquad \frac{\mathrm{d}\beta}{\mathrm{d}T} = -\frac{1}{k_{\mathrm{B}}T^2} = -k_{\mathrm{B}}\beta^2.$$

Further, since $\ln\hat{\rho} = -\beta H - \ln Z$,

$$S = -k_{\mathrm{B}}\langle -\beta H - \ln Z\rangle = \frac{1}{T}\left(\langle H\rangle + k_{\mathrm{B}}T\ln Z\right) = \frac{1}{T}\left(\langle H\rangle - F\right),$$

i.e. $F = \langle H\rangle - TS$ [47, Eqs. (2.6.45), (2.6.48)].

Second identity. With $\partial_T \ln Z = \frac{\mathrm{d}\beta}{\mathrm{d}T}\partial_\beta \ln Z = \langle H\rangle/(k_{\mathrm{B}}T^2)$ one finds

$$\left(\frac{\partial F}{\partial T}\right)_{V,N} = -k_{\mathrm{B}}\ln Z - k_{\mathrm{B}}T\frac{\langle H\rangle}{k_{\mathrm{B}}T^2} = \frac{1}{T}\left(F - \langle H\rangle\right) = -S,$$

which is the T-component of $\mathrm{d}F = -S\,\mathrm{d}T - P\,\mathrm{d}V$ [47, Eq. (2.6.49)]. Therefore $C_{V,N} = T\,(\partial S/\partial T)_{V,N} = -T\,\partial_T^2 F$.

First identity. Differentiating $\langle H\rangle = F + TS$ w.r.t. T and using $\partial_T F = -S$ yields

$$\partial_T\langle H\rangle = \partial_T F + S + T\partial_T S = T\left(\frac{\partial S}{\partial T}\right)_{V,N} = C_{V,N}(T),$$

which corresponds to $\mathrm{d}\langle H\rangle = T\,\mathrm{d}S - P\,\mathrm{d}V$ [47, Eq. (2.6.50a)].

Third identity. Following [40, p. 73, Eq. (1.148)] (there for classical systems, the quantum case is identical with the above Z) we find

$$\begin{aligned} C_{V,N} &= \frac{\partial\langle H\rangle}{\partial T} = \frac{\mathrm{d}\beta}{\mathrm{d}T}\frac{\partial\langle H\rangle}{\partial\beta} = k_{\mathrm{B}}\beta^2\frac{\partial^2}{\partial\beta^2}\ln Z = k_{\mathrm{B}}\beta^2\frac{\partial}{\partial\beta}\left(\frac{1}{Z}\frac{\partial Z}{\partial\beta}\right) \\ &= k_{\mathrm{B}}\beta^2\left[\frac{1}{Z}\frac{\partial^2 Z}{\partial\beta^2} - \frac{1}{Z^2}\left(\frac{\partial Z}{\partial\beta}\right)^2\right] = k_{\mathrm{B}}\beta^2\left(\langle H^2\rangle - \langle H\rangle^2\right). \end{aligned}$$

Moreover $\left\langle (H - \langle H\rangle)^2\right\rangle = \langle H^2\rangle - 2\langle H\rangle^2 + \langle H\rangle^2 = \langle H^2\rangle - \langle H\rangle^2$, and by Theorem 9.10 in the eigenbasis of H

$$\left\langle (H - \langle H\rangle)^2\right\rangle = \frac{1}{Z}\sum_n \mathrm{e}^{-\beta E_n}\left(E_n - \langle H\rangle\right)^2 \geq 0.$$

This is the thermal stability criterion $C_V \geq 0$ [40, Eq. (1.147)].

On the exception. The Tong lecture notes are not part of the literature folder. Notice only that the positivity derived above relies on the existence of the canonical state ($Z < \infty$, equilibrium with a heat bath). Systems with negative heat capacity, such as black holes, do not admit such a description, so there is no contradiction.

Notation 9.55 For a crystal[3] at hand we introduce ...

- the *total mass of the crystal* m (with unit kg)
- the *molar mass of the crystal* M (with unit kg/mol)
- the *number of moles of the crystal* n (with unit mol)

Fact 9.56 One has for the number of moles the identity

$$n = \frac{m}{M} \tag{9.53}$$

Notation 9.57 We enumerate the masses of the r atoms in the unit cell as $m_1, m_2, \dots, m_r$.

Fact 9.58 The total mass m of the crystal is given as

$$m = N_x N_y N_z \cdot \sum_{j=1}^{r} m_j. \tag{9.54}$$

Example: A monoatomic crystal, e.g. lead (Pb) in an fcc-lattice with a single atom per unit cell.

- The molar mass M of lead is

$$M_{\text{Pb}} = 207.2\,\text{g/mol} = 207.2 \cdot 10^{-3}\,\text{kg/mol} \tag{9.55}$$

- The total mass m of a lead-crystal (with monoatomic basis in an fcc-lattice) is given as the total number of cells multiplied with the number of lead-atoms per cell (i.e. one) multiplied with the mass of a lead atom

  i.e.

$$m_{\text{Pb}} = N_x N_y N_z \cdot m_{\text{Pb-atom}} \tag{9.56}$$

  with

$$m_{\text{Pb-atom}} = 207.2\,\text{u} = 207.2 \cdot 1.66 \cdot 10^{-27}\,\text{kg} \tag{9.57}$$

[3] Notice that one can also introduce these definitions for materials that are not crystalline. However, in this document, we will not be concerned with those materials.

Combining these two equations yields for the number of moles n in a crystal with mass m the equation

$$n = \frac{m_{\mathrm{Pb}}}{M_{\mathrm{Pb}}} = N_x N_y N_z \cdot \frac{1.66 \cdot 10^{-27}}{10^{-3}} \mathrm{mol} = N_x N_y N_z \cdot 1.66 \cdot 10^{-24}\,\mathrm{mol} \tag{9.58}$$

Definition 9.59 We define the *molar heat capacity* $C_{V,N,\mathrm{molar}}(T)$ as the amount of heat required to raise the temperature of one mole of a substance by one Kelvin, i.e.

$$C_{V,N,\mathrm{molar}}(T) = \frac{C_{V,N}(T)}{n} \tag{9.59}$$

whereas n is the amount of substance in moles.

Remark 9.59.1 Identities analogous to Lemma 9.54 follow immediately.

Theorem 9.60 TBD

See 03 page 41, 42 for a nice summary of potentials and partition functions.

TBD: 02: page 129 (useful formulae).

TBD: 03: page 22 (equilibrium is found by maximizing the entropy).

(The references "03" and "02" could not be matched unambiguously to books of the literature folder; the following summary is compiled from [47, Tables 2.1 and 3.1, Sect. 3.1.3] and [40, Sects. 1.5.2 and 2.5].)

1. *Summary of the ensembles* [47, Table 2.1]:

	microcanonical	canonical	grand canonical
Physical situation	isolated	energy exchange	energy and particle exchange
Density	$\frac{1}{\Omega}\sum_{E_m\in\mathscr{E}} \lvert E_m\rangle\langle E_m\rvert$	$\frac{1}{Z}\mathrm{e}^{-\beta\hat{H}}$	$\frac{1}{\Xi}\mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}$
Normalization	$\Omega(E,V,N)=\lvert\mathscr{E}\rvert$	$Z(T,V,N)=\mathrm{Tr}\ \mathrm{e}^{-\beta\hat{H}}$	$\Xi(T,V,\mu)=\mathrm{Tr}_{\mathscr{F}}\ \mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}$
Natural variables	E,V,N	T,V,N	T,V,μ
Potential	$S=k_\mathrm{B}\ln\Omega$	$F=-k_\mathrm{B}T\ln Z$	$\Omega=-k_\mathrm{B}T\ln\Xi$
Extremal principle	S maximal	F minimal	Ω minimal

   In all three ensembles $S=-k_\mathrm{B}\,\mathrm{Tr}(\hat{\rho}\ln\hat{\rho})$, and the differentials of the potentials are listed in Corollary 9.45.

2. *Useful formulae* (with $U=\langle\hat{H}\rangle$, and $z=\mathrm{e}^{\beta\mu}$):

$$U=-\frac{\partial}{\partial\beta}\ln Z=-\left(\frac{\partial}{\partial\beta}\ln\Xi\right)_{z,V}, \qquad P=k_\mathrm{B}T\frac{\partial}{\partial V}\ln Z=k_\mathrm{B}T\frac{\partial}{\partial V}\ln\Xi,$$
$$S=k_\mathrm{B}\frac{\partial}{\partial T}\left(T\ln Z\right), \qquad C_{V,N}=k_\mathrm{B}\beta^2\left\langle\left(\hat{H}-U\right)^2\right\rangle_{\mathrm{CE}},$$
$$\langle\hat{N}\rangle=\frac{1}{\beta}\frac{\partial}{\partial\mu}\ln\Xi, \qquad \left\langle\left(\hat{N}-\langle\hat{N}\rangle\right)^2\right\rangle=k_\mathrm{B}T\frac{\partial\langle\hat{N}\rangle}{\partial\mu}.$$

3. *Homogeneous systems (Gibbs-Duhem)*: if the entropy is extensive, $S(\alpha E,\alpha V,\alpha N)=\alpha S(E,V,N)$, then [47, Eqs. (3.1.24), (3.1.24')], [40, Eq. (1.180)]

$$E=TS-PV+\mu N, \qquad G=\mu N, \qquad \Omega=-PV, \quad \text{i.e.} \quad \frac{PV}{k_\mathrm{B}T}=\ln\Xi, \qquad S\,\mathrm{d}T-V\,\mathrm{d}P+N\,\mathrm{d}\mu=0.$$

4. *Equilibrium maximizes the entropy*: let $\mathscr{H}_{\mathscr{E}}=\mathrm{span}\{\lvert E_m\rangle \mid E_m\in\mathscr{E}\}$. For every density $\hat{\rho}'$ that is compatible with the constraints of the microcanonical ensemble (i.e. whose eigenstates lie in $\mathscr{H}_{\mathscr{E}}$), one has $S'=-k_\mathrm{B}\,\mathrm{Tr}(\hat{\rho}'\ln\hat{\rho}')\le S_{\mathrm{MCE}}$ [40, Eq. (2.104)].

Proof 9.60 *Item 1* collects Theorems 9.27 and 9.32, Definition 9.33, Remark 9.11.1, Theorem 9.52 and the extremal principles of Theorems 9.29, 9.35 and Item 4.

Item 2. The formulae for U (canonical), S and $C_{V,N}$ are shown in the proof of Lemma 9.54 (with $S = -\partial_T F$), the one for U (grand canonical) is [40, Eq. (1.174)], those for $\langle \hat{N} \rangle$ and its fluctuations are Lemma 9.41, and those for P follow from $P = -\partial_V F$ (Theorem 9.52) and $P = -\partial_V \Omega$ (Corollary 9.34).

Item 3. Differentiating $S(\alpha E, \alpha V, \alpha N) = \alpha S(E, V, N)$ w.r.t. α at $\alpha = 1$ gives with Equation (9.33) $\frac{1}{T}E + \frac{P}{T}V - \frac{\mu}{T}N = S$, i.e. $E = TS - PV + \mu N$ [47, p. 81]. Inserting this into the definitions of Corollary 9.45 yields $G = \mu N$ and $\Omega = -PV$, and with Definition 9.33 $PV/(k_B T) = \ln \Xi$. Comparing $\mathrm{d}E = T\,\mathrm{d}S + S\,\mathrm{d}T - P\,\mathrm{d}V - V\,\mathrm{d}P + \mu\,\mathrm{d}N + N\,\mathrm{d}\mu$ with Equation (9.48) yields the Gibbs-Duhem relation $S\,\mathrm{d}T - V\,\mathrm{d}P + N\,\mathrm{d}\mu = 0$.

Item 4. We follow [40, Sect. 2.5.3]. Step 1 of the proof of Theorem 9.29 applies on the subspace $\mathscr{H}_{\mathscr{E}}$, on which $\hat{\rho}_{\mathrm{MCE}}$ has the positive eigenvalue Ω^{-1}, and gives

$$\mathcal{H} = \mathrm{Tr}\left[\hat{\rho}'\left(\ln \hat{\rho}_{\mathrm{MCE}} - \ln \hat{\rho}'\right)\right] \leq 0.$$

Since $k_B \,\mathrm{Tr}(\hat{\rho}' \ln \hat{\rho}_{\mathrm{MCE}}) = k_B \ln(\Omega^{-1}) \,\mathrm{Tr}(\hat{\rho}') = -S_{\mathrm{MCE}}$, one finds $k_B \mathcal{H} = S' - S_{\mathrm{MCE}} \leq 0$. Hence all processes that can still occur in an isolated system (and lead into equilibrium) do not decrease the entropy, which is the second law of thermodynamics, $\mathrm{d}S \geq 0$ [40, Eqs. (2.104), (2.105)].

9.8.3. Transitioning from Canonical Ensemble to the Grand Canonical Ensemble

TBElaborated.

We follow [40, Sect. 1.5.2], [47, Sects. 2.7 and 3.1], and Section 9.7.

Remark 9.60.1 *Thermodynamic level.* The grand canonical potential $\Omega(T, V, \mu)$ is the Legendre transform of the free energy $F(T, V, N)$ w.r.t. the particle number [40, Eq. (1.183)], [47, Eq. (3.1.16)],

$$\Omega = F - \mu N, \qquad \mu = \left(\frac{\partial F}{\partial N}\right)_{T,V}, \qquad \mathrm{d}\Omega = -S\,\mathrm{d}T - P\,\mathrm{d}V - N\,\mathrm{d}\mu,$$

cf. Corollary 9.45.

Remark 9.60.2 *Statistical level.* The grand canonical partition function is a generating function of the canonical ones [47, Eq. (2.7.8)],

$$\Xi(T, V, \mu) = \sum_{N=0}^{\infty} \mathrm{e}^{\beta\mu N} Z_N(T, V) = \sum_{N=0}^{\infty} \mathrm{e}^{\beta(\mu N - F(T,V,N))},$$

where $Z_N = \mathrm{e}^{-\beta F(T,V,N)}$ was used. For macroscopic systems the sum is dominated by its maximal term (Theorem 9.42), which is located where the exponent $\mu N - F(T, V, N)$ is maximal w.r.t. N, i.e. where $\mu = (\partial F/\partial N)_{T,V}$. At this point

$$\Omega(T, V, \mu) = -k_B T \ln \Xi \approx F(T, V, N) - \mu N,$$

i.e. the "Laplace-transform" on the statistical level becomes the Legendre transformation on the thermodynamic level (cf. the saddle point evaluation in [40, Aufgabe 2.4.3], which leads to $F = \Omega + \mu\langle \hat{N} \rangle$).

Remark 9.60.3 *Practical recipe.* To compute canonical quantities for a fixed particle number N_{CN} within the (often more convenient) grand canonical ensemble, one determines the chemical potential $\mu(T,V)$ from

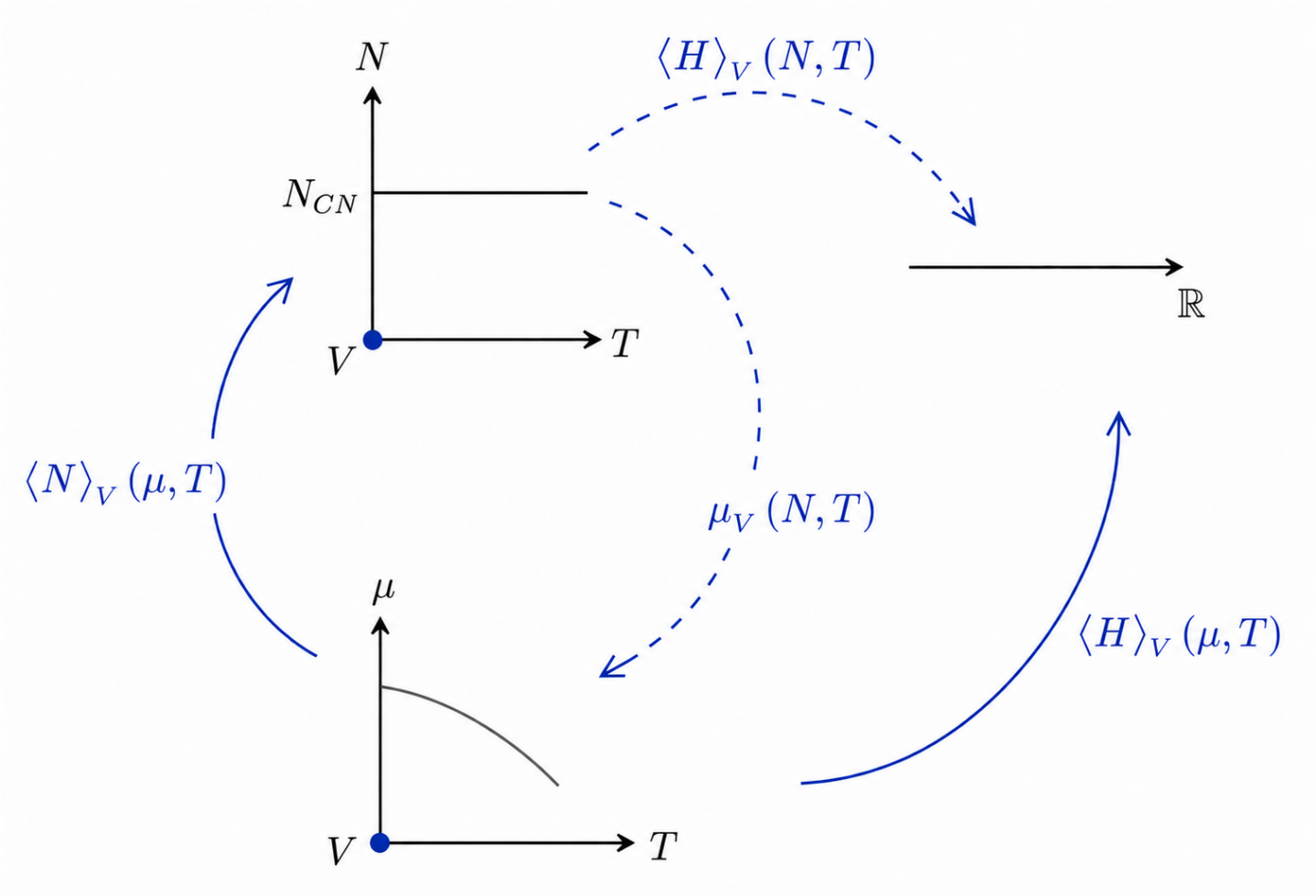
$$\langle \hat{N} \rangle (\mu(T,V),T,V) = N_{\mathrm{CN}},$$

which is possible by the monotonicity of Theorem 9.37 [40, Eq. (1.169)]. By the equivalence of the ensembles (Theorem 9.42), canonical quantities are then given by grand canonical ones evaluated at $\mu = \mu(T,V)$, e.g. $\langle \hat{H} \rangle (N_{\mathrm{CN}},T,V) \approx \langle \hat{H} \rangle (\mu(T,V),T,V)$ and $F = \Omega + \mu N_{\mathrm{CN}}$. Derivatives w.r.t. T or V at fixed N_{CN} then have to be computed with the chain rule, since μ depends on T and V [40, Eqs. (1.184), (1.185)]. This is exactly what is done in the following Corollary.

Corollary 9.61 Computing the specific heat capacity in the grand canonical ensemble one finds

$$\begin{aligned} C_{N,V}(T) &= \partial_T \langle H \rangle (N,T,V) \\ &= \left(\partial_T \langle H \rangle\right)(\mu(T,V),T,V) + \left(\partial_\mu \langle H \rangle\right)(\mu(T,V),T,V) \cdot \left(\partial_T \mu\right)(N,V,T) \end{aligned} \tag{9.60}$$

whereas the particle number N is kept constant.



Proof 9.61 For a fixed N_{CN} we introduce the map $(T,V) \mapsto \mu(T,V)$ such that

$$\langle N \rangle(\mu(T,V),T,V) = N_{\mathrm{CN}} \tag{9.61}$$

and we omit the N_{CN} in μ for notational simplicity. Now we recall, that by equivalence of the ensembles, one finds

$$\langle H \rangle(N,T,V) \equiv \langle H \rangle(\mu(T,V),T,V) \tag{9.62}$$

Now the promised equality follows from the chain-rule, i.e. by introducing the map $T \mapsto g(T) \equiv (\mu(T),T)$ etc.

Might be Interesting later:

- Callen - Thermodynamics and an Introduction to Thermostatistics, Wiley Sons
- Texier Roux - Physique Statistique, Dunod
- Diu, Guthmann, Lederer, Roulet - Physique Statistique, Hermann
- Jancovici - Statistical Physics and Thermodynamics, McGraw-Hill
- Landau Lifschitz - Statistical Physics, Pergamon Press
- K. Huang - Statistical Mechanics, Wiley
- Barrat Hansen - Basic Concepts for Simple and Complex Fluids, Cambridge University Press
- Somewhere page 13, 14: Stirlings approximation.
- Somewhere page 19, 20, 22: Entropy and Temperature for two combined systems.
- Somewhere page 27, 28: Chapter 4 Canonical Ensemble; Same book page 35, 36 Chapter 5 Grand canonical ensemble.
- Somewhere pdfpage44: "Ueberlässt man ein abgeschlossenes Vielteilchensystem sich selbst, so streben die makroskopisch messbaren Groeszen gegen zeitlich konstante Werte. Dies ist ein Erfahrungssatz."
- Somewhere page 39: "Die Energie E kann nur mit einer endlichen Genauigkeit δE bestimmt werden (...)".
- Page 157 in the template: minimization of the grand canonical potential.

9.9. Auxiliary Identities

For later use we introduce the following notation

Notation 9.62 We introduce analoga for the [F]ermi- / [B]ose- / [ζ]-functions that take dimensionless arguments as

$$\mathrm{F}(x) = \frac{1}{\mathrm{e}^x + 1} \qquad / \qquad \mathrm{B}(x) = \frac{1}{\mathrm{e}^x - 1} \qquad / \qquad \mathrm{n}^\zeta(x) = \frac{1}{\mathrm{e}^x - \zeta} \tag{9.63}$$

with $\zeta \in \{-1, +1\}$ as usual.

Lemma 9.63 One obtains the identities

$$\frac{\mathrm{d}}{\mathrm{d}x}\mathrm{n}^\zeta(x) = -\mathrm{n}^\zeta(x)\left(1 + \zeta\mathrm{n}^\zeta(x)\right) \equiv -\frac{1}{4}\zeta\mathrm{ch}^2(x/2) \equiv \begin{cases} -\frac{1}{4}\,\mathrm{sech}^2\,(x/2) & \text{for } \zeta = -1 \\ -\frac{1}{4}\,\mathrm{csch}^2\,(x/2) & \text{for } \zeta = +1 \end{cases} \tag{9.64}$$

Proof 9.63 See Appendix, Proofs, page 516.

Notation 9.64 For a temperature $\beta = \frac{1}{k_\mathrm{B}T}$ we write for the [F]ermi- / [B]ose- / [ζ]-functions

$$\mathrm{F}_{\hbar\beta}(\omega) = \frac{1}{\mathrm{e}^{\hbar\beta\omega} + 1} \qquad / \qquad \mathrm{B}_{\hbar\beta}(\omega) = \frac{1}{\mathrm{e}^{\hbar\beta\omega} - 1} \qquad / \qquad \mathrm{n}^\zeta_{\hbar\beta}(\omega) = \frac{1}{\mathrm{e}^{\hbar\beta\omega} - \zeta} \tag{9.65}$$

with $\zeta \in \{-1, +1\}$ as usual.

Remark 9.64.1 Notice that one has the relation $\mathrm{n}^\zeta_{\hbar\beta}(\omega) = \mathrm{n}^\zeta(\beta\hbar\omega)$, etc.

For reasons that are difficult to motivate in advance[4], we will need the following identities in later chapters.

Lemma 9.65 For $\mathrm{i}\omega_n \in \mathrm{i}\Omega_{-1}$ one has the identities

$$\mathrm{F}_{\hbar\beta}(\bullet + \mathrm{i}\omega_n) = -\mathrm{B}_{\hbar\beta}(\bullet), \qquad \mathrm{F}_{\hbar\beta}(\mathrm{i}\omega_n - \bullet) = \mathrm{B}_{\hbar\beta}(\bullet) + 1 \tag{9.66}$$

further one has

$$\mathrm{F}_{\hbar\beta}(-\bullet) = 1 - \mathrm{F}_{\hbar\beta}(\bullet). \tag{9.67}$$

Proof 9.65 See Appendix, Proofs, page 517.

[4] These identities will be needed in different situations, for example to compute the self-energy or the heat capacity of an interacting electron-phonon-system.

Remark 9.65.1 Notice further that one also has the trivial identities for $\omega_n \in \Omega_{+1}$

$$\mathrm{F}_{\hbar\beta}(\bullet \pm \mathrm{i}\omega_n) = \mathrm{F}_{\hbar\beta}(\bullet) \tag{9.68}$$

Lemma 9.66 One has the derivatives

$$\frac{\mathrm{d}}{\mathrm{d}T}\,\mathrm{n}_\beta^\zeta(\hbar\omega) = \frac{\hbar\omega}{k_\mathrm{B}T^2}\,\mathrm{n}_\beta^\zeta(\hbar\omega)\left(1+\zeta\,\mathrm{n}_\beta^\zeta(\hbar\omega)\right) = \begin{cases} \dfrac{\hbar\omega}{4k_\mathrm{B}T^2}\,\mathrm{sech}^2\left(\dfrac{\hbar\omega}{2k_\mathrm{B}T}\right) & \text{for } \zeta=-1 \\ \dfrac{\hbar\omega}{4k_\mathrm{B}T^2}\,\mathrm{csch}^2\left(\dfrac{\hbar\omega}{2k_\mathrm{B}T}\right) & \text{for } \zeta=+1 \end{cases} \tag{9.69}$$

Proof 9.66 See Appendix, Proofs, page 517.

Corollary 9.67 For $z \in \mathbb{C}$ we find the identity

$$\frac{\mathrm{d}}{\mathrm{d}z}\mathrm{n}_{\hbar\beta}^\zeta(z) = -\hbar\beta\mathrm{n}_{\hbar\beta}^\zeta(z)\left(1+\zeta\mathrm{n}_{\hbar\beta}^\zeta(z)\right) \equiv -\frac{\hbar\beta}{4}\zeta\mathrm{ch}^2(\hbar\beta z/2) \equiv \begin{cases} -\dfrac{\hbar\beta}{4}\,\mathrm{sech}^2\left(\hbar\beta z/2\right) & \text{for } \zeta=-1 \\ -\dfrac{\hbar\beta}{4}\,\mathrm{csch}^2\left(\hbar\beta z/2\right) & \text{for } \zeta=+1 \end{cases} \tag{9.70}$$

Proof 9.67 Follows directly from Lemma 9.63 with the chain-rule. Alternatively, by direct computation, see Appendix, Proofs, page 517.

10. Teaser for Equilibrium Green-Functions

"The Green's function method is one of the most powerful and versatile formalisms in physics"

The very first sentence in the book from Stefanucci and van Leuween [51].

The ultimate goal of equilibrium Green-function-techniques is to *describe* (in the widest sense of the word) systems as in Notation 8.1 in the canonical ensemble, or in the grand canonical ensemble, or in hybrid ensembles.

10.1. General Setup - Pure Systems

Ingredient I: Many-Particle-Hilbert-Space, States and Operators

Notation 10.1 We consider a system with statistics ζ and nature η, and an underlying many-particle Hilbert-space $\mathscr{H} \equiv \mathscr{H}_\eta$ that is generated by creation- and annihilation-operators

$$\mathscr{H} = \mathrm{span}_{\mathbb{C}} \left\{ \prod_{j=1}^{\mathrm{d}_\eta} \frac{1}{\sqrt{n_j!}} \left(c_j^\dagger \right)^{n_j} \mid \mathrm{vac.} \rangle \equiv |n_1, n_2, \dots, n_{\mathrm{d}_\eta}\rangle \,\middle|\, n_1, n_2, \dots, n_{\mathrm{d}_\eta} \in \mathbb{N}_\zeta \right\} \tag{10.1}$$

with a number of states to occupy

$$\mathrm{d}_\eta = \begin{cases} \mathrm{d}_{m=0} & \text{for } \eta = 0, \\ \mathrm{d}_{\mathcal{H}} & \text{for } \eta = 1, \end{cases} \tag{10.2}$$

generated through creation- and annihilation-operators acting on a vacuum. The Hamiltonian of the system is then given by a contribution H_0 that we believe to understand and perturbations V as

$$\begin{aligned} H &= H_0 &+ \quad & V \\ &= \sum_{i,j} H_{0\,ij} c_i^\dagger c_j &+ \quad & V(\mathbf{c}^\dagger, \mathbf{c}) \end{aligned} \tag{10.3}$$

with creation- and annihilation-operators $\left\{ c_1, c_1^\dagger, c_2, c_2^\dagger, \dots, c_{\mathrm{d}_\eta}, c_{\mathrm{d}_\eta}^\dagger \right\}$ obey the statistical commutation-relations

$$\left[c_i, c_j\right]_\zeta = \left[c_i^\dagger, c_j^\dagger\right]_\zeta = 0, \qquad \left[c_i, c_j^\dagger\right]_\zeta = \delta_{i,j} \tag{10.4}$$

Remark 10.1.1 Usually one switches the notation to a more *generic case*, and just writes generalized (system-specific) indices $\left\{ c_1, c_1^\dagger, c_2, c_2^\dagger, \dots, c_{\mathrm{d}_\eta}, c_{\mathrm{d}_\eta}^\dagger \right\} \equiv \bigcup_{\alpha \in \mathscr{A}} \left\{ c_\alpha, c_\alpha^\dagger \right\}$ with some index-set $\mathscr{A}$.

Ingredient II: The Natural Ensemble for Pure Systems

For systems with nature $\eta = 0$, we want to use the canonical ensemble and ignore the particle-number dependence, which is (on an enumerational level) equivalent to the grand canonical ensemble with $\mu = 0$. For systems with nature $\eta = 1$, we want to use the grand canonical ensemble with μ dictating the particle number. We combine these two cases into a single notation, by introducing the "natural ensemble".

Notation 10.2 We consider a system with nature $\eta \in \{0, 1\}$ in the grand canonical ensemble, with a volume V, temperature T and chemical potential

$$\begin{cases} \mu = 0 & \text{for } \eta = 0 \\ \mu \underset{\text{in general}}{\neq} 0 & \text{for } \eta = 1. \end{cases} \tag{10.5}$$

This gives us $2 + \eta$ natural variables.

Fact 10.3 In the absence of „spontaneous symmetry breaking“[1] expectation-values in the grand canonical ensemble are evaluated w.r.t. the density

$$\rho = \frac{\mathrm{e}^{-\beta(H-\eta\mu N)}}{\mathrm{Tr}_{\mathscr{H}}\, \mathrm{e}^{-\beta(H-\eta\mu N)}} \equiv \frac{1}{Z_\eta}\mathrm{e}^{-\beta(H-\eta\mu N)} \equiv \begin{cases} \frac{1}{Z}\mathrm{e}^{-\beta H} & \text{for } \eta = 0 \\ \frac{1}{Z}\mathrm{e}^{-\beta(H-\mu N)} & \text{for } \eta = 1. \end{cases}, \tag{10.6}$$

whereas we introduced the *natural partition-function*

$$Z_\eta \equiv \begin{cases} Z(T, V) & \text{for } \eta = 0 \\ Z(\mu, T, V) & \text{for } \eta = 1. \end{cases} \tag{10.7}$$

Remark 10.3.1 Recall that the state above represents a solution to the stationary von Neumann equation.

Remark 10.3.2 Although in the case of „spontaneous symmetry breaking“, the evaluation of observables w.r.t. the state above yields incorrect results, one can oftentimes however use the state above, and break the underlying symmetry „by hand“, in order to recover the „correct“ physical (ground) state (or, in the case that we will encounter later, the correct physical „field theory“) again.

Fact 10.4 The thermodynamic potential[2] in the natural ensemble is given by the so-called *natural energy*

$$\Omega_\eta \equiv \begin{cases} \Omega(T, V) = -\dfrac{\mathrm{Log}\, Z(T, V)}{\beta} & \text{for } \eta = 0 \\ \Omega(\mu, T, V) = -\dfrac{\mathrm{Log}\, Z(\mu, T, V)}{\beta} & \text{for } \eta = 1, \end{cases} \tag{10.8}$$

[1] We will introduce this concept in the chapter about superconductivity.

[2] Recall that the thermodynamic potential is a scalar-quantity which is used to represent the thermodynamic state of a system.

from which one can conclude the usual relations for the entropy, pressure and, in case of $\eta = 1$, the conjugated variable of N as

$$\frac{\partial \Omega_\eta}{\partial T} = -S, \qquad \frac{\partial \Omega_\eta}{\partial V} = -P, \quad \text{and if } \eta = 1: \quad \frac{\partial \Omega_\eta}{\partial \mu} = -N \tag{10.9}$$

whereas both sides of these respective equations depend on the $2 + \eta$ variables, which has been omitted for notational clarity.

Remark 10.4.1 Notice that the thermodynamic potential reduces to the Helmholtz free energy F for $\eta = 0$, and to the Landau-potential Ω for $\eta = 1$.

10.2. General Setup - Mixed Systems

We discuss the case of mixed systems at the example of mixture with massive and massless particles. The generalizations to other mixtures is straight-forward.

Ingredient I: Hilbert-Space, States and Operators

Notation 10.5 We consider a system, which is made of two subsystems, one with Fock-space $\mathscr{H}_{m>0} \equiv \mathscr{F}_\zeta$ with generators $\left\{ c_{\alpha_1}, c^\dagger_{\alpha_1}, c_{\alpha_2}, c^\dagger_{\alpha_2}, \ldots, c_{\alpha_{d_{m>0}}}, c^\dagger_{\alpha_{d_{m>0}}} \right\}$ and statistical operators, and another one with Hilbert-space $\mathscr{H}_{m=0}$ with bosonic generators $\left\{ c_{\beta_1}, c^\dagger_{\beta_1}, c_{\beta_2}, c^\dagger_{\beta_2}, \ldots, c_{\beta_{d_{m=0}}}, c^\dagger_{\beta_{d_{m=0}}} \right\}$. The total Hilbert-space $\mathscr{H}$ of the system is given as tensor-product

$$\mathscr{H} = \mathscr{H}_{m>0} \otimes \mathscr{H}_{m=0}$$

with basis[3] and scalar-product as usual. The generic Hamiltonian reads

$$\begin{aligned} H_{\text{tot}} &\equiv & H_{m>0} &+ & H_{m=0} &+ V_{\text{int}} \\ &\equiv & H_{\substack{0 \\ m>0}} &+ V_{m>0} &+ H_{\substack{0 \\ m=0}} &+ V_{m=0} &+ V_{\text{int}} \\ &\equiv \sum_{i,j} H_{\substack{0,ij \\ m>0}} c^\dagger_{\alpha_i} c_{\alpha_j} &+ V_{m>0}(\mathbf{c}^\dagger_\alpha, \mathbf{c}_\alpha) &+ \sum_{i,j} H_{\substack{0,ij \\ m=0}} c^\dagger_{\beta_i} b_{\beta_j} &+ V_{m=0}(\mathbf{c}^\dagger_\beta, \mathbf{c}_\beta) &+ V_{\text{int}}(\mathbf{c}^\dagger, \mathbf{c}) \end{aligned} \tag{10.10}$$

with interactions as in Fact 8.4.

Ingredient II: The Hybrid Ensemble

Notation 10.6 We further restrict our attention to the case in which the above mentioned system is made up of two sub-systems which have a mutual volume V and temperature T and a chemical potential μ for the massive particles. This gives us the three natural variables (μ, T, V).

[3] Cf. Flensberg page 276.

Fact 10.7 In the absence of „spontaneous symmetry breaking“ (to be introduced in a later chapter) expectation-values in the hybrid ensemble are evaluated w.r.t. the *hybrid density*

$$\rho = \frac{\mathrm{e}^{-\beta\left(H_{m>0}-\mu N_{m>0}+H_{\mathrm{w}}+V_{\mathrm{int}}\right)}}{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta\left(H_{\mathrm{p}}-\mu N+H_{\mathrm{w}}+V_{\mathrm{int}}\right)}} \equiv \frac{1}{Z}\mathrm{e}^{-\beta\left(H_{\mathrm{p}}-\mu N+H_{\mathrm{w}}+V_{\mathrm{int}}\right)}, \tag{10.11}$$

whereas we introduced the *mixed partition-function* $Z \equiv Z(N,\mu,T,V)$.

Remark 10.7.1 Recall that the state above represents a solution to the stationary von Neumann equation.

Remark 10.7.2 Although in the case of „spontaneous symmetry breaking“, the evaluation of observables w.r.t. the state above yields incorrect results, one can oftentimes however use the state above, and break the underlying symmetry „by hand“, in order to recover the „correct“ physical state (or, in the case that we will encounter later, the correct physical „field theory“) again.

Remark 10.7.3 Thermodynamic Relations?

10.3. Applications (Teaser)

In [38]:

> *"The ultimate objective of the quantum theory of many-particle systems is to understand experimentally observable properties of a diverse range of physical systems."*

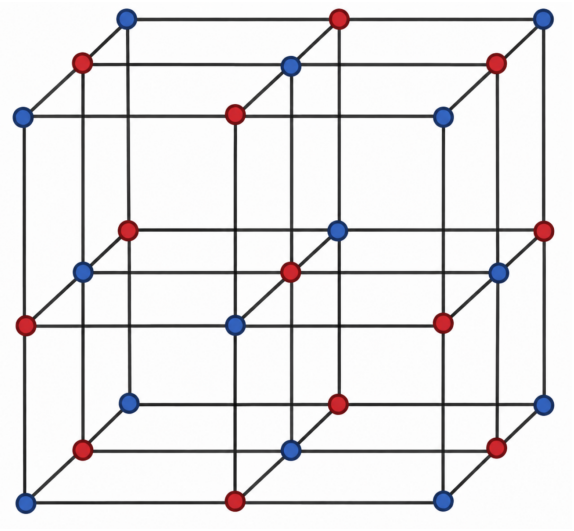
This quote from Negele and Orland is hitting very hard, because most of the theory and formalism presented in this work can be applied to *any crystalline system* (there are more than 200.000 known crystals in the Inorganic Crystal Structure Database[4]). Lying out the tools to study all of these systems is apparently a very powerful formalism.

It is a standard-fact, that in many experimental setups that are in some sense "close" to thermal equilibrium, observable quantities can be expressed as "equilibrium Green-functions" (will be introduced later). We list some examples whereas the meaning of the individual symbols will become clear throughout this document.

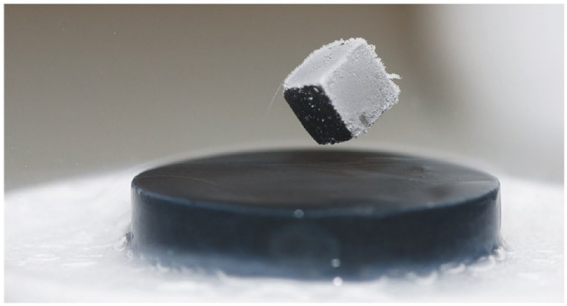
[4] `https://icsd.fiz-karlsruhe.de/`

System ("Cartoon"):

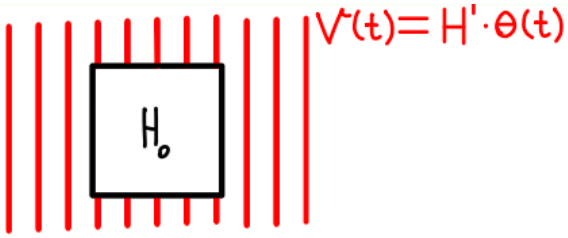
- **Any arbitrary Crystal:**



- **Superconductor**[7]:



- **An *arbitrary* observable A of a System subjected to a „weak“ Perturbation H':**



Observable(s):

- **Electronic Density of States / Band-Structure:**

$$\rho_{n\mathbf{k}}(\omega) = -\frac{\hbar}{\pi}\,\mathrm{Im}\lim_{\epsilon\to 0} G^{\mathrm{ret}}_{\substack{n,n\\ \mathbf{k},\mathbf{k}}}(\omega + \mathrm{i}\epsilon)$$

- **Magnetization**[5]**:**

$$\langle M\rangle \propto \sum_{\substack{\mathbf{k}\in\mathrm{Q}\\ n\in\{1,2,\dots\}\\ \omega\in(-\infty,+\infty)}} G^{<}_{\substack{n,n\\ \mathbf{k},\mathbf{k}\\ \uparrow,\uparrow}}(\omega) - G^{<}_{\substack{n,n\\ \mathbf{k},\mathbf{k}\\ \downarrow,\downarrow}}(\omega)$$

- **Electronic / Phononic / Total Heat Capacity:**

$C_{N,V}(T) = \partial_T \langle H\rangle_{N,T}$ = "sum of Green-functions"[6]

- **Electronic Conductivity Tensor:**

$\sigma(\omega)$ = "Green-function with current operators"

- **Thermal Conductivity Tensor:**

κ = "Green-function with energy-current operators"

- **Order Parameter**[8] **(in Eliashberg-Theory):**

$$\Delta_n(k) \propto \hat{\mathscr{G}}^{\ n}_{1,2}(k)$$
Gorkov

- **Kubo-Formula:**

$$\langle A\rangle(t) = \langle A\rangle(t=-\infty) + \int \mathrm{d}t'\, G^{\mathrm{ret}}_{AH'}(t,t') + \mathcal{O}(H')^2$$

[5] Note that for this to be unequal to zero one has to have spin orbit coupling or spontaneous symmetry breaking or another mechanism.
[6] Depending on the model, there can be a different number and different types of Green-functions.
[7] The picture was taken from [56].
[8] Here again, one has to ("spontaneously") break a symmetry in order to get non-zero values.

11. Green-Functions at Zero Temperature

Can be obtained from Green-Functions at Finite-Temperature (see next chapter) and taking the limit $T \to 0$, as elucidated in the Appendix, Section 29.3. A derivation of some standard-identities that one oftentimes encounters in literature on many-body-Green-function-techniques is also provided in the Appendix.

12. Real-Time-Two-Operator-Green-Functions at Finite Temperature

12.1. Two-Operator Green-Functions without Periodicity

For reasons that are impossible to motivate in advance, we introduce the following notations and functions.

Definition 12.1 For a pair of two operators (X, X') and times $t, t' \in \mathbb{R}$ we define the *real-time-two-operator-Green-function* in its various notations as *expectation-value*

$$\begin{aligned} G^{++}_{XX'}(t,t') \equiv G^{\mathbb{T}}_{XX'}(t,t') &\equiv G_{XX'}(t,t') \\ &\equiv -\frac{\mathrm{i}}{\hbar}\left\langle \mathrm{T}_t\, X\,(t)\, X'\left(t'\right)\right\rangle \\ &\equiv -\frac{\mathrm{i}}{\hbar}\frac{\mathrm{Tr}_{\mathscr{H}}\, \mathrm{e}^{-\beta\Xi}\, \mathrm{T}_t\, X\,(t)\, X'\,(t')}{\mathrm{Tr}_{\mathscr{H}}\, \mathrm{e}^{-\beta\Xi}} \\ &\equiv -\frac{\mathrm{i}}{\hbar}\frac{\mathrm{Tr}_{\mathscr{H}}\, \mathrm{e}^{-\beta\Xi}\left[\theta(t-t')\, X\,(t)\, X'\,(t') + \mathrm{S}_{X,X'}\,\theta(t'-t) X'\,(t')\, X\,(t)\right]}{\mathrm{Tr}_{\mathscr{H}}\, \mathrm{e}^{-\beta\Xi}} \end{aligned} \tag{12.1}$$

with time-ordering-operator and ensemble-Heisenberg-time-evolution as usual.

Definition 12.2 We introduce various *Green-functions corresponding to the operator-pair* (X, X') as

- $G_{X,X'}(t,t') \equiv G^{++}_{X,X'}(t,t') \equiv G^{\mathbb{T}}_{X,X'}(t,t') \equiv -\frac{\mathrm{i}}{\hbar}\langle \mathrm{T}_t\, X(t) X'(t')\rangle$
- $G^{+-}_{X,X'}(t,t') \equiv G^{<}_{X,X'}(t,t') \equiv -\frac{\mathrm{i}}{\hbar} S_{X,X'}\langle X'(t') X(t)\rangle$
- $G^{-+}_{X,X'}(t,t') \equiv G^{>}_{X,X'}(t,t') \equiv -\frac{\mathrm{i}}{\hbar}\langle X(t) X'(t)\rangle$
- $G^{--}_{X,X'}(t,t') \equiv G^{\overline{\mathbb{T}}}_{X,X'}(t,t') \equiv -\frac{\mathrm{i}}{\hbar}\langle \overline{\mathrm{T}}_t X(t) X'(t')\rangle$
- $G^{\mathrm{ret}}_{X,X'}(t,t') = -\frac{\mathrm{i}}{\hbar}\theta(t-t')\langle\left[X(t),\, X'(t')\right]_{\mathrm{S}}\rangle$
- $G^{\mathrm{adv}}_{X,X'}(t,t') = +\frac{\mathrm{i}}{\hbar}\theta(t'-t)\langle\left[X(t),\, X'(t')\right]_{\mathrm{S}}\rangle$

Lemma 12.3 The Green-functions defined above only depend on the time-difference, hence one can write

$$G^{\blacksquare}_{X,X'}(t,t') \equiv G^{\blacksquare}_{X,X'}(t-t'). \tag{12.2}$$

Proof 12.3 See Appendix, Proofs, page 518.

Remark 12.3.1 For the discussion of Feynman-diagrams, it is fruitful to introduce this redundant, extra time-argument.

Lemma 12.4 The following identities are immediate, if one neglects boundary-conditions[1]

- $G^{\mathbb{T}}_{X,X'}(t,t') = +\theta(t-t')\,G^{>}_{X,X'}(t,t') + \theta(t'-t)\,G^{<}_{X,X'}(t,t')$,
- $G^{\overline{\mathbb{T}}}_{X,X'}(t,t') = +\theta(t'-t)\,G^{>}_{X,X'}(t,t') + \theta(t-t')\,G^{<}_{X,X'}(t,t')$,
- $G^{\mathrm{ret}}_{X,X'}(t,t') = \left(G^{++}_{X,X'} - G^{+-}_{X,X'}\right)(t,t') = \left(G^{-+}_{X,X'} - G^{--}_{X,X'}\right)(t,t') = \theta(t-t')\left(G^{-+}_{X,X'} - G^{+-}_{X,X'}\right)(t,t')$,
- $G^{\mathrm{adv}}_{X,X'}(t,t') = \left(G^{++}_{X,X'} - G^{-+}_{X,X'}\right)(t,t') = \left(G^{+-}_{X,X'} - G^{--}_{X,X'}\right)(t,t') = \theta(t'-t)\left(G^{+-}_{X,X'} - G^{-+}_{X,X'}\right)(t,t')$,
- $G^{\mathbb{T}}_{X,X'}(t,t') + G^{\overline{\mathbb{T}}}_{X,X'}(t,t') = G^{>}_{X,X'}(A,A') + G^{<}_{X,X'}(t,t')$,
- $G^{\mathrm{ret}}_{X,X'}(t,t') - G^{\mathrm{adv}}_{X,X'}(t,t') = G^{>}_{X,X'}(t,t') - G^{<}_{X,X'}(t,t')$,

and if one has $X^{\dagger} = X'$ one also finds

- $G^{\mathrm{ret}}_{X,X'}(t,t') = G^{\mathrm{adv}}_{X,X'}(t',t)^{\dagger}$.

whereas the last equation is to be understood as a generalized matrix.

Proof 12.4 See Appendix, Proofs, page 518.

Remark 12.4.1 We emphasize a comment from Kamenev [28]:

> *"I can see how one can be overwhelmed by a number of different Green-functions, rules to follow and by the length of the calculations."*

[1] This is what one usually does in thermal quantum field theory. There are some comments about this in [Mahan].

12.2. Pure One-Body Green-Functions without Periodicity

Definition 12.5 We consider $X = c_\alpha$ and $X' = c^\dagger_{\alpha'}$ for multi-indices $A \equiv (\alpha, t) \in \mathscr{A} \times \mathbb{R}$, with

$$\left[c_\alpha, c^\dagger_{\alpha'}\right]_\zeta = \delta_{\alpha,\alpha'}, \qquad \mathrm{S}(c_\alpha) = \mathrm{S}(c^\dagger_{\alpha'}) = \zeta.$$

Then we write for the *real-time-one-body-Green-function*[2], *the lesser, greater, anti-time-ordered, retarded and advanced Green's-functions* in their various shapes as *expectation-value*

$$\begin{aligned}
&\bullet\ G(A,A') \equiv G^{++}(A,A') \equiv G^{\mathbb{T}}(A,A') \equiv -\frac{\mathrm{i}}{\hbar}\left\langle \mathrm{T}_t\, c_\alpha(t) c^\dagger_{\alpha'}(t')\right\rangle,\\
&\bullet\quad G^{+-}(A,A') \equiv G^{<}(A,A') \equiv -\frac{\mathrm{i}}{\hbar}\zeta\left\langle c^\dagger_{\alpha'}(t') c_\alpha(t)\right\rangle,\\
&\bullet\quad G^{-+}(A,A') \equiv G^{>}(A,A') \equiv -\frac{\mathrm{i}}{\hbar}\left\langle c_\alpha(t) c^\dagger_{\alpha'}(t')\right\rangle,\\
&\bullet\quad G^{--}(A,A') \equiv G^{\overline{\mathbb{T}}}(A,A') \equiv -\frac{\mathrm{i}}{\hbar}\left\langle \overline{\mathrm{T}}_t c_\alpha(t) c^\dagger_{\alpha'}(t')\right\rangle,\\
&\bullet\quad G^{\mathrm{ret}}(A,A') = -\frac{\mathrm{i}}{\hbar}\theta(t-t')\left\langle \left[c_\alpha(t),\, c^\dagger_{\alpha'}(t')\right]_\zeta\right\rangle,\\
&\bullet\quad G^{\mathrm{adv}}(A,A') = +\frac{\mathrm{i}}{\hbar}\theta(t'-t)\left\langle \left[c_\alpha(t),\, c^\dagger_{\alpha'}(t')\right]_\zeta\right\rangle.
\end{aligned}$$

with time-ordering-operator and ensemble-Heisenberg-time-evolution as usual.

Remark 12.5.1 Among physicists, the usual *interpretation* of the causal Green-function is as follows[3]

> *The one-particle Green's function describes a Gedankenexperiment which can never happen in practice. One creates a particle at time t' in the state α' and then (if $t > t'$) annihilates another particle at time t in the state α.*

Lemma 12.6 We obtain for the time-ordered, the anti-time-ordered, the retarded and the advanced Green-functions the equations of motion, and write them in wise foresight in sets as

$$\partial_t G^{\mathbb{T}}_{\alpha,\alpha'}(t) = -\frac{\mathrm{i}}{\hbar}\delta(t)\delta_{\alpha,\alpha'} \quad - \quad \frac{1}{\hbar}\left\langle \mathrm{T}_t\left[c_\alpha, \frac{\Xi}{\hbar}\right]_{\mathrm{H}}(t) c^\dagger_{\alpha'}(0)\right\rangle, \tag{12.3}$$

$$\partial_t G^{\mathrm{ret}}_{\alpha,\alpha'}(t) = -\frac{\mathrm{i}}{\hbar}\delta(t)\delta_{\alpha,\alpha'} \quad - \quad \frac{1}{\hbar}\theta(t)\left\langle \left[\left[c_\alpha, \frac{\Xi}{\hbar}\right]_{\mathrm{H}}(t), c^\dagger_{\alpha'}(0)\right]_\zeta\right\rangle, \tag{12.4}$$

and as

$$\partial_t G^{\overline{\mathbb{T}}}_{\alpha,\alpha'}(t) = \frac{\mathrm{i}}{\hbar}\delta(t)\delta_{\alpha,\alpha'} \quad - \quad \frac{1}{\hbar}\left\langle \overline{\mathrm{T}}_t\left[c_\alpha, \frac{\Xi}{\hbar}\right]_{\mathrm{H}}(t) c^\dagger_{\alpha'}(0)\right\rangle, \tag{12.5}$$

[2] Other names of this function are *time-ordered Green-function*, or *causal Green-function*. One also calls this Green-function the *propagator* of the underlying physical system.

[3] From [32], p. 167, with adapted notation to fit our purposes.

$$\partial_t G^{\mathrm{adv}}_{\alpha,\alpha'}(t) = -\frac{\mathrm{i}}{\hbar}\delta(-t)\delta_{\alpha,\alpha'} \quad + \quad \frac{1}{\hbar}\theta(-t)\left\langle\left[\left[c_\alpha, \frac{\Xi}{\hbar}\right]_{\mathrm{H}}(t), c^\dagger_{\alpha'}(0)\right]_\zeta\right\rangle. \tag{12.6}$$

Proof 12.6 See Appendix, Proofs, page 520.

Remark 12.6.1 Notice the symmetric behaviour of total minus-signs in these expressions.

Change of Basis

Notation 12.7 We consider a change of basis[4] with a unitary transformation

$$\widetilde{c}^\dagger_\alpha = \sum_i U_{i,\alpha} c^\dagger_i, \qquad \widetilde{c}_\alpha = \sum_i U^*_{i,\alpha} c_i \tag{12.7}$$

Remark 12.7.1 Notice that this can equivalently be rewriten by regarding the total sets of operators as column-vectors

$$\widetilde{\mathbf{c}} = U^\dagger \mathbf{c}, \qquad \widetilde{\mathbf{c}}^\dagger = \mathbf{c}^\dagger U \tag{12.8}$$

Corollary 12.8 We obtain for the two Green-functions w.r.t. to the two basis sets the relationship

$$\widetilde{G}^{\blacksquare} = U^\dagger G^{\blacksquare} U \quad \Longleftrightarrow \quad U \widetilde{G}^{\blacksquare} U^\dagger = G^{\blacksquare} \tag{12.9}$$

whereas $\blacksquare$ represents *any* of the double upper indices in Definition 12.5.

Proof 12.8 See Appendix, Proofs, page 522.

[4] Notice that in the case of $\eta = 1$ this might originate from a basis-change of the underlying snigle-particle Hilbert-space.

Examples: Pure, Non-Interacting Systems

Example: A Quantum Dot with Nature η and Statistics ζ

We consider the system from Definition 8.25. It's Green-functions can be inferred as a special case of the diagonal gas in Theorem 12.9 below.

Example: A Diagonal Gas with Nature η and Statistics ζ

We consider the system from Definition 8.27.

Theorem 12.9 Introducing the variables $\xi_\alpha \equiv \epsilon_\alpha - \eta\mu$ it follows

$$
\begin{aligned}
G^{\mathbb{T}}{}_{0\,\alpha,\alpha'}(t) &= -\frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}t\xi_\alpha/\hbar}\delta_{\alpha,\alpha'}\Big[\theta(t)\left(1+\zeta\,\mathrm{n}^\zeta_\beta(\xi_\alpha)\right)+\theta(-t)\zeta\mathrm{n}^\zeta_\beta(\xi_\alpha)\Big], & G^{\mathbb{T}}{}_{0\,\alpha,\alpha'}(\omega) &= +\frac{1}{\hbar}\delta_{\alpha,\alpha'}\lim_{\epsilon\to 0}\frac{1+\zeta\mathrm{n}^\zeta_{\hbar\beta}(\omega)}{\left(\omega+\mathrm{i}\epsilon-\xi_\alpha/\hbar\right)}-\frac{\zeta\mathrm{n}^\zeta_{\hbar\beta}(\omega)}{\left(\omega-\mathrm{i}\epsilon-\xi_\alpha/\hbar\right)},\\
G^{<}{}_{0\,\alpha,\alpha'}(t) &= -\frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}t\xi_\alpha/\hbar}\delta_{\alpha,\alpha'}\zeta\mathrm{n}^\zeta_\beta(\xi_\alpha), & G^{<}{}_{0\,\alpha,\alpha'}(\omega) &= -\frac{\mathrm{i}}{\hbar}\delta_{\alpha,\alpha'}\zeta\mathrm{n}^\zeta_\beta(\xi_\alpha)2\pi\delta(\omega-\xi_\alpha/\hbar),\\
G^{>}{}_{0\,\alpha,\alpha'}(t) &= -\frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}t\xi_\alpha/\hbar}\delta_{\alpha,\alpha'}\left(1+\zeta\,\mathrm{n}^\zeta_\beta(\xi_\alpha)\right), & G^{>}{}_{0\,\alpha,\alpha'}(\omega) &= -\frac{\mathrm{i}}{\hbar}\delta_{\alpha,\alpha'}\left(1+\zeta\,\mathrm{n}^\zeta_\beta(\xi_\alpha)\right)2\pi\delta(\omega-\xi_\alpha/\hbar),\\
G^{\overline{\mathbb{T}}}{}_{0\,\alpha,\alpha'}(t) &= -\frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}t\xi_\alpha/\hbar}\delta_{\alpha,\alpha'}\Big[\theta(-t)\left(1+\zeta\,\mathrm{n}^\zeta_\beta(\xi_\alpha)\right)+\theta(+t)\zeta\mathrm{n}^\zeta_\beta(\xi_\alpha)\Big], & G^{\overline{\mathbb{T}}}{}_{0\,\alpha,\alpha'}(\omega) &= +\frac{1}{\hbar}\delta_{\alpha,\alpha'}\lim_{\epsilon\to 0}-\frac{1+\zeta\mathrm{n}^\zeta_{\hbar\beta}(\omega)}{\left(\omega-\mathrm{i}\epsilon-\xi_\alpha/\hbar\right)}+\frac{\zeta\mathrm{n}^\zeta_{\hbar\beta}(\omega)}{\left(\omega+\mathrm{i}\epsilon-\xi_\alpha/\hbar\right)},\\
G^{\mathrm{ret}}{}_{0\,\alpha,\alpha'}(t) &= -\frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}t\xi_\alpha/\hbar}\delta_{\alpha,\alpha'}\theta(t), & G^{\mathrm{ret}}{}_{0\,\alpha,\alpha'}(\omega+\mathrm{i}\epsilon) &= +\frac{1}{\hbar}\delta_{\alpha,\alpha'}\frac{1}{\omega+\mathrm{i}\epsilon-\xi_\alpha/\hbar},\\
G^{\mathrm{adv}}{}_{0\,\alpha,\alpha'}(t) &= -\frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}t\xi_\alpha/\hbar}\delta_{\alpha,\alpha'}\theta(-t), & G^{\mathrm{adv}}{}_{0\,\alpha,\alpha'}(\omega-\mathrm{i}\epsilon) &= +\frac{1}{\hbar}\delta_{\alpha,\alpha'}\frac{1}{\omega-\mathrm{i}\epsilon-\xi_\alpha/\hbar}.
\end{aligned}
\tag{12.10}
$$

Proof 12.9 See Appendix, Proofs, page 522.

Remark 12.9.1 Notice that we can conclude the expectation-value for the number-operator from the lesser Green-function as

$$\langle c^\dagger_\alpha c_\alpha\rangle = -\frac{\hbar}{\mathrm{i}}\zeta G^<_{\alpha,\alpha}(t=0) = \mathrm{n}^\zeta_\beta(\xi_\alpha). \tag{12.11}$$

which will come handy in many situations.

Remark 12.9.2 Notice that this can be rewritten as a matrix-equation:

- We introduce the matrix $\Xi_{\alpha,\alpha'} \equiv \delta_{\alpha,\alpha'}\xi_\alpha$ and correspondingly we define the matrix-valued distributions

$$\mathbf{n}^\zeta_\beta(\boldsymbol{\Xi}) \equiv \left(\mathbf{n}^\zeta_\beta(\boldsymbol{\Xi})\right)_{\alpha,\alpha'} = \delta_{\alpha,\alpha'}\,\mathrm{n}^\zeta_\beta(\xi_\alpha), \qquad \boldsymbol{\delta}(\omega\mathbf{1}-\boldsymbol{\Xi}/\hbar) \equiv (\boldsymbol{\delta}(\omega\mathbf{1}-\boldsymbol{\Xi}/\hbar))_{\alpha,\alpha'} = \delta_{\alpha,\alpha'}\delta(\omega-\xi_\alpha/\hbar) \tag{12.12}$$

- and matrix-valued notation

$$\left[\left((\omega\pm\mathrm{i}\epsilon)\mathbf{1}-\frac{\boldsymbol{\Xi}}{\hbar}\right)^{-1}\right]_{\alpha,\alpha'} = \frac{\delta_{\alpha,\alpha'}}{\omega\pm\mathrm{i}\epsilon-\xi_\alpha/\hbar} \tag{12.13}$$

Corollary 12.10 Introducing the matrix-notation as above we find

$$\begin{aligned}
\mathbf{G}_0^{\mathbb{T}}(t) &= -\frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}t\Xi/\hbar}\left[\theta(t)\left(\mathbf{1}+\zeta\,\mathbf{n}_\beta^\zeta(\Xi)\right)+\theta(-t)\zeta\mathbf{n}_\beta^\zeta(\Xi)\right], & \boldsymbol{G}_0^{\mathbb{T}}(\omega) &= +\frac{1}{\hbar}\lim_{\epsilon\to 0}\frac{1+\zeta\mathrm{n}_{\hbar\beta}^\zeta(\omega)}{(\omega+\mathrm{i}\epsilon)\mathbf{1}-\Xi/\hbar}-\frac{\zeta\mathrm{n}_{\hbar\beta}^\zeta(\omega)}{(\omega-\mathrm{i}\epsilon)\mathbf{1}-\Xi/\hbar},\\
\boldsymbol{G}_0^{<}(t) &= -\frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}t\Xi/\hbar}\zeta\mathbf{n}_\beta^\zeta(\Xi), & \boldsymbol{G}_0^{<}(\omega) &= -\frac{\mathrm{i}}{\hbar}\zeta\mathbf{n}_\beta^\zeta(\Xi)2\pi\boldsymbol{\delta}(\omega\mathbf{1}-\Xi/\hbar),\\
\boldsymbol{G}_0^{>}(t) &= -\frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}t\Xi/\hbar}\left(\mathbf{1}+\zeta\,\mathbf{n}_\beta^\zeta(\Xi)\right), & \boldsymbol{G}_0^{>}(\omega) &= -\frac{\mathrm{i}}{\hbar}\left(\mathbf{1}+\zeta\,\mathbf{n}_\beta^\zeta(\Xi)\right)2\pi\boldsymbol{\delta}(\omega\mathbf{1}-\Xi/\hbar),\\
\boldsymbol{G}_0^{\overline{\mathbb{T}}}(t) &= -\frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}t\Xi/\hbar}\left[\theta(-t)\left(\mathbf{1}+\zeta\,\mathrm{n}_\beta^\zeta(\Xi)\right)+\theta(+t)\zeta\mathrm{n}_\beta^\zeta(\Xi)\right], & \boldsymbol{G}_0^{\overline{\mathbb{T}}}(\omega) &= +\frac{1}{\hbar}\lim_{\epsilon\to 0}-\frac{1+\zeta\mathrm{n}_{\hbar\beta}^\zeta(\omega)}{(\omega-\mathrm{i}\epsilon)\mathbf{1}-\Xi/\hbar}+\frac{\zeta\mathrm{n}_{\hbar\beta}^\zeta(\omega)}{(\omega+\mathrm{i}\epsilon)\mathbf{1}-\Xi/\hbar},\\
\boldsymbol{G}_0^{\mathrm{ret}}(t) &= -\frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}t\Xi/\hbar}\theta(t), & \boldsymbol{G}_0^{\mathrm{ret}}(\omega+\mathrm{i}\epsilon) &= +\frac{1}{\hbar}\frac{1}{(\omega+\mathrm{i}\epsilon)\mathbf{1}-\Xi/\hbar},\\
\boldsymbol{G}_0^{\mathrm{adv}}(t) &= -\frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}t\Xi/\hbar}\theta(-t), & \boldsymbol{G}_0^{\mathrm{adv}}(\omega-\mathrm{i}\epsilon) &= +\frac{1}{\hbar}\frac{1}{(\omega-\mathrm{i}\epsilon)\mathbf{1}-\Xi/\hbar}.
\end{aligned} \tag{12.14}$$

Proof 12.10 Follows from applying the matrix-identities.

Example: A Non-Diagonal Gas with Nature η and Statistics ζ

We consider the system from Definition 8.29.

Hypothesis 12.11 A direct (analytical) computation of all the individual Green-functions from the definition is (to the authors knowledge) impossible (unless one is referring to the matrices that diagonalize the Hamiltonian). One can however determine the individual Green-functions by first determining the Matsubara- or the imaginary time Green-function and subsequently using Green's chart (Figure 14.2) to determine the individual Green-functions.

Fermionic Examples

Example: A Spin-$\frac{1}{2}$-Particle

We consider the system from Definition 8.26. Notice that this is an obvious special case of the system considered in [26].

Fact 12.12 We can compute the Green-functions of this system very efficiently, by combining Corollaries 12.8 and 12.10. To this end, we only need to find the transformation matrices that diagonalize the Hamiltonian.

Lemma 12.13 In order to find the eigenvalues of

$$H \equiv \begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix}^\dagger \begin{pmatrix} \epsilon_0+\epsilon_1^z & -\mathrm{i}\epsilon_1^y+\epsilon_1^x \\ +\mathrm{i}\epsilon_1^y+\epsilon_1^x & \epsilon_0-\epsilon_1^z \end{pmatrix} \begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix} \tag{12.15}$$

it suffices to find the eigenvalues of the matrix

$$h = \begin{pmatrix} n_z & -\mathrm{i}n_y+n_x \\ +\mathrm{i}n_y+n_x & -n_z \end{pmatrix}, \quad \text{with } \vec{n} = \boldsymbol{\epsilon}/\epsilon \in \mathrm{S}^2\,. \tag{12.16}$$

Proof 12.13 See Appendix, Proofs, page 525.

Fact 12.14 The unit-vector $\mathbf{n}$ can be expressed in spherical coordinates $(r, \phi, \theta) \in 1 \times (0, 2\pi) \times (0, \pi)$ as:

$$\mathbf{n} = \begin{pmatrix} \cos(\phi)\sin(\theta) \\ \sin(\phi)\sin(\theta) \\ \cos(\theta) \end{pmatrix}.$$

Lemma 12.15 The matrix

$$h = \begin{pmatrix} n_z & -\mathrm{i}n_y + n_x \\ +\mathrm{i}n_y + n_x & -n_z \end{pmatrix}, \quad \text{with } |\vec{n}| = 1. \tag{12.17}$$

possesses the eigenvalues ± 1 with eigenvectors

$$|\uparrow_n\rangle = \cos\frac{\theta}{2}|\uparrow\rangle + \sin\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\phi}|\downarrow\rangle, \qquad |\downarrow_n\rangle = \sin\frac{\theta}{2}|\uparrow\rangle - \cos\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\phi}|\downarrow\rangle \tag{12.18}$$

whereas

$$\left\{ |\uparrow\rangle \equiv \mathbf{e}_x = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |\downarrow\rangle \equiv \mathbf{e}_y = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\} \subset \mathbb{R}^2$$

represent the eigenstates of the third Pauli-matrix.

Proof 12.15 See Appendix, Proofs, page 525.

Corollary 12.16 It follows

$$|\uparrow\rangle = \cos\frac{\theta}{2}|\uparrow_n\rangle + \sin\frac{\theta}{2}|\downarrow_n\rangle, \qquad |\downarrow\rangle = \sin\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\phi}|\uparrow_n\rangle - \cos\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\phi}|\downarrow_n\rangle$$

Proof 12.16 See Appendix, Proofs, page 527.

Remark 12.16.1 Notice that we obtain for the corresponding creation- (and annihilation-) operators

$$c_\uparrow = \cos\frac{\theta}{2}c_{\uparrow_n} + \sin\frac{\theta}{2}c_{\downarrow_n}, \qquad c_\downarrow = \sin\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\phi}c_{\uparrow_n} - \cos\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\phi}c_{\downarrow_n}$$

whereas we denote $c_{\uparrow_n} \equiv c_{\uparrow_n}$ etc for notational convenience.

Remark 12.16.2 Since this is a unitary transformation, these new operators $\left\{ c_{\sigma_n}, c^\dagger_{\sigma_n} \right\}_{\sigma\in\{\downarrow,\uparrow\}}$ also obey the CAR.

Remark 12.16.3 Notice that we have now found the spectral decomposition of the Hamiltonian

$$H = \sum_{\sigma\in\{\uparrow,\downarrow\}} E_\sigma c^\dagger_{\sigma_n} c_{\sigma_n} \tag{12.19}$$

with $E_\sigma \equiv \epsilon_0 \pm \epsilon$ and we write as usual $\xi_\sigma \equiv E_\sigma - \mu$.

Remark 12.16.4 It follows from Lemma 8.28 for the grand-canonical-time-evolution

$$c_{\sigma_n}(t) = \mathrm{e}^{-\mathrm{i}\xi_\sigma t/\hbar} c_{\sigma_n}, \qquad c^\dagger_{\sigma_n}(t) = \mathrm{e}^{+\mathrm{i}\xi_\sigma t/\hbar} c^\dagger_{\sigma_n}$$

Fact 12.17 We can now use Corollary 12.8 by remarking that the expansion in Equation (12.7) is represented exactly through the one in Equation (12.18). This gives us the unitary transformation-matrix

$$U = \begin{pmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\phi} \\ \sin\frac{\theta}{2} & -\cos\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\phi} \end{pmatrix} \quad \Longleftrightarrow \quad U^\dagger = \begin{pmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2} \\ \sin\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\phi} & -\cos\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\phi} \end{pmatrix} \tag{12.20}$$

it is therefore sufficient to determine the individual Green-functions in the diagonal basis. For this, we can refer to Theorem 12.9.

Remark 12.17.1 Notice that we could have also computed the individual Green-functions in the "pedestrian-way". This is elaborated in the Appendix, subsection 29.11.

12.3. Phononic Displacement-Green-Functions without Periodicity

We consider ...

- either the system from Remark 8.28.4 (which represents a special case from the system in Definition 8.27),
- or the system from Remark 8.31.2 (which represents a special case from the system in Definition 8.31),
- or the phononic part of the system from Definitions 8.35, 8.36, 8.39, 8.40
- or reasonable generalizations or special cases of these systems.

Notice that we have $\zeta = +1$ and $\eta = 0$ for all of these systems.

Definition 12.18 For $\nu \in \{1, \dots, rd_{\mathbf{x}}\}$ and $\mathbf{q} \in \mathrm{Q}$, we introduce the *phononic-displacement-operator* $A_\nu(\mathbf{q})$ as

$$A_\nu(\mathbf{q}) = c_\nu(\mathbf{q}) + c_\nu^\dagger(-\mathbf{q}). \tag{12.21}$$

Remark 12.18.1 Notice that it is a little bit *misleading* to call these objects displacement / position-operators, since in Lemma 5.29, in particular in Equation (5.41) we see that there are prefactors missing. However... This notation is all over the literature, which is why we will also stick to it, leaving it with this word of warning.

Remark 12.18.2 Notice that $A_\nu(\mathbf{q}) = A_\nu^\dagger(-\mathbf{q}) \iff A_\nu(-\mathbf{q}) = A_\nu^\dagger(\mathbf{q})$

Definition 12.19 We consider $X = A_\nu(\mathbf{q})$ and $X' = A_{\nu'}^\dagger(\mathbf{q}')$ for multi-indices

$$(\alpha, t) \equiv (\mathbf{q}, \nu, t) \in \mathrm{Q} \times \{1, \dots, rd_{\mathbf{x}}\} \times \mathbb{R} \tag{12.22}$$

we introduce the different *real-time-[D]isplacement-Green-functions*[5]

$$\begin{aligned}
&\bullet\ D(A, A') \equiv D^{++}(A, A') \equiv D^{\mathbb{T}}(A, A') \equiv -\frac{\mathrm{i}}{\hbar} \left\langle \mathrm{T}_t\, A_\alpha(t) A_{\alpha'}^\dagger(t') \right\rangle, \\
&\bullet\ D^{+-}(A, A') \equiv D^{<}(A, A') \equiv -\frac{\mathrm{i}}{\hbar} \left\langle A_{\alpha'}^\dagger(t') A_\alpha(t) \right\rangle, \\
&\bullet\ D^{-+}(A, A') \equiv D^{>}(A, A') \equiv -\frac{\mathrm{i}}{\hbar} \left\langle A_\alpha(t) A_{\alpha'}^\dagger(t') \right\rangle, \\
&\bullet\ D^{--}(A, A') \equiv D^{\overline{\mathbb{T}}}(A, A') \equiv -\frac{\mathrm{i}}{\hbar} \left\langle \overline{\mathrm{T}}_t A_\alpha(t) A_{\alpha'}^\dagger(t') \right\rangle, \\
&\bullet\ D^{\mathrm{ret}}(A, A') = -\frac{\mathrm{i}}{\hbar} \theta(t - t') \left\langle \left[A_\alpha(t),\ A_{\alpha'}^\dagger(t') \right] \right\rangle, \\
&\bullet\ D^{\mathrm{adv}}(A, A') = +\frac{\mathrm{i}}{\hbar} \theta(t' - t) \left\langle \left[A_\alpha(t),\ A_{\alpha'}^\dagger(t') \right] \right\rangle,
\end{aligned}$$

with canonical time-evolution-operator as usual.

[5] Cf. Cuevas p. 233 vs Mahan p. 99 and Negele p. 245, whereas there is a typo (missing minus-sign) in the first literature.

Remark 12.19.1 The fact that this is a reasonable definition is far from obvious and will be discussed further later on. See also Remark 13.9.1.

Remark 12.19.2 Since these Green-functions represent a special usecase of Lemma 12.3 one also obtains (in the stationary states) the simplifcation for the temporal argument

$$D^{\blacksquare}_{\nu,\nu'}\left(t,\mathbf{q}\,|\,t',\mathbf{q}'\right) \equiv D^{\blacksquare}_{\substack{\mathbf{q},\mathbf{q}'\\ \nu,\nu'}}\left(t\,|\,t'\right) \equiv D^{\blacksquare}_{\substack{\mathbf{q},\mathbf{q}'\\ \nu,\nu'}}\left(t-t',0\right) \equiv D^{\blacksquare}_{\substack{\mathbf{q},\mathbf{q}'\\ \nu,\nu'}}\left(t-t'\right) \tag{12.23}$$

Remark 12.19.3 In Chapter 18 we will see (i.e. *prove*), that due to the translation-invariance of crystals, typical Hamiltonians, as the ones in Equations (8.30), (8.34), (8.42), (8.43), one obtains phononic Green-functions which are *diagonal in the crystal-momentum*, implying that one can write

$$D^{\blacksquare}(A,A') \equiv D^{\blacksquare}_{\nu,\nu'}\left(t,\mathbf{q}\,|\,t',\mathbf{q}'\right) = \delta_{\mathbf{q},\mathbf{q}'} D^{\blacksquare}_{\nu,\nu'}\left(t,\mathbf{q}\,|\,t',\mathbf{q}'\right) \equiv \delta_{\mathbf{q},\mathbf{q}'} D^{\blacksquare}_{\substack{\mathbf{q}\\ \nu,\nu'}}\left(t\,|\,t'\right) \tag{12.24}$$

Since these Green-functions represent a special usecase of Lemma 12.3 one also obtains (in the stationary states) the further simplifcation

$$D^{\blacksquare}(A,A') \equiv \delta_{\mathbf{q},\mathbf{q}'} D^{\blacksquare}_{\substack{\mathbf{q}\\ \nu,\nu'}}\left(t\,|\,t'\right) \equiv \delta_{\mathbf{q},\mathbf{q}'} D^{\blacksquare}_{\substack{\mathbf{q}\\ \nu,\nu'}}\left(t-t',0\right) \equiv \delta_{\mathbf{q},\mathbf{q}'} D^{\blacksquare}_{\substack{\mathbf{q}\\ \nu,\nu'}}\left(t-t'\right) \tag{12.25}$$

Remark 12.19.4 In [44], page 66, it is elaborated, that the free phonon Green-functions obey in the so-called "position basis" (to be introduced later) common differential equations.

Example: A Diagonal Phonon Gas

We consider the system Remark 8.28.4 (which represents a special case from the system in Definition 8.27).

Fact 12.20 Notice first that due to the structure of the non-interacting Hamiltonian the phononic Green-functions are diagonal in the branches, i.e.

$$D^{\blacksquare}_{\substack{\mathbf{q}\\ \nu,\nu'}}(t) \equiv \delta_{\nu,\nu'} D^{\blacksquare}_{\mathbf{q}\nu}(t) \tag{12.26}$$

Theorem 12.21 It follows[6]

$$
\begin{aligned}
D^{\mathbb{T}}_{\substack{0\\ \alpha,\alpha'}}(t) &= -\frac{\mathrm{i}}{\hbar}\delta_{\nu,\nu'}\delta_{\mathbf{q},\mathbf{q}'}\sum_{\sigma\in\{+,-\}}\theta(\sigma t)\Big[\left(1+\mathrm{B}_{\hbar\beta}(\omega_{\mathbf{q}\nu})\right)\mathrm{e}^{-\sigma\omega_{\mathbf{q}\nu}\mathrm{i}t}+\mathrm{B}_{\hbar\beta}(\omega_{\mathbf{q}\nu})\mathrm{e}^{+\sigma\omega_{\mathbf{q}\nu}\mathrm{i}t}\Big], & D^{\mathbb{T}}_{\substack{0\\ \alpha,\alpha'}}(\omega) &= +\frac{1}{\hbar}\delta_{\nu,\nu'}\delta_{\mathbf{q},\mathbf{q}'}\lim_{\eta\to 0^+}\sum_{\sigma\in\{+,-\}}\left[\sigma\frac{\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})+1}{\omega-\sigma\omega_{\mathbf{q}\nu}+\sigma\mathrm{i}\eta}+\sigma\frac{\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})}{\omega+\sigma\omega_{\mathbf{q}\nu}+\sigma\mathrm{i}\eta}\right],\\
D^{<}_{\substack{0\\ \alpha,\alpha'}}(t) &= -\frac{\mathrm{i}}{\hbar}\delta_{\nu,\nu'}\delta_{\mathbf{q},\mathbf{q}'}\left[\left(\mathrm{B}_{\beta}(\Omega_{\mathbf{q}\nu})+1\right)e^{+\mathrm{i}\omega_{\mathbf{q}\nu}t}+\mathrm{B}_{\beta}(\Omega_{\mathbf{q}\nu})e^{-\mathrm{i}\omega_{\mathbf{q}\nu}t}\right], & D^{<}_{\substack{0\\ \alpha,\alpha'}}(\omega) &= -\frac{\mathrm{i}}{\hbar}\delta_{\nu,\nu'}\delta_{\mathbf{q},\mathbf{q}'}2\pi\Big[\left(\mathrm{B}_{\hbar\beta}(\omega_{\mathbf{q}\nu})+1\right)\delta(\omega+\omega_{\mathbf{q}\nu})+\mathrm{B}_{\hbar\beta}(\omega_{\mathbf{q}\nu})\delta(\omega-\omega_{\mathbf{q}\nu})\Big],\\
D^{>}_{\substack{0\\ \alpha,\alpha'}}(t) &= -\frac{\mathrm{i}}{\hbar}\delta_{\nu,\nu'}\delta_{\mathbf{q},\mathbf{q}'}\left[\left(\mathrm{B}_{\beta}(\omega_{\mathbf{q}\nu})+1\right)e^{-\mathrm{i}\omega_{\mathbf{q}\nu}t}+\mathrm{B}_{\beta}(\omega_{\mathbf{q}\nu})e^{+\mathrm{i}\omega_{\mathbf{q}\nu}t}\right], & D^{>}_{\substack{0\\ \alpha,\alpha'}}(\omega) &= -\frac{\mathrm{i}}{\hbar}\delta_{\nu,\nu'}\delta_{\mathbf{q},\mathbf{q}'}2\pi\Big[\left(\mathrm{B}_{\hbar\beta}(\omega_{\mathbf{q}\nu})+1\right)\delta(\omega-\omega_{\mathbf{q}\nu})+\mathrm{B}_{\hbar\beta}(\omega_{\mathbf{q}\nu})\delta(\omega+\omega_{\mathbf{q}\nu})\Big],\\
D^{\overline{\mathbb{T}}}_{\substack{0\\ \alpha,\alpha'}}(t) &= -\frac{\mathrm{i}}{\hbar}\delta_{\nu,\nu'}\delta_{\mathbf{q},\mathbf{q}'}\sum_{\sigma\in\{+,-\}}\theta(-\sigma t)\Big[\left(1+\mathrm{B}_{\hbar\beta}(\omega_{\mathbf{q}\nu})\right)\mathrm{e}^{-\sigma\omega_{\mathbf{q}\nu}\mathrm{i}t}+\mathrm{B}_{\hbar\beta}(\omega_{\mathbf{q}\nu})\mathrm{e}^{+\sigma\omega_{\mathbf{q}\nu}\mathrm{i}t}\Big], & D^{\overline{\mathbb{T}}}_{\substack{0\\ \alpha,\alpha'}}(\omega) &= +\frac{1}{\hbar}\delta_{\nu,\nu'}\delta_{\mathbf{q},\mathbf{q}'}\lim_{\eta\to 0^+}\sum_{\sigma\in\{+,-\}}\left[\sigma\frac{\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})}{\omega-\sigma\omega_{\mathbf{q}\nu}+\sigma\mathrm{i}\eta}+\sigma\frac{\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})+1}{\omega+\sigma\omega_{\mathbf{q}\nu}+\sigma\mathrm{i}\eta}\right],\\
D^{\mathrm{ret}}_{\substack{0\\ \alpha,\alpha'}}(t) &= -\frac{2}{\hbar}\delta_{\nu,\nu'}\delta_{\mathbf{q},\mathbf{q}'}\theta(+t)\sin\left(\omega_{\mathbf{q}\nu}t\right), & D^{\mathrm{ret}}_{\substack{0\\ \alpha,\alpha'}}(\omega+\mathrm{i}\epsilon) &= +\frac{1}{\hbar}\delta_{\nu,\nu'}\delta_{\mathbf{q},\mathbf{q}'}\frac{2\omega_{\nu}(\mathbf{q})}{(\omega+\mathrm{i}\epsilon)^2-\omega_{\nu}^2(\mathbf{q})},\\
D^{\mathrm{adv}}_{\substack{0\\ \alpha,\alpha'}}(t) &= +\frac{2}{\hbar}\delta_{\nu,\nu'}\delta_{\mathbf{q},\mathbf{q}'}\theta(-t)\sin\left(\omega_{\mathbf{q}\nu}t\right), & D^{\mathrm{adv}}_{\substack{0\\ \alpha,\alpha'}}(\omega-\mathrm{i}\epsilon) &= +\frac{1}{\hbar}\delta_{\nu,\nu'}\delta_{\mathbf{q},\mathbf{q}'}\frac{2\omega_{\nu}(\mathbf{q})}{(\omega-\mathrm{i}\epsilon)^2-\omega_{\nu}^2(\mathbf{q})}.
\end{aligned}
\tag{12.27}
$$

Proof 12.21 See Appendix, Proofs, page 528.

[6] Notice that we have a different sign than in the literature [32] page 99 for the advanced Green-function $D^{\mathrm{adv}}_{\mathbf{q}\nu}(t)$. Notice apart from this typo from Mahan, our results are in harmony with the literature: For D^{ret} and $D^{<}$: See [23] page 73 and also [32] page 116 with Wick-transformation.

13. Imaginary-Time-Two-Operator-Green-Functions at Finite Temperature

13.1. Two-Operator Green-Functions with Periodicity

Definition 13.1 For a pair of two operators (X, X') and some imaginary time $\tau \in \mathbb{R}$ we define the *imaginary-time two-operator Green-function* in its various shapes

$$\begin{aligned}\mathscr{G}_{X,X'}(\tau,\tau') &\equiv -\frac{1}{\hbar}\left\langle \mathrm{T}_\tau\, X(\tau)\, X'(\tau')\right\rangle \\ &\equiv -\frac{1}{\hbar}\frac{\mathrm{Tr}_{\mathscr{H}}\, \mathrm{e}^{-\beta\Xi}\, \mathrm{T}_\tau\, X(\tau)\, X'(\tau')}{\mathrm{Tr}_{\mathscr{H}}\, \mathrm{e}^{-\beta\Xi}} \\ &\equiv -\frac{1}{\hbar}\frac{\mathrm{Tr}_{\mathscr{H}}\, \mathrm{e}^{-\beta\Xi}\Big[\theta(\tau-\tau')\, X(\tau)\, X'(\tau') + S_{X,X'}\,\theta(\tau'-\tau)\, X'(\tau')\, X(\tau)\Big]}{\mathrm{Tr}_{\mathscr{H}}\, \mathrm{e}^{-\beta\Xi}}\end{aligned}$$

with imaginary-time-ordering-operator and ensemble-Heisenberg-imaginary-time-evolution as usual.

Theorem 13.2 It follows

$$\mathscr{G}_{X,X'}(\tau,\tau') \equiv \mathscr{G}_{X,X'}(\tau-\tau',0) \equiv \mathscr{G}_{X,X'}(\tau-\tau') \equiv S_{X,X'}\mathscr{G}_{X,X'}(\tau-\tau'+\hbar\beta), \tag{13.1}$$

which implies that the function

$$(-\hbar\beta,\, \hbar\beta) \ni \tau \mapsto \mathscr{G}_{X,X'}(\tau) \in \mathbb{C} \tag{13.2}$$

is periodic.

Proof 13.2 See Appendix, Proofs, page 538

Remark 13.2.1 This periodicity-property is known as the *Kubo-Martin-Schwinger-relation* [37].

Remark 13.2.2 Notice that this implies, with Lemma 1.11, that there exists a Matsubara-Fourier-transformation of the Green-function

$$\mathrm{i}\Omega_{S_{X,X'}} \ni \mathrm{i}\omega_n \mapsto \mathscr{G}_{X,X'}(\mathrm{i}\omega_n) \equiv \int_0^{\hbar\beta} \mathrm{d}\tau\, \mathscr{G}_{X,X'}(\tau)\, \mathrm{e}^{\mathrm{i}\omega_n\tau} \in \mathbb{C}. \tag{13.3}$$

13.2. Pure One-Body Green-Functions with Periodicity

Definition 13.3 We consider $X = c_\alpha$ and $X' = c^\dagger_{\alpha'}$ for multi-indices $A \equiv (\alpha, t) \in \mathscr{A} \times \mathbb{R}$, with

$$\left[c_\alpha, c^\dagger_{\alpha'}\right]_\zeta = \delta_{\alpha,\alpha'}, \qquad \mathrm{S}(c_\alpha) = \mathrm{S}(c^\dagger_{\alpha'}) = \zeta.$$

Then we write for the *imaginary-time one-body Green-function* in its various shapes

$$\mathscr{G}(A, A') \equiv \mathscr{G}_{\alpha,\alpha'}(\tau, \tau') \equiv -\frac{1}{\hbar} \frac{\mathrm{Tr}_{\mathscr{H}}\, \mathrm{e}^{-\beta\Xi}\left[\theta(\tau - \tau')\, c_\alpha(\tau)\, c^\dagger_{\alpha'}(\tau') + \zeta\, \theta(\tau' - \tau)\, c^\dagger_{\alpha'}(\tau')\, c_\alpha(\tau)\right]}{\mathrm{Tr}_{\mathscr{H}}\, \mathrm{e}^{-\beta\Xi}} \tag{13.4}$$

with *imaginary-time*-ordering-operator and ensemble-Heisenberg-imaginary-time-evolution as usual[1]

Theorem 13.4 It follows

$$\mathscr{G}_{\alpha,\alpha'}(\tau, \tau') \equiv \mathscr{G}_{\alpha,\alpha'}(\tau - \tau', 0) \equiv \mathscr{G}_{\alpha,\alpha'}(\tau - \tau') \equiv \zeta \mathscr{G}_{\alpha,\alpha'}(\tau - \tau' + \hbar\beta), \tag{13.5}$$

which implies that the function

$$(-\hbar\beta,\, \hbar\beta) \ni \tau \mapsto \mathscr{G}_{\alpha,\alpha'}(\tau) \in \mathbb{C} \tag{13.6}$$

is periodic.

Proof 13.4 See Appendix, Proofs, page 538

Lemma 13.5 An useful identity is the so-called *equation of motion*

$$\partial_\tau \mathscr{G}_{\alpha\alpha'}(\tau) = -\frac{1}{\hbar}\delta(\tau)\delta_{\alpha,\alpha'} \quad + \quad \frac{1}{\hbar}\left\langle \mathrm{T}_\tau \left[c_\alpha, \frac{\Xi}{\hbar}\right]_{\mathrm{H}}(\tau) c^\dagger_{\alpha'}(0)\right\rangle. \tag{13.7}$$

Proof 13.5 See Appendix, Proofs, page 539

Remark 13.5.1 A common strategy to solve this differential equation is the so-called "integrating-factor method".

[1] Notice that in the imaginary-time case, the creation- and annihilation-operators are no longer complex-conjugates to each other:

$$c_\bullet(\tau) = \mathrm{e}^{\tau(H-\eta\mu N)/\hbar} c_\bullet \mathrm{e}^{-\tau(H-\eta\mu N)/\hbar}, \qquad c^\dagger_\bullet(\tau) = \mathrm{e}^{\tau(H-\eta\mu N)/\hbar} c^\dagger_\bullet \mathrm{e}^{-\tau(H-\eta\mu N)/\hbar}.$$

One of the (in the authors opinion) very few instances where this becomes actually an important subtelty regarding a calculation is, for example, in the derivation of the Eliashberg-equations [35].

Example: Pure, Non-Interacting Systems

Example: A Quantum Dot with Nature η and Statistics ζ

We consider the system from Definition 8.25. The Green-functions of this system can be inferred as a special case of the diagonal gas below.

Example: A Diagonal Gas with Nature η and Statistics ζ

We consider the system from Definition 8.27.

Theorem 13.6 Omitting convergence-generating factors, and introducing the variable $\xi_\alpha \equiv \epsilon_\alpha - \eta\mu$, it follows

$$\mathscr{G}^{\ 0}_{\alpha,\alpha'}(\mathrm{i}\omega_n) = \frac{1}{\hbar}\frac{\delta_{\alpha,\alpha'}}{\mathrm{i}\omega_n - \xi_\alpha/\hbar}, \qquad \mathscr{G}^{\ 0}_{\alpha,\alpha'}(\tau) = -\frac{1}{\hbar}\mathrm{e}^{-\tau\xi_\alpha/\hbar}\delta_{\alpha,\alpha'}\left[\theta(\tau)\left(1+\zeta\ \mathrm{n}^\zeta_\beta(\xi_\alpha)\right) + \theta(-\tau)\,\zeta\ \mathrm{n}^\zeta_\beta(\xi_\alpha)\right]. \tag{13.8}$$

Proof 13.6 See Appendix, Proofs, page 539

Example: A Non-Interacting Gas with Nature η and Statistics ζ

We consider the system from Definition 8.29.

Theorem 13.7 Omitting convergence-generating factors it follows

$$\mathscr{G}^{\ 0}_{\alpha,\alpha'}(\mathrm{i}\omega_n) = \frac{1}{\hbar}\left(\left[\mathrm{i}\omega_n - \frac{H_0-\eta\mu}{\hbar}\right]^{\mathrm{inv}}\right)_{\alpha,\alpha'}, \qquad \mathscr{G}^{\ 0}_{\alpha,\alpha'}(\tau) = \frac{1}{\hbar\beta}\sum_{\omega_n\in\Omega_\zeta}\frac{1}{\hbar}\left(\frac{\mathrm{e}^{-\mathrm{i}\omega_n\tau}}{\mathrm{i}\omega_n - \frac{H_0-\eta\mu}{\hbar}}\right)_{\alpha,\alpha'}. \tag{13.9}$$

Proof 13.7 See Appendix, Proofs, page 540

Remark 13.7.1 Notice that we can write this in matrix-notation as

$$\mathscr{G}_0(\mathrm{i}\omega_n) = \frac{1}{\hbar}\frac{1}{\mathrm{i}\omega_n - \left(H_0-\eta\mu\right)/\hbar} \tag{13.10}$$

Remark 13.7.2 Note that within the proof of this we found the solution of the differential equation[2]

$$\left(\partial_\tau + \frac{H-\eta\mu}{\hbar}\right)\mathscr{G}(\tau) = -\delta(\tau)\,\delta_{\alpha,\alpha'}/\hbar \tag{13.11}$$

with $\mathscr{G}$ defined on the interval $(-\hbar\beta, +\hbar\beta)$, subject to the boundary-condition

$$\mathscr{G}(\tau+\hbar\beta) = -\mathscr{G}(\tau). \tag{13.12}$$

[2] Cf. [38], p. 73 and [6] p. Exercises for Chapter 9

Fermionic Systems

Example: A Spin-$\frac{1}{2}$-Particle

We consider the system from Definition 8.26.

Theorem 13.8 It follows for $\omega_- \neq \omega_+$

$$\mathscr{G}(\tau) = \frac{1}{\hbar}\sum_{k=\pm}\frac{\left(z-(\epsilon_0-\mu)/\hbar\right)\sigma_0+\boldsymbol{\epsilon}\cdot\boldsymbol{\sigma}/\hbar}{\left(z-\omega_+\right)\left(z-\omega_-\right)}\mathrm{e}^{-z\tau}\left(z-\omega_k\right)\mathrm{F}_{\hbar\beta}(z)\Big|_{z=\omega_k}, \qquad \mathscr{G}(\mathrm{i}\omega_n) = \frac{1}{\hbar}\frac{\left(\mathrm{i}\omega_n-\frac{\epsilon_0-\mu}{\hbar}\right)\sigma_0+(\boldsymbol{\epsilon}/\hbar)\cdot\boldsymbol{\sigma}}{\left(\mathrm{i}\omega_n-\omega_+\right)\left(\mathrm{i}\omega_n-\omega_-\right)}, \tag{13.13}$$

with

$$\omega_\xi \equiv \frac{\xi\epsilon+\epsilon_0-\mu}{\hbar} \qquad \text{for } \xi\in\{-,+\}.$$

Proof 13.8 See Appendix, Proofs, page 542

13.3. Phononic Displacement-Green-Functions with Periodicity

We consider ...

- either the system from Remark 8.28.4 (which represents a special case from the system in Definition 8.27),
- or the system from Remark 8.31.2 (which represents a special case from the system in Definition 8.31),
- or the phononic part of the system from Definitions 8.35, 8.36, 8.39, 8.40
- or reasonable generalizations or special cases of these systems.

Notice that we have $\zeta = +1$ and $\eta = 0$ for all of these systems.

Definition 13.9 We consider $X = A_\nu(\mathbf{q})$ and $X' = A^\dagger_{\nu'}(\mathbf{q}')$ for multi-indices

$$(\alpha, \tau) \equiv (\mathbf{q}, \nu, \tau) \in \mathrm{Q} \times \{1, \dots, rd_{\mathbf{x}}\} \times \mathbb{R} \tag{13.14}$$

we introduce the *imaginary-time-[D]isplacement-Green-function* as

$$\mathscr{D}_{\alpha,\alpha'}(\tau, \tau') = -\frac{1}{\hbar} \left\langle \mathrm{T}_\tau \, A_\alpha(\tau) A^\dagger_{\alpha'}(\tau') \right\rangle \quad \Longleftrightarrow \quad \mathscr{D}_{\nu,\nu'}(\tau, \mathbf{q} \mid \tau', \mathbf{q}') = -\frac{1}{\hbar} \left\langle \mathrm{T}_\tau \, A_\nu(\tau, \mathbf{q}) A^\dagger_{\nu'}(\tau', \mathbf{q}') \right\rangle . \tag{13.15}$$

Remark 13.9.1 It is far from obvious that this definition is a reasonable choice for a Green-function. It will turn out however, that this Green-function appears quite naturally in the functional integral formalism of the theory, after one has performed a suitable change of variables resulting in Theorem 29.80. It will also become useful in the discussion of Feynman-diagrams, cf. the proof of Theorem 21.3.

Remark 13.9.2 Analogously to Remark 12.19.2 we obtain with Theorem 13.2 that this Green-function is periodic and only depends on the time-difference, such that we can write

$$\mathscr{D}_{\nu,\nu'}(\tau, \mathbf{q} \mid \tau', \mathbf{q}') \equiv \underset{\nu,\nu'}{\mathscr{D}_{\mathbf{q},\mathbf{q}'}}(\tau, \tau') \equiv \underset{\nu,\nu'}{\mathscr{D}_{\mathbf{q},\mathbf{q}'}}(\tau - \tau') \tag{13.16}$$

and

$$\mathscr{D}_{\alpha,\alpha'}(\tau, \tau') \equiv \mathscr{D}_{\alpha,\alpha'}(\tau - \tau', 0) \equiv \mathscr{D}_{\alpha,\alpha'}(\tau - \tau') = +\mathscr{D}_{\alpha,\alpha'}(\tau - \tau' + \hbar\beta) \tag{13.17}$$

which implies that the function

$$(0, \hbar\beta) \ni \tau \mapsto \mathscr{D}_{\alpha,\alpha'}(\tau) \in \mathbb{C} \tag{13.18}$$

is periodic.

Remark 13.9.3 Analogously to Remark 12.19.3 we promise to prove in the later chapters that one obtains in typical crystalline systems simplifications as

$$\underset{\nu,\nu'}{\mathscr{D}_{\mathbf{q},\mathbf{q}'}}(\tau, \tau') \equiv \delta_{\mathbf{q},\mathbf{q}'} \underset{\nu,\nu'}{\mathscr{D}_{\mathbf{q}}}(\tau, \tau') \tag{13.19}$$

Example: A d-dimensional Phononic Gas

We consider the system from Remark 8.28.4.

Theorem 13.10 It follows

$$\begin{aligned}\mathscr{D}^{\ 0}_{\alpha,\alpha'}(\tau) &= -\frac{1}{\hbar}\delta_{\alpha,\alpha'}\sum_{\nu\in\{+,-\}}\theta(\nu\tau)\Big[\left(1+\mathrm{B}_{\hbar\beta}(\omega_\alpha)\right)\,\mathrm{e}^{-\nu\,\omega_\alpha\tau}+\mathrm{B}_{\hbar\beta}(\omega_\alpha)\,\mathrm{e}^{\nu\,\omega_\alpha\tau}\Big]\\ \mathscr{D}^{\ 0}_{\alpha\alpha'}(\mathrm{i}\omega_n) &= -\frac{1}{\hbar}\frac{2\omega_\alpha\delta_{\alpha,\alpha'}}{\omega_n^2+\omega_\alpha^2}\end{aligned} \tag{13.20}$$

Proof 13.10 See Appendix, Proofs, page 543

Remark 13.10.1 Notice that this can be rewritten using hyperbolic functions[3].

Remark 13.10.2 Notice also, that in the non-interacting case, the periodic standard-continuation of the function is symmetric, i.e. satisfies the equation

$$\mathscr{D}^{\ 0}_{\alpha\alpha'}(\tau) = \mathscr{D}^{\ 0}_{\alpha\alpha'}(-\tau). \tag{13.21}$$

This relation is integral, when one writes down and computes Feynman-diagrams related to electron-phonon theories.

Remark 13.10.3 We now recall that we can rewrite the bare phonon-propagator

$$\mathscr{D}_{0,\nu}(\mathrm{i}\omega_n,\mathbf{q}) = \frac{1}{\hbar}\frac{2\omega_\nu(\mathbf{q})}{(\mathrm{i}\omega_n)^2-\omega_\nu^2(\mathbf{q})} = \frac{1}{\hbar}\int_0^\infty \mathrm{d}\omega\frac{2\omega}{(\mathrm{i}\omega_n)^2-\omega^2}\delta\left(\omega-\omega_\nu(\mathbf{q})\right) \tag{13.22}$$

and therefore conclude, that the electron-phonon coupling-strength contains the phonon-propagator as a factor of the integrand.

Remark 13.10.4 Notice further the decomposition

$$\begin{aligned}\mathscr{D}_{0,\nu}(\mathrm{i}\omega_n,\mathbf{q}) &= -\frac{1}{\hbar}\left(\frac{1}{\mathrm{i}\omega_n-\omega_\nu(\mathbf{q})}-\frac{1}{\mathrm{i}\omega_n+\omega_\nu(\mathbf{q})}\right)\\ &= -\frac{1}{\hbar}\left(\frac{-\mathrm{i}\omega_n-\omega_\nu(\mathbf{q})}{(\mathrm{i}\omega_n)^2-\omega_\nu^2(\mathbf{q})}-\frac{-\mathrm{i}\omega_n+\omega_\nu(\mathbf{q})}{(\mathrm{i}\omega_n)^2-\omega_\nu^2(\mathbf{q})}\right)\\ &= -\frac{1}{\hbar}\frac{2\omega_\nu(\mathbf{q})}{\omega_n^2+\omega_\nu^2(\mathbf{q})}\end{aligned}$$

[3] https://physics.stackexchange.com/questions/202672/free-phonon-propagator-in-imaginary-time?rq=1

which is useful when one has the intention of continuing this expression analytically to the real axis.

Theorem 13.11 The imaginary-time-displacement-Green-function of a phononic gas solves the differential equation

$$\left(\partial_\tau^2 - \omega_\alpha^2\right) \mathscr{D}_{\substack{0 \\ \alpha,\alpha'}}(\tau) = 2\frac{\omega_\alpha}{\hbar}\delta(\tau)\,\delta_{\alpha,\alpha'} \tag{13.23}$$

with $\mathscr{D}$ defined on the interval $(0, +\hbar\beta)$, subject to the boundary-condition

$$\mathscr{D}(\tau + \hbar\beta) = +\mathscr{D}(\tau). \tag{13.24}$$

Proof 13.11 See Appendix, Proofs, page 544

Lemma 13.12 It follows

$$2\langle a^\dagger_{\nu,\mathbf{q}} a_{\nu,\mathbf{q}}\rangle + 1 = \langle A^\dagger_{\nu,\mathbf{q}} A_{\nu,\mathbf{q}}\rangle = \lim_{\epsilon\to 0}\int_{-\infty}^{+\infty} \mathrm{d}\omega\, \mathrm{B}_{\hbar\beta}(\omega)\left(-\frac{\hbar}{\pi}\,\mathrm{Im}\, D^{\mathrm{ret}}_{\substack{\nu,\nu \\ \mathbf{q},\mathbf{q}}}(\omega + \mathrm{i}\epsilon)\right) \tag{13.25}$$

Remark 13.12.1 Notice that this is the diagonal element ($\nu' = \nu$, $\mathbf{q}' = \mathbf{q}$) of the phononic spectral matrix from Section 14.3, and that the prefactor is $\mathrm{d}\omega$, not $\mathrm{d}\omega/(2\pi)$, since the latter would be off by a factor of 2π, as one can check explicitly using Theorem 13.10.

Proof 13.12 See Appendix, Proofs, page 546

14. Lehmann-Representation and more Green-Functions

Notation 14.1 The *Lehmann-representation*, refers to the following algebraic trick: We introduce the exact eigenbasis of the Hamiltonian

$$\mathscr{B} \equiv \{|\,0\,\rangle, |\,1\,\rangle, |\,2\,\rangle, \ldots\} \quad \text{s.t.} \quad \mathscr{H} = \operatorname{span}_{\mathbb{C}} \mathscr{B} \tag{14.1}$$

with eigenvalues

$$\xi_n |\,n\,\rangle \equiv \Xi |\,n\,\rangle \equiv \begin{cases} (H - \eta\mu N)\,|\,n\,\rangle & \text{for systems with nature } \eta \\ \left(H_{\mathrm{p}} - \mu N + H_{\mathrm{w}} + V_{\mathrm{int}}\right)|\,n\,\rangle & \text{for wave-particle-mixtures} \\ \vdots \end{cases} \tag{14.2}$$

Remark 14.1.1 The existence of this basis is guaranteed, if we introduce some cutoff for our basis, since then we have an hermitian operator on a finite dimensional complex vector space.

Remark 14.1.2 Notice that we capture all three cases from Notation 8.1.

Remark 14.1.3 Notice further, that ξ denotes here *not* the non-interacting energies relative to the chemical potential, but the relative energies of the full many body Hamiltonian!

With this eigenbasis, we can now formally derive integral identities that connect the various Green-functions.

Fact 14.2 Recall also the *Sokhotski-Plemelj-theorem* a.k.a. the *Dirac-identity* for integrals over the frequency ω

$$\frac{1}{\omega \pm \mathrm{i}\epsilon + \text{const.}} = \mathrm{P}\,\frac{1}{\omega + \text{const.}} \mp \mathrm{i}\pi\delta(\omega + \text{const.}) \tag{14.3}$$

in the distributional sense for $\epsilon \to 0$.

Proof 14.2 For a fully fleshed proof, see, for example, [17] in the Appendix.

Remark 14.2.1 Notice that in the literature it seems to be quite "popular" to state this identity without any proof. See for example [4] Equation (7.19) or [1] above Equation (7.6) or [30] Equation (31.24), or [39] Equation (3.152), or [12] Equation (1.20), or [32] below Equation (3.115).

14.1. Identities for Two-Operator-Green-Functions

Definition 14.3 For reasons that are difficult to motivate in advance, we introduce the *spectral function corresponding to the operator pair* (X, X') as

$$A_{X,X'}(\omega) \equiv -\frac{\hbar}{\pi} \operatorname{Im} \lim_{\epsilon \to 0} G^{\text{ret}}_{X,X'}(\omega + \mathrm{i}\epsilon). \tag{14.4}$$

Whereas this limit is to be understood in the distributional sense[1].

Remark 14.3.1 Notice that we defined these functions by their frequency-dependencies, and not by their time-dependencies (in constrast to the Green-functions).

Remark 14.3.2 Special cases of this spectral function will correspond to so-called "densities of states" for various systems. We will elaborate on this in the next sections.

Lemma 14.4 With the Lehmann-representation one finds the expansion

$$\mathscr{G}_{X,X'}(\mathrm{i}\omega_l) = \frac{1}{Z} \sum_{(n,m) \in \mathbb{N}^2} \langle n|X|m\rangle\langle m|X'|n\rangle \, \frac{e^{-\beta\xi_n} - S_{X,X'} e^{-\beta\xi_m}}{\hbar} \, \frac{1}{\mathrm{i}\omega_l + (\xi_n - \xi_m)/\hbar} \tag{14.5}$$

and similar identities for all the other Green-functions (and the spectral function).

Proof 14.4 See Appendix, Proofs, page 548

Theorem 14.5 The Matsubara-Green-function can be analytically continued down to the real axis to the retarded / advanced Green-functions as

$$\begin{aligned} \mathrm{i}\omega_n \mapsto \omega + \mathrm{i}\epsilon \quad &\Rightarrow \quad \mathscr{G}_{X,X'}(\mathrm{i}\omega_n) \mapsto G^{\text{ret}}_{X,X'}(\omega + \mathrm{i}\epsilon), \\ \mathrm{i}\omega_n \mapsto \omega - \mathrm{i}\epsilon \quad &\Rightarrow \quad \mathscr{G}_{X,X'}(\mathrm{i}\omega_n) \mapsto G^{\text{adv}}_{X,X'}(\omega - \mathrm{i}\epsilon). \end{aligned}$$

Proof 14.5 Follows immediately from the Lehmann-representations in Eqs. (33.150)-(33.157) and the Carlson-theorem[2].

Theorem 14.6 One also obtains an adapted version of the *Fluctuation-Dissipation-Theorem*:

[1] This means, that this object needs to be integrated over.
[2] Cf. [38].

$$\begin{aligned} G^{<}_{X,X'}(\omega) &= 2\mathrm{i}\ \mathrm{S}_{X,X'}\, \mathrm{n}^{\mathrm{S}_{X,X'}}_{\hbar\beta}(\omega)\, \mathrm{Im} \lim_{\epsilon\to 0} G^{\mathrm{ret}}_{X,X'}(\omega + \mathrm{i}\epsilon), \\ G^{>}_{X,X'}(\omega) &= 2\mathrm{i} \left(1 + \mathrm{S}_{X,X'}\, \mathrm{n}^{\mathrm{S}_{X,X'}}_{\hbar\beta}(\omega)\right) \mathrm{Im} \lim_{\epsilon\to 0} G^{\mathrm{ret}}_{X,X'}(\omega + \mathrm{i}\epsilon). \end{aligned} \tag{14.6}$$

Proof 14.6 See Appendix, Proofs, page 557

Theorem 14.7 One finds the *Lehmann-identities*

$$\begin{aligned} \mathrm{Re}\, G_{X,X'}(\omega) &= +\mathrm{Re}\, G^{\mathrm{ret}}_{X,X'}(\omega) && = +\mathrm{Re}\, G^{\mathrm{adv}}_{X,X'}(\omega), \\ \mathrm{Im}\, G_{X,X'}(\omega) &= +\mathrm{Im}\, G^{\mathrm{ret}}_{X,X'}(\omega) \cdot \left(\tanh \frac{\beta\hbar\omega}{2}\right)^{\mathrm{S}_{X,X'}} && = -\mathrm{Im}\, G^{\mathrm{adv}}_{X,X'}(\omega) \cdot \left(\tanh \frac{\beta\hbar\omega}{2}\right)^{\mathrm{S}_{X,X'}}, \end{aligned} \tag{14.7}$$

Proof 14.7 See Appendix, Proofs, page 558

Theorem 14.8 We conclude the so-called *Kramers-Kronig-relations* a.k.a. *dispersion-relations* as

$$\begin{aligned} \mathrm{Re}\, G^{\mathrm{ret}}_{X,X'}(\omega) &= \frac{1}{\pi} \int \mathrm{d}\omega'\ \mathrm{Im}\, G^{\mathrm{ret}}_{X,X'}(\omega')\, \mathrm{P}\, \frac{1}{\omega' - \omega} \\ \mathrm{Im}\, G^{\mathrm{ret}}_{X,X'}(\omega) &= \frac{1}{\pi} \int \mathrm{d}\omega'\ \mathrm{Re}\, G^{\mathrm{ret}}_{X,X'}(\omega')\, \mathrm{P}\, \frac{1}{\omega' - \omega} \end{aligned}$$

Proof 14.8 See, for example, [4], Equation (7.34).

Remark 14.8.1 There are more identities that one can conclude, for example, by combining the results of this section with Theorem 12.21. See, for example, [32] Equations (3.327) and (3.328) or [48] Equations (4.2.14a) and (4.2.14b). They are however not needed for any further discussions, which is the reason why we omit them.

Theorem 14.9 In the case that $X' = X^\dagger$ we obtain ...

- for $\mathrm{S}_{X,X^\dagger} = -1$ the implication

$$\omega \in \mathbb{R} \quad \Rightarrow \quad 0 < A_{X,X^\dagger}(\omega) \tag{14.8}$$

- for $\mathrm{S}_{X,X^\dagger} = +1$ the implication

$$\omega > 0 \quad \Rightarrow \quad 0 < A_{X,X^\dagger}(\omega) \tag{14.9}$$

Proof 14.9 Follows immediately by combining Remark 8.11.2 with Equation (33.149) since $\exp -\hbar\beta\omega < 1$ for $\omega > 0$.

Remark 14.9.1 We emphasize at this point, something, that is usually swiped under the carpet: In the case of *bosonic* statistics, it is completely fine for a bosonic "density of states" to be *negative* at negative frequencies. There is nothing wrong about this! The *physically reasonable region* however is usually (for example in the case of phonons) at positive frequencies.

We summarize the different identities in *Green's Chart* which graphically depicts how one can determine every two-operator Green-function from the imaginary-time or (inclusive) Matsubara-Green-function.

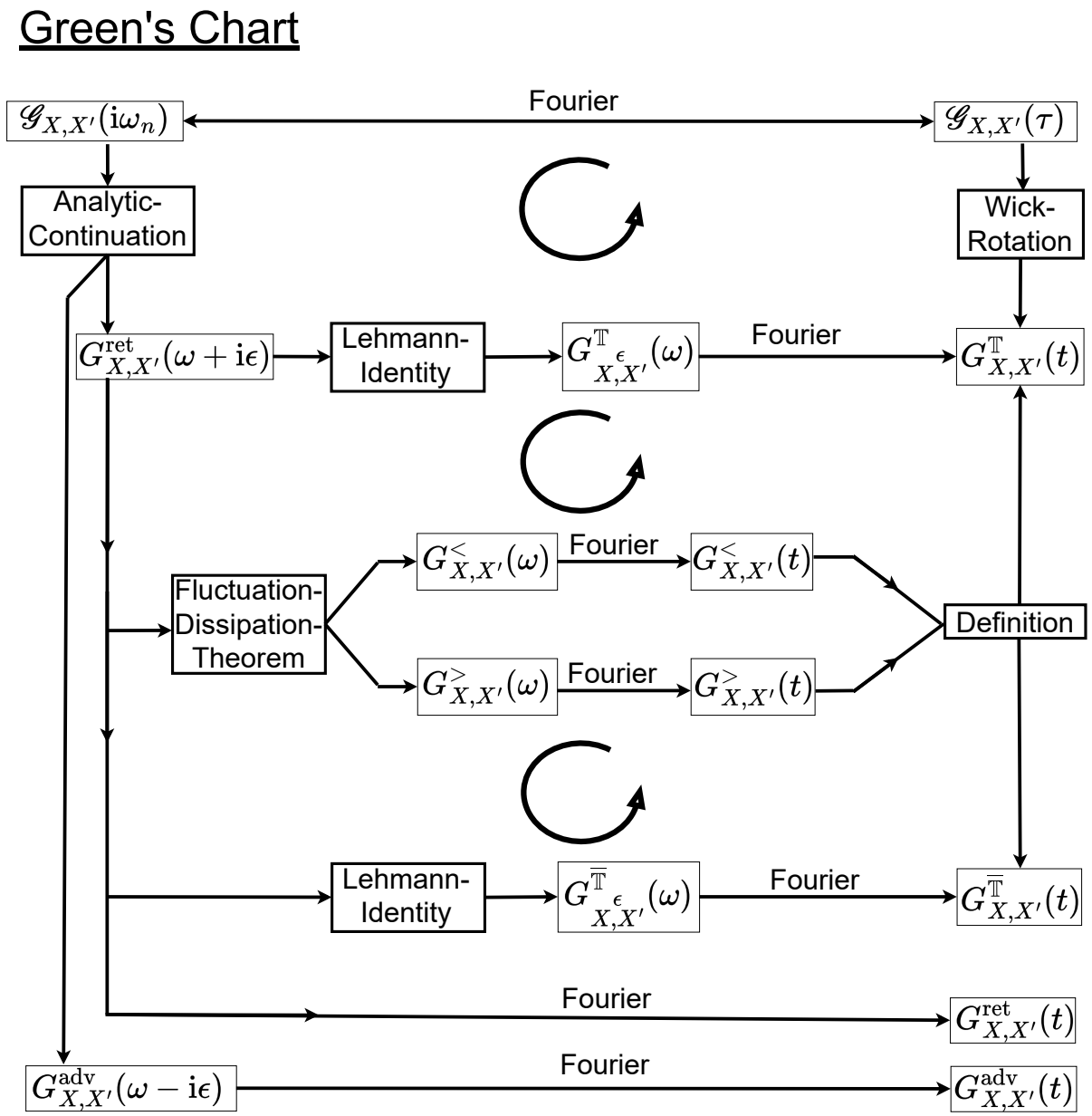


Figure 14.1.: Summarizing the different relationships of the various two-operator Green-functions.

14.2. Identities for Pure One-Body-Green-Functions

In this section, we consider $X = c_\alpha$ and $X' = c^\dagger_{\alpha'}$ for multi-indices $A \equiv (\alpha, t) \in \mathscr{A} \times \mathbb{R}$, with

$$\left[c_\alpha, c^\dagger_{\alpha'}\right]_\zeta = \delta_{\alpha,\alpha'}, \qquad \mathrm{S}(c_\alpha) = \mathrm{S}(c^\dagger_{\alpha'}) = \zeta.$$

Definition 14.10 For reasons that are difficult to motivate in advance, we introduce the *spectral matrix* or the *generalized spectral functions* $A_{\alpha\alpha'}(\omega)$ defined by

$$A_{\alpha\alpha'}(\omega) := -\frac{\hbar}{\pi} \operatorname{Im} \lim_{\epsilon\to 0} G^{\mathrm{ret}}_{\alpha\alpha'}(\omega + \mathrm{i}\epsilon).$$

Whereas this limit is to be understood in the distributional sense[3].

Remark 14.10.1 Notice that we defined these functions by their frequency-dependencies, and not by their time-dependencies (in constrast to the Green-functions).

Lemma 14.11 With the Lehmann-representation one finds the expansion

$$\mathscr{G}_{\alpha,\alpha'}(\mathrm{i}\omega_l) = \frac{1}{Z} \sum_{(n,m)\in\mathbb{N}^2} \langle n|c_\alpha|m\rangle\langle m|c^\dagger_{\alpha'}|n\rangle \, \frac{e^{-\beta\xi_n} - \zeta e^{-\beta\xi_m}}{\hbar} \, \frac{1}{\mathrm{i}\omega_l + (\xi_n - \xi_m)/\hbar} \tag{14.10}$$

and similar identities for all the other Green-functions (and the generalized spectral functions).

Proof 14.11 See Appendix, Proofs, page 548

Remark 14.11.1 In the derivation of these identities, it also becomes clear why there will always be the need to introduce convergence-generating factors for some of the Green-functions.

Theorem 14.12 The Matsubara-Green-function can be analytically continued down to the real axis to the retarded / advanced Green-functions as

$$\begin{aligned} \mathrm{i}\omega_n \mapsto \omega + \mathrm{i}\epsilon \quad &\Rightarrow \quad \mathscr{G}_{\alpha,\alpha'}(\mathrm{i}\omega_n) \mapsto G^{\mathrm{ret}}_{\alpha,\alpha'}(\omega + \mathrm{i}\epsilon) \\ \mathrm{i}\omega_n \mapsto \omega - \mathrm{i}\epsilon \quad &\Rightarrow \quad \mathscr{G}_{\alpha,\alpha'}(\mathrm{i}\omega_n) \mapsto G^{\mathrm{adv}}_{\alpha,\alpha'}(\omega - \mathrm{i}\epsilon) \end{aligned}$$

Proof 14.12 Follows immediately from Theorem 14.5.

[3] As explained earlier.

Remark 14.12.1 Notice however, that one has to be a little bit careful when one wants to perform the analytic continuation. The function has to be rewritten w.r.t. simple poles, or functions that decay „fast enough“ at infinity.

Theorem 14.13 The *fluctuation-dissipation-theorem*[4] states the two *Lehmann-identities*

$$\begin{aligned} G^{<}_{\alpha\alpha'}(\omega) &= 2\mathrm{i}\,\zeta\,\mathrm{n}^{\zeta}_{\hbar\beta}(\omega)\,\mathrm{Im}\lim_{\epsilon\to 0} G^{\mathrm{ret}}_{\alpha\alpha'}(\omega+\mathrm{i}\epsilon), \\ G^{>}_{\alpha\alpha'}(\omega) &= 2\mathrm{i}\left(1+\zeta\,\mathrm{n}^{\zeta}_{\hbar\beta}(\omega)\right)\mathrm{Im}\lim_{\epsilon\to 0} G^{\mathrm{ret}}_{\alpha\alpha'}(\omega+\mathrm{i}\epsilon). \end{aligned} \tag{14.11}$$

Proof 14.13 Follows from Theorem 14.6.

Lemma 14.14 For a given chemical potential μ, we can compute the average number of particles as

$$\langle N\rangle = \frac{-1}{\pi}\lim_{\epsilon\to 0}\sum\!\!\!\!\!\!\int_{\substack{\alpha\in\mathscr{A}\\ E\in(-\infty,+\infty)}} \mathrm{n}^{\zeta}_{\beta}(E)\ \mathrm{Im}\ G^{\mathrm{ret}}_{\alpha,\alpha}(E+\mathrm{i}\epsilon)$$

Proof 14.14 See Appendix, Proofs, page 560

Remark 14.14.1 Analogously one can compute the expectation-value for the particle numbers associated to a certain type of state, for example for electrons in a crystal, one can compute the number of spin-up or spin-down electrons. One can also compute the expectation-value of the holes.

Lemma 14.15 The spectral function fulfills the following identities

- $\delta_{\alpha,\alpha'} = \int \mathrm{d}\omega\, A_{\alpha,\alpha'}(\omega)$
- $\mathrm{d} = \int \mathrm{d}\omega\,\mathrm{Tr}\,A(\omega) \equiv \int \mathrm{d}\omega\,\rho(\omega)$
- For fermions ($\zeta = -1$) one finds the density

$$0 < \frac{\mathrm{d}N_{\mathrm{states}}}{\mathrm{d}\omega} \equiv \rho(\omega) \equiv \mathrm{Tr}\,A(\omega) = -\frac{\hbar}{\pi}\,\mathrm{Im}\lim_{\epsilon\to 0}\mathrm{Tr}\,G^{\mathrm{ret}}(\omega+\mathrm{i}\epsilon) \quad \text{for all } \omega\in\mathbb{R} \tag{14.12}$$

Proof 14.15 See Appendix, Proofs, page 560

Remark 14.15.1 Noting that the spectral function is in the fermionic case positive definite, one usually[5] proposes the interpretation of the spectral function as a *density (of states)* or (after renormalization) *probability-density* by generalizing from the non-interacting case. Although these are, strictly speaking, just single-particle-states, and not many-particle-states, that are being counted when one integrates this object.

[4] In [23], p. 46 the origin of this name is motivated. Another proof is provided (for the fermionic case) in [6] page 136.
[5] Cf. [32], p. 123

Remark 14.15.2 For systems, where the index can be decomposed one can also introduce specific densities. One has additional indices $i \in I$, for example ...

- electronic spin-up and spin-down-component $\mathscr{A} \ni \alpha \equiv (i, \sigma) \in I \times \{\downarrow, \uparrow\}$,
- electronic Wannier-states $\mathscr{A} \ni \alpha \equiv (\mathbf{R}_j, n, i) \in \mathrm{L_f} \times \{1, 2, 3, \ldots\} \times I$,
- electronic Bloch-states $\mathscr{A} \ni \alpha \equiv (\mathbf{k}, n, i) \in \mathrm{Q} \times \{1, 2, 3, \ldots\} \times I$.

Corollary 14.16 Notice that this interpretation allows us, in the fermionic case, to write the expectation-value of the particle-number in the intuitive form

$$\langle N \rangle = \int_{-\infty}^{+\infty} \mathrm{d}E \, \mathrm{F}_\beta(E) \, \rho(E) \tag{14.13}$$

Proof 14.16 Follows immediately from combining the lemmata.

Theorem 14.17 Another useful set of *Lehmann-identities* is

$$\begin{aligned}
\mathrm{Re}\, G^{\ \epsilon}_{\alpha,\alpha'}(\omega) &= +\mathrm{Re}\, G^{\mathrm{ret}}_{\alpha,\alpha'}(\omega + \mathrm{i}\epsilon) &&= +\mathrm{Re}\, G^{\mathrm{adv}}_{\alpha,\alpha'}(\omega - \mathrm{i}\epsilon), \\
\mathrm{Im}\, G^{\ \epsilon}_{\alpha,\alpha'}(\omega) &= +\mathrm{Im}\, G^{\mathrm{ret}}_{\alpha,\alpha'}(\omega + \mathrm{i}\epsilon) \cdot \left(\coth \frac{\beta\hbar\omega}{2} \right)^{\zeta} &&= -\mathrm{Im}\, G^{\mathrm{adv}}_{\alpha,\alpha'}(\omega - \mathrm{i}\epsilon) \cdot \left(\coth \frac{\beta\hbar\omega}{2} \right)^{\zeta},
\end{aligned}$$

in the limit $\epsilon \to 0$.

Proof 14.17 Follows from Theorem 14.7.

We summarize the different identities in *Green's Chart* which graphically depicts how one can determine every one-body Green-function from the imaginary-time or (inclusive) Matsubara-Green-function.

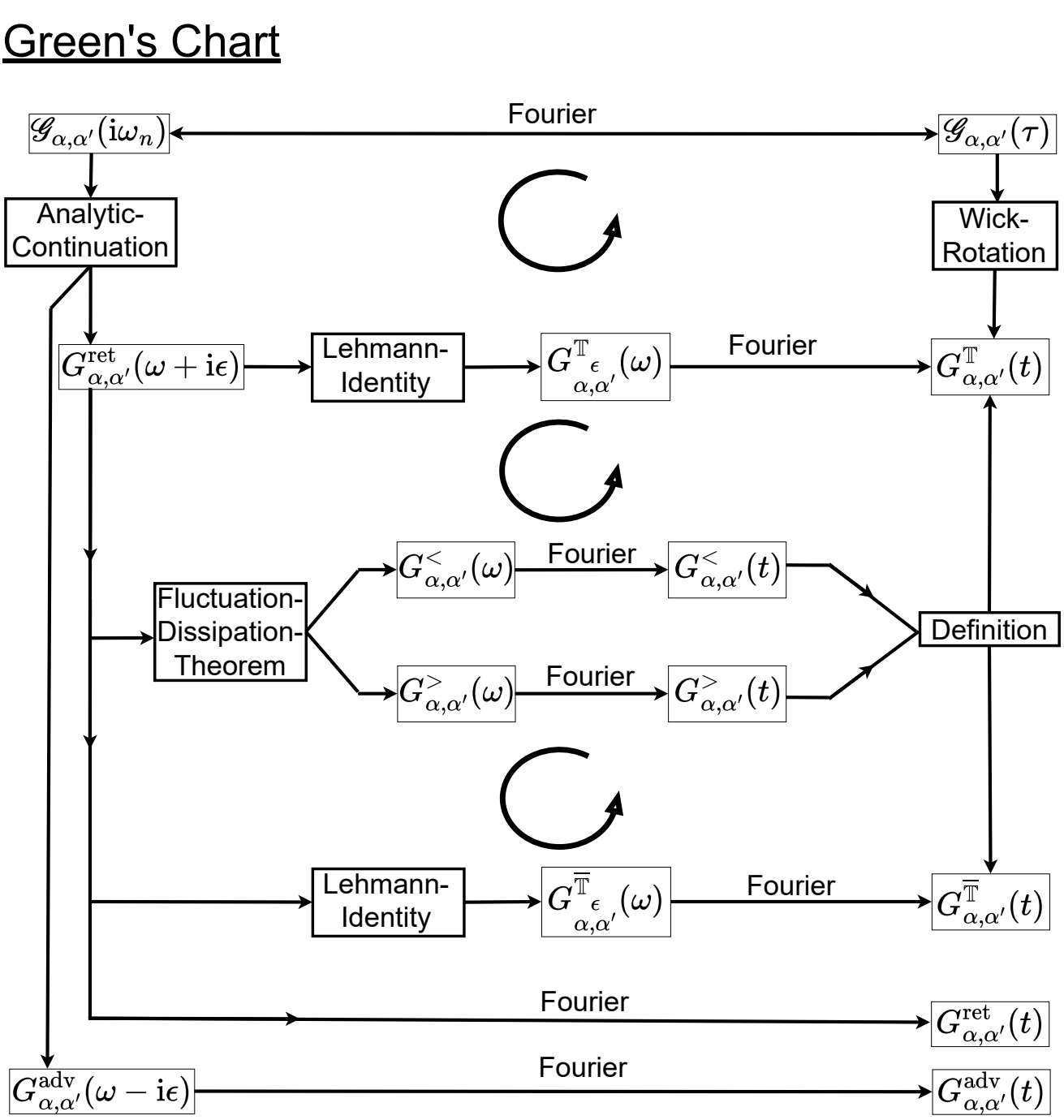


Figure 14.2.: Summarizing the different relationships of the various pure one-body Green-functions.

14.3. Identities for Phononic Displacement-Green-Functions

Definition 14.18 For reasons that are difficult to motivate in advance, we introduce the *phononic spectral matrix* or the *phononic generalized spectral functions* $\underset{\alpha,\alpha'}{\rho}_{\text{ph}}(\omega)$ defined by

$$\underset{\alpha,\alpha'}{\rho}_{\text{ph}}(\omega) \equiv -\frac{\hbar}{\pi} \operatorname{Im} \lim_{\epsilon \to 0} D^{\text{ret}}_{\alpha,\alpha'}(\omega + \mathrm{i}\epsilon).$$

Whereas this limit is to be understood in the distributional sense[6].

Remark 14.18.1 Notice that we defined these functions by their frequency-dependencies, and not by their time-dependencies (in constrast to the Green-functions).

Remark 14.18.2 Notice that emphasizing all the individual indices that are inside this function, it actually reads as

$$\underset{\substack{\nu,\nu' \\ \mathbf{q},\mathbf{q}'}}{\rho}_{\text{ph}}(\omega) \equiv A_{A_\nu(\mathbf{q}),A^\dagger_{\nu'}(\mathbf{q}^\dagger)}(\omega) \equiv -\frac{\hbar}{\pi} \operatorname{Im} \lim_{\epsilon \to 0} \underset{\mathbf{q},\mathbf{q}'}{D^{\text{ret}}_{\nu,\nu'}}(\omega + \mathrm{i}\epsilon).$$

Theorem 14.19 One obtains that

$$0 < \omega \quad \Rightarrow \quad 0 < \underset{\substack{\nu,\nu \\ \mathbf{q},\mathbf{q}}}{\rho}_{\text{ph}}(\omega) \tag{14.14}$$

Proof 14.19 This is simply a special case of Theorem 14.9.

Remark 14.19.1 Notice that the phononic spectral function is only neccessarily positive definite for $\omega > 0$. For frequencies that are smaller than zero it can (from a mathematical perspective) surely happen that it becomes negative, and *there is nothing unphysical about this*, if one restricts the interpretation of it being a probability dsitribution to positive frequencies. It is actually itself *unphysical to even consider negative frequencies* here, since the argument ω corresponds to the oscillation-frequency with which the ions in a crystal are moving.

Remark 14.19.2 Following the literature [32] (page 125), the factor $\mathrm{B}_{\hbar\beta}(\omega)\underset{\substack{\nu,\nu \\ \mathbf{q},\mathbf{q}}}{\rho}_{\text{ph}}(\omega)$ is interpreted as *the temperature-dependent probability of having phonons with crystal-momentum* $\mathbf{q}$ *and frequency* ω *in the branch* ν.

[6] As explained earlier.

Theorem 14.20 The Matsubara-Green-function can be analytically continued down to the real axis to the retarded / advanced Green-functions as

$$\begin{aligned} \mathrm{i}\omega_n \mapsto \omega + \mathrm{i}\epsilon \quad &\Rightarrow \quad \mathscr{D}_{\alpha,\alpha'}(\mathrm{i}\omega_n) \mapsto D^{\mathrm{ret}}_{\alpha,\alpha'}(\omega + \mathrm{i}\epsilon) \\ \mathrm{i}\omega_n \mapsto \omega - \mathrm{i}\epsilon \quad &\Rightarrow \quad \mathscr{D}_{\alpha,\alpha'}(\mathrm{i}\omega_n) \mapsto D^{\mathrm{adv}}_{\alpha,\alpha'}(\omega - \mathrm{i}\epsilon) \end{aligned}$$

Proof 14.20 Follows immediately from Theorem 14.5.

Remark 14.20.1 Notice however, that one has to be a little bit careful when one wants to perform the analytic continuation. The function has to be rewritten w.r.t. simple poles, or functions that decay „fast enough“ at infinity.

Theorem 14.21 The *fluctuation-dissipation-theorem*[7] states the two *Lehmann-identities*

$$\begin{aligned} D^{<}_{\alpha\alpha'}(\omega) &= 2\mathrm{i}\mathrm{B}_{\hbar\beta}(\omega)\,\mathrm{Im}\lim_{\epsilon\to 0} D^{\mathrm{ret}}_{\alpha\alpha'}(\omega + \mathrm{i}\epsilon), \\ D^{>}_{\alpha\alpha'}(\omega) &= 2\mathrm{i}\left(1 + \mathrm{B}_{\hbar\beta}(\omega)\right)\mathrm{Im}\lim_{\epsilon\to 0} D^{\mathrm{ret}}_{\alpha\alpha'}(\omega + \mathrm{i}\epsilon). \end{aligned} \tag{14.15}$$

Proof 14.21 Follows from Theorem 14.6.

Theorem 14.22 Another useful set of *Lehmann-identities* is

$$\begin{aligned} \mathrm{Re}\, D_{\substack{\epsilon \\ \alpha,\alpha'}}(\omega) &= +\mathrm{Re}\, D^{\mathrm{ret}}_{\alpha,\alpha'}(\omega + \mathrm{i}\epsilon) &&= +\mathrm{Re}\, D^{\mathrm{adv}}_{\alpha,\alpha'}(\omega - \mathrm{i}\epsilon), \\ \mathrm{Im}\, D_{\substack{\epsilon \\ \alpha,\alpha'}}(\omega) &= +\mathrm{Im}\, D^{\mathrm{ret}}_{\alpha,\alpha'}(\omega + \mathrm{i}\epsilon) \cdot \coth\frac{\beta\hbar\omega}{2} &&= -\mathrm{Im}\, D^{\mathrm{adv}}_{\alpha,\alpha'}(\omega - \mathrm{i}\epsilon) \cdot \coth\frac{\beta\hbar\omega}{2}, \end{aligned}$$

in the limit $\epsilon \to 0$.

Proof 14.22 Follows from Theorem 14.7.

We summarize the different identities in *Green's Chart* which graphically depicts how one can determine every one-body Green-function from the imaginary-time or (inclusive) Matsubara-Green-function.

[7] In [23], p. 46 the origin of this name is motivated.

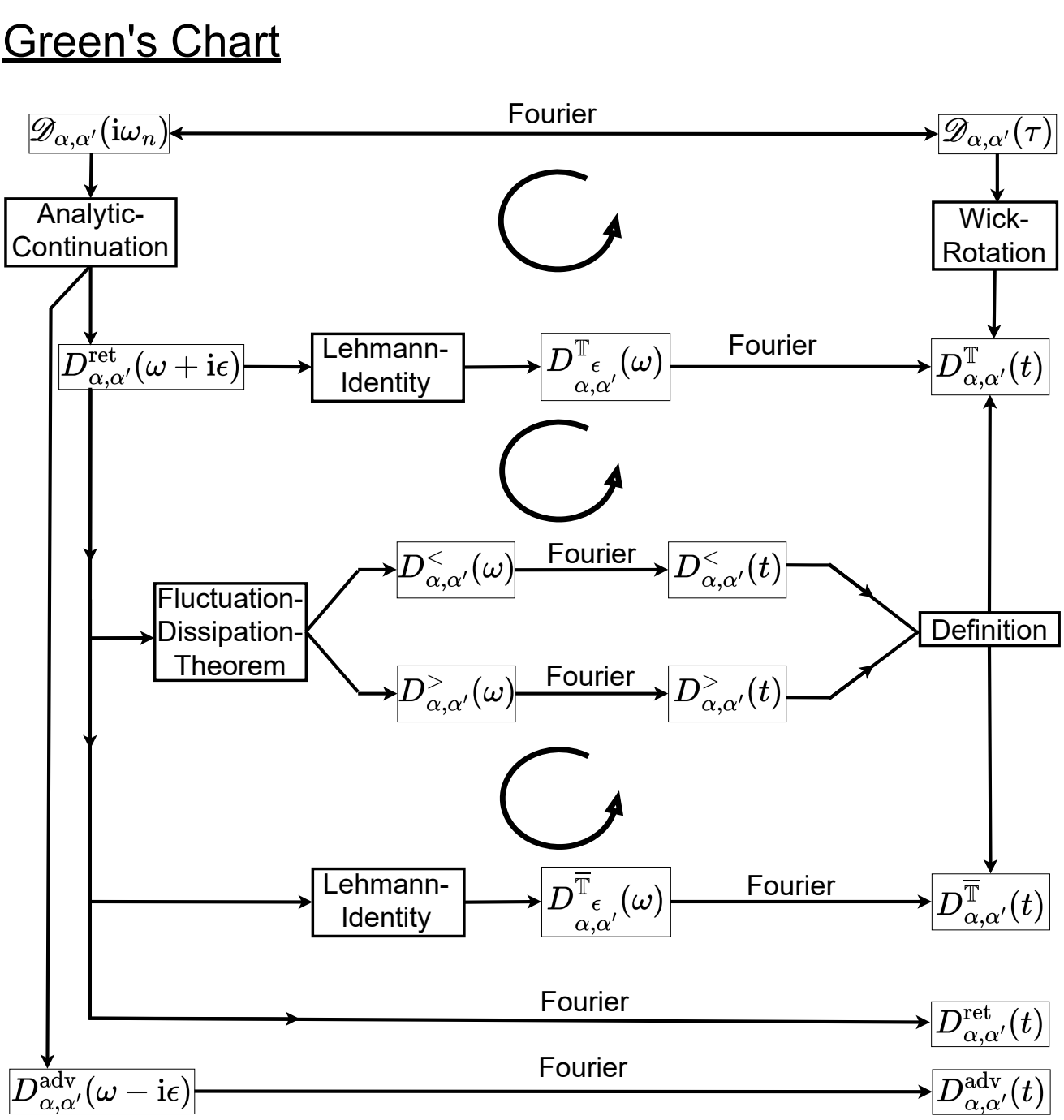


Figure 14.3.: Summarizing the different relationships of the various phononic Green-functions.

14.4. Definitions of Pure n-Body Green-Functions

For reasons that are difficult to motivate in advance, we introduce generalize the one-body Green-functions from Equation (13.4) to n-body Green-functions as follows.

Definition 14.23 We define *real- and imaginary-time n-body Green-functions* as

$$G^n(A_1, \dots A_n \mid A'_n, \dots A'_1) \equiv \left(-\frac{\mathrm{i}}{\hbar}\right)^n \langle \mathrm{T}_t \, c_{\alpha_1}(t_1) \dots c_{\alpha_n}(t_n) \, c^\dagger_{\alpha'_1}(t'_1) \dots c^\dagger_{\alpha'_n}(t'_n) \rangle, \tag{14.16}$$

$$\mathscr{G}^n(A_1, \dots A_n \mid A'_n, \dots A'_1) \equiv \left(-\frac{1}{\hbar}\right)^n \langle \mathrm{T}_\tau \, c_{\alpha_1}(\tau_1) \dots c_{\alpha_n}(\tau_n) \, c^\dagger_{\alpha'_1}(\tau'_1) \dots c^\dagger_{\alpha'_n}(\tau'_n) \rangle. \tag{14.17}$$

Remark 14.23.1 Notice that we use another sign-convention here than Negele and Orland on page 53.

15. Systematic Calculation of Imaginary-Time and Matsubara-Green-Functions for Interacting Systems

15.1. S-Matrix-Expansion for the Two-Operator Green-Functions

In this whole section, we consider a situation as in Equation (10.3) or its mixed system generalization, where the total system is written as

$$H = H_0 + V \quad \Longleftrightarrow \quad \Xi = \Xi_0 + V \tag{15.1}$$

whereas H_0 is a Hamiltonian of which the Green-functions are accessible, and V is a perturbation of some kind.

Definition 15.1 For $\tau \in \mathbb{R}$, we define the *time-evolution operator in the interaction representation* as

$$U_{\text{int}}(\tau) = \mathrm{e}^{\tau\Xi_0/\hbar}\mathrm{e}^{-\tau\Xi/\hbar} \quad \Longleftrightarrow \quad U_{\text{int}}^{-1}(\tau) = \mathrm{e}^{\tau\Xi/\hbar}\mathrm{e}^{-\tau\Xi_0/\hbar} \tag{15.2}$$

Lemma 15.2 We obtain for the derivative of the time-evolution operator in the interaction representation the equation

$$\partial_\tau U_{\text{int}}(\tau) = -\frac{1}{\hbar} V_{\mathrm{H}_{\Xi_0}}(\tau) U_{\text{int}}(\tau) \tag{15.3}$$

Proof 15.2 See Appendix, Proofs, page 561

Corollary 15.3 One can (formally) solve the differential-equation for $U_{\text{int}}(\tau)$ for the boundary condition $U(0) = 1$ with the *time-ordered exponential* as

$$U_{\text{int}} = \sum_{n=0}^{\infty} \left(-\frac{1}{\hbar}\right)^n \frac{1}{n!} \int_0^\tau \mathrm{d}\tau_1 \cdots \int_0^\tau \mathrm{d}\tau_n \, \mathrm{T}_\tau \left[V_{\mathrm{H}_{\Xi_0}}(\tau_1) \dots V_{\mathrm{H}_{\Xi_0}}(\tau_n) \right] \equiv \mathrm{T}_\tau \exp\left[-\frac{1}{\hbar} \int_0^\tau \mathrm{d}\tilde{\tau} \, V_{\mathrm{H}_{\Xi_0}}(\tilde{\tau}) \right] \tag{15.4}$$

Proof 15.3 See Appendix, Proofs, page 561

Lemma 15.4 We can rewrite a two-operator Green-function from Definition 13.1 for $\tau \in (0, \hbar\beta)$ as

$$\begin{aligned}\mathscr{G}_{X,X'}(\tau) &\equiv -\frac{1}{\hbar}\left\langle \mathrm{T}_\tau\, X(\tau)\, X'(0)\right\rangle \\ &= -\frac{1}{\hbar}\frac{\mathrm{Tr}_{\mathscr{H}}\, \mathrm{e}^{-\beta\Xi_0} U_{\mathrm{int}}(\beta) U_{\mathrm{int}}^{-1}(\tau) X_{\mathrm{H}_{\Xi_0}}(\tau)\, U_{\mathrm{int}}(\tau) X'(0)}{\mathrm{Tr}_{\mathscr{H}}\, \mathrm{e}^{-\beta\Xi_0} U(\beta)}\end{aligned} \tag{15.5}$$

Proof 15.4 See Appendix, Proofs, page 561

Definition 15.5 For $\tau_1, \tau_2 \in (0, \hbar\beta)$, we now introduce the *S-matrix* as

$$S(\tau_1, \tau_2) = \mathrm{T}_\tau \exp\left[-\frac{1}{\hbar}\int_{\tau_1}^{\tau_2} \mathrm{d}\tilde{\tau}\, V_{\mathrm{H}_{\Xi_0}}(\tilde{\tau})\right] \tag{15.6}$$

Remark 15.5.1 Notice that we obtain immediately the equality

$$U_{\mathrm{int}}(\tau) = S(\tau, 0) \equiv S(\tau). \tag{15.7}$$

Lemma 15.6 For $\tau_{1,2,3} \in \mathbb{R}$ we obtain the identities

$$S(\tau_2, \tau_1) = U_{\mathrm{int}}(\tau_2) U_{\mathrm{int}}^{-1}(\tau_1), \qquad S(\tau_3, \tau_2) S(\tau_2, \tau_1) = S(\tau_3, \tau_1) \tag{15.8}$$

Proof 15.6 See, for example, [32], page 130.

Theorem 15.7 For $\tau \in (0, \hbar\beta)$ the two-operator Green-function can be rewritten as

$$\mathscr{G}_{X,X'}(\tau) \equiv -\frac{1}{\hbar}\left\langle \mathrm{T}_\tau\, X(\tau)\, X'(0)\right\rangle = -\frac{1}{\hbar}\frac{\left\langle \mathrm{T}_\tau\, S(\beta) X_{\mathrm{H}_{\Xi_0}}(\tau)\, X'_{\mathrm{H}_{\Xi_0}}(0)\right\rangle_0}{\langle S(\beta)\rangle_0} \tag{15.9}$$

Proof 15.7 See Appendix, Proofs, page 562

Corollary 15.8 One finds for $\tau \in (0, \hbar\beta)$ the *S-matrix-expansion of the various Green-functions*

$$\begin{aligned}
\mathscr{G}_{X,X'}(\tau) &= -\frac{1}{\hbar}\frac{\left\langle \mathrm{T}_\tau\, S(\beta) X_{\Xi_0}(\tau) X'_{\Xi_0}(0)\right\rangle_0}{\langle S(\beta)\rangle_0} \\
\mathscr{G}_{\alpha\alpha'}(\tau) &= -\frac{1}{\hbar}\frac{\left\langle \mathrm{T}_\tau\, S(\beta) c_{\alpha\Xi_0}(\tau) c^\dagger_{\alpha'\Xi_0}(0)\right\rangle_0}{\langle S(\beta)\rangle_0} \\
\mathscr{D}_{\alpha\alpha'}(\tau) &= -\frac{1}{\hbar}\frac{\left\langle \mathrm{T}_\tau\, S(\beta) \hat{A}_{\alpha\Xi_0}(\tau) \hat{A}^\dagger_{\alpha'\Xi_0}(0)\right\rangle_0}{\langle S(\beta)\rangle_0}
\end{aligned} \tag{15.10}$$

Proof 15.8 Follows by considering special cases of the Theorem above.

Remark 15.8.1 The S-matrix-expansion of the Green-functions can be derived in a much more straightforward way, by referring to the quantum field theory of the underlying system. We will present this in Equation (16.36).

Remark 15.8.2 Notice a peculiarity here that is oftentimes swiped under the carpet: This expansion holds *only* for $\tau \in (0, \hbar\beta)$, i.e. $\mathscr{G}_{X,X'}(\tau) \equiv \mathscr{G}_{X,X'}(\tau, 0)$, etc. This same peculiarity will re-appear (in the same way!), when we rederive the the imaginary-time correlation-function in the field-integral formalism.

Theorem 15.9 *Wick-Theorem from an operator-formalism.* states that

$$\mathscr{G}^n_0(A_1, \dots A_n \mid A'_1, \dots A'_n) = \begin{vmatrix} \mathscr{G}_0(A_1|A'_1) & \cdots & \mathscr{G}_0(A_1|A'_n) \\ \vdots & \ddots & \vdots \\ \mathscr{G}_0(A_n|A'_1) & \cdots & \mathscr{G}_0(A_n|A'_n) \end{vmatrix}_\zeta . \tag{15.11}$$

Proof 15.9 We refer to [6]: Notice first that Equation (14.17) in our document coincides (up to a factor of $\hbar$) with Equation (10.65) in the literature, and Equation (13.4) in our document coincides (again, up to the factor of $\hbar$) with Equation (10.33b) in the literature. We refer then to section 10.6 in the literature for a proof with the equation of motion technique.

Theorem 15.10 The *linked cluster theorem* states that the formulae in eq. (15.10) can be simplified to

$$\begin{aligned}
\mathscr{G}_{X,X'}(\tau) &= -\frac{1}{\hbar}\sum_{n=0}^{\infty}\left(\frac{-1}{\hbar}\right)^n \int_0^{\hbar\beta} \mathrm{d}\tau_1 \cdots \int_0^{\hbar\beta} \mathrm{d}\tau_n \left\langle \mathrm{T}_\tau\, X_{\Xi_0}(\tau) X'_{\Xi_0}(0) V_{\Xi_0}(\tau_1)\cdots V_{\Xi_0}(\tau_n)\right\rangle_0^{\mathrm{DCD}} \\
\mathscr{G}_{\alpha\alpha'}(\tau) &= -\frac{1}{\hbar}\sum_{n=0}^{\infty}\left(\frac{-1}{\hbar}\right)^n \int_0^{\hbar\beta} \mathrm{d}\tau_1 \cdots \int_0^{\hbar\beta} \mathrm{d}\tau_n \left\langle \mathrm{T}_\tau\, c_{\alpha\Xi_0}(\tau) c^\dagger_{\alpha'\Xi_0}(0) V_{\Xi_0}(\tau_1)\cdots V_{\Xi_0}(\tau_n)\right\rangle_0^{\mathrm{DCD}} \\
\mathscr{D}_{\alpha,\alpha'}(\tau) &= -\frac{1}{\hbar}\sum_{n=0}^{\infty}\left(\frac{-1}{\hbar}\right)^n \int_0^{\hbar\beta} \mathrm{d}\tau_1 \cdots \int_0^{\hbar\beta} \mathrm{d}\tau_n \left\langle \mathrm{T}_\tau\, A_{\alpha\Xi_0}(\tau) A^\dagger_{\alpha'\Xi_0}(\tau') V_{\Xi_0}(\tau_1)\cdots V_{\Xi_0}(\tau_n)\right\rangle_0^{\mathrm{DCD}}
\end{aligned}$$

where only DCD ≡ "[D]ifferent [C]onnected [D]iagrams" are evaluated

Proof 15.10 This is (unfortunately) a folklore-theorem that is always stated, but never proven in the generality in which one claims its radius of applicability: In the book from Mahan (cf. [32], page 132) this theorem is basically stated as a fact without a proof, and also only for the case of an electron-gas. In the book from Bruus and Flensberg (cf. [6], chapter 12) this theorem is only proven in the case of an electron-gas with electron-electron-interactions (and even there are, in my opinion, some gaps in the argument). In the book from Altland (cf. [4], chapter 5) this theorem is only proven with several examples, but one time without a proof, and another time (in the case of an electron gas) only until second order. In the book from Salmhofer (cf. [46], chapter 2) this statement *is* proven for a general case, but only for scalar field theories, not fermionic or mixed field theories. In the book from Negele and Orland (cf. [38], chapter 2 section 3) it is also only proven for pure systems (not for mixed systems). The list goes on... We will use this theorem therefore without a rigorous proof, and when we come to the computation of self-energies (where this theorem does matter) we will notice that a straight-forward expansion of the numerators and denominators indeed gives such a factorization that allows for a cancellation.

Remark 15.10.1 The straight-forward evaluation of these infinite series is cumbersome and basically never done in practice. There is a much more elegant way to compute Green-functions by identifying proper kernels in the so-called "Dyson-equation" (to be introduced below). This process involves the identification of "good" Green-functions, which can be linked to many observable quantities one the one hand, and possess a kernel that is easy to compute on the other hand.

15.2. The Dyson-Equation for Pure One-Body Green-Functions

Notation 15.11 For reasons that will become clear in a later chapter[1] we assume the existence of a function[2]

$$\begin{aligned} \Sigma : \mathrm{i}\Omega_\xi &\longrightarrow \mathrm{Mat}_{\mathrm{d}\times\mathrm{d}}(\mathbb{C}) \\ \mathrm{i}\omega_n &\longmapsto \Sigma(\mathrm{i}\omega_n) \end{aligned}$$

which we call the *(statistical) self-energy* s.t. the *Dyson-equation* for the one-body Green-function is fulfilled

$$\mathscr{G}(\mathrm{i}\omega_n) = \mathscr{G}_0(\mathrm{i}\omega_n) + \left(\mathscr{G}_0 \cdot \Sigma \cdot \mathscr{G}\right)(\mathrm{i}\omega_n), \tag{15.12}$$

where the dot inside the parenthesis corresponds to matrix-multiplication.

Remark 15.11.1 It should be noted, that there are different sign-conventions for the self-energy in the literature. We are following the one from [4, 43][3] in contrast to [38, 29][4]. We will however motivate the here chosen convention below.

[1] When we have introduced the effective action formalism, it will become clear that one can conclude the existence and shape of this function from symmetry-considerations for *most* fermionic and bosonic systems. For phonons however one can not conclude the existence of a self-energy. Phonons will be discussed in the next section.

[2] Note that the self-energy depends on the statistics of the system $\Sigma_\zeta \equiv \Sigma$.

[3] See explicitly in [4] Equation (5.38) and in [43] under Equation (25).

[4] See explicitly in [38] under Equation (3.37) and in [29] Equation (4.35).

Remark 15.11.2 Recall from Theorem 29.107 that this implies the existence of a corresponding imaginary-time-version of this equation[5] and that the Matsubara-Fourier-transformed self-energy does not have the unit of an energy.

Remark 15.11.3 The justification for the name „self-energy“ can be seen in the following way: A formal inversion of the equation above yields

$$\begin{aligned}\mathscr{G}(\mathrm{i}\omega_n) = \left(1 - \mathscr{G}_0 \cdot \Sigma\right)^{-1}(\mathrm{i}\omega_n) \cdot \mathscr{G}_0(\mathrm{i}\omega_n) = \frac{1}{\left(\mathscr{G}_0^{-1} - \Sigma\right)(\mathrm{i}\omega_n)} &= \frac{1}{\hbar}\frac{1}{\mathrm{i}\omega_n - \left(H_0 + \Sigma(\mathrm{i}\omega_n) - \eta\mu\right)/\hbar}, \\ &= \frac{1}{\mathrm{i}\hbar\omega_n - \left(H_0 + \Sigma(\mathrm{i}\omega_n) - \eta\mu\right)}.\end{aligned} \tag{15.13}$$

The self-energy is therefore a term, that is formally being added on top of the Hamiltonian-matrix.

Remark 15.11.4 Notice that in the equation-system of the last remark we found the identity

$$\mathscr{G}^{-1}(\mathrm{i}\omega_n) = \mathscr{G}_0^{-1}(\mathrm{i}\omega_n) - \Sigma(\mathrm{i}\omega_n) \tag{15.14}$$

If we now generalize the one-body Green-function to possess two Matsubara-frequencies, i.e.

$$\mathscr{G}\left(A|A'\right) \equiv \mathscr{G}\left(\mathrm{i}\omega_n, \alpha|\mathrm{i}\omega_{n'}, \alpha'\right) \equiv \mathscr{G}_{\substack{\alpha,\alpha' \\ \mathrm{i}\omega_n,\mathrm{i}\omega_{n'}}} \equiv \delta_{\omega_n,\omega_{n'}}\mathscr{G}_{\alpha,\alpha'}(\mathrm{i}\omega_n), \qquad \text{etc.} \tag{15.15}$$

then we see, that we can write the *generalized Dyson-equation*

$$\mathscr{G}^{-1} = \mathscr{G}_0^{-1} - \Sigma. \tag{15.16}$$

Corollary 15.12 With the von Neumann-series, one concludes

$$\mathscr{G}(\mathrm{i}\omega_n) = \left(1 - \mathscr{G}_0 \cdot \Sigma\right)^{-1}(\mathrm{i}\omega_n) \cdot \mathscr{G}_0(\mathrm{i}\omega_n) = \sum_{n=0}^{\infty}\left(\left[\mathscr{G}_0 \cdot \Sigma\right]^n \cdot \mathscr{G}_0\right)(\mathrm{i}\omega_n),$$

Proof 15.12 Follows immediately from using the von Neumann-series.

[5] More concretely

$$\begin{aligned}\Sigma\colon (0,\hbar\beta)^2 &\to \mathrm{Mat}_{\mathrm{d}_{\mathcal{H}}\times\mathrm{d}_{\mathcal{H}}}(\mathbb{C}) \\ (\tau,\tau') &\mapsto \Sigma(\tau,\tau')\end{aligned}$$

s.t. the Dyson-equation in (imaginary-)time-space the (connected or unconnected) one-body Green-function is fulfilled

$$\mathscr{G}(\tau,\tau') = \mathscr{G}_0(\tau,\tau') + \left(\mathscr{G}_0 \cdot \Sigma \cdot \mathscr{G}\right)(\tau,\tau'),$$

where the dot inside the parenthesis is to be understood as a generalized product as in Definition 29.103.

Remark 15.12.1 It will turn out, that depending on the situation, it is advantegous to make use of the first or second equation-sign.

Remark 15.12.2 It will also turn out, that the self-energy of the system, which seems like a very abstract concept here, can be calculated quite straight-forward. The self-energy Σ of a particle will turn out to be the sum of „all the connected irreducible diagrams“, whereas we will carefully explain what is meant by this statement in the following subsections. We will need all the identities presented here for the computation of the self-energy.

15.3. The Dyson-Equation for Phononic Displacement-Green-Functions

Notation 15.13 For reasons that will become clear in a later chapter we assume the existence of a function

$$\begin{aligned}\Pi:\ \mathrm{i}\Omega_{+1} &\longrightarrow \mathrm{Mat}_{d_{\max}\times d_{\max}}(\mathbb{C})\\ \mathrm{i}\omega_n &\longmapsto \Pi(\mathrm{i}\omega_n)\end{aligned}$$

with $d_{\max} = rd_{\mathbf{x}}N_p$, which we call the *polarization* s.t. the *Dyson-equation* of the phononic displacement-Green-function is fulfilled

$$\mathscr{D}(\mathrm{i}\omega_n) = \mathscr{D}_0(\mathrm{i}\omega_n) + \left(\mathscr{D}_0 \cdot \Pi \cdot \mathscr{D}\right)(\mathrm{i}\omega_n),$$

where the dot inside the parenthesis corresponds to matrix-multiplication.

Remark 15.13.1 In contrast to its electronic counterpart, this equation is unique within the literature.

Remark 15.13.2 Recall from Theorem 29.107 that this implies the existence of a corresponding imaginary-time-version version of this equation[6] which again has not the unit of an energy.

Remark 15.13.3 Notice that a formal inversion of the equation above yields[7]

[6] More concretely

$$\begin{aligned}\Pi:\ (0,\hbar\beta)^2 &\longrightarrow \mathrm{Mat}_{d_{\max}\times d_{\max}}(\mathbb{C})\\ (\tau,\tau') &\mapsto \Pi(\tau,\tau')\end{aligned}$$

s.t. the Dyson-equation in (imaginary-)time for phononic displacement-Green-function is fulfilled

$$\mathscr{D}(\tau,\tau') = \mathscr{D}_0(\tau,\tau') + \left(\mathscr{D}_0 \cdot \Pi \cdot \mathscr{D}\right)(\tau,\tau'),$$

where the dot inside the parenthesis is to be understood as a generalized product as in Definition 29.103.

[7] Cf. [3].

$$\begin{aligned} \mathscr{D}(\mathrm{i}\omega_n) &= \left(1 - \mathscr{D}_0 \cdot \Pi\right)^{-1}(\mathrm{i}\omega_n) \cdot \mathscr{D}_0(\mathrm{i}\omega_n) = \frac{1}{\left(\mathscr{D}_0^{-1} - \Pi\right)(\mathrm{i}\omega_n)} \\ \iff \quad \mathscr{D}^{-1}_{\nu,\nu'}(\mathbf{q}, \mathrm{i}\omega_n) &= \underset{\nu,\nu'}{\mathscr{D}^{-1}_0}(\mathbf{q}, \mathrm{i}\omega_n) - \Pi_{\nu,\nu'}(\mathbf{q}, \mathrm{i}\omega_n) \end{aligned} \tag{15.17}$$

Lemma 15.14 For typical phononic systems in crystals, this equation can be rewritten to become

$$\mathscr{D}(\mathbf{q}, \mathrm{i}\omega_n) = -\frac{1}{\hbar} \frac{2\boldsymbol{\omega}(\mathbf{q})}{\left(\omega_n^2 \mathbb{1}_{rd_\mathrm{x} \times rd_\mathrm{x}} + \boldsymbol{\omega}^2(\mathbf{q})\right) + \frac{2}{\hbar}\boldsymbol{\omega}(\mathbf{q})\,\Pi(\mathbf{q}, \mathrm{i}\omega_n)} \tag{15.18}$$

Proof 15.14 See Appendix, Proofs, page 562

Corollary 15.15 With the von Neumann-series, one concludes

$$\mathscr{D}(\mathrm{i}\omega_n) = \left(1 - \mathscr{D}_0 \cdot \Pi\right)^{-1}(\mathrm{i}\omega_n) \cdot \mathscr{D}_0(\mathrm{i}\omega_n) = \sum_{n=0}^{\infty} \left(\left[\mathscr{D}_0 \cdot \Pi\right]^n \cdot \mathscr{D}_0\right)(\mathrm{i}\omega_n),$$

Proof 15.15 Follows from a formal inversion with the von Neumann-series.

Remark 15.15.1 It will turn out, that depending on the situation, it is advantegous to make use of the first or second equation-sign.

Remark 15.15.2 Just as for the self-energy of the system, the polarization can be calculated quite straight-forward.

15.4. The Bethe-Salpeter-Equation for Two-Body Green-Functions of Particle-Nature

For pedagogical reasons (we just presented a formula with which one can compute the one-body Green-function of an interacting system; Now we should present the formula for the two-body Green-function of an interacting system) we will now present the Bethe-Salpeter-Equation for the two-body Green-function and refer to the proof that is being carried out several chapters later.

Theorem 15.16 Under the proper circumstances, we can conclude the existence of a so-called *effective interaction* Vert which solves the equation

$$\begin{aligned}\mathcal{G}(i_1, i_2 \mid i_1', i_2') &= \mathcal{G}(i_1 \mid i_1')\mathcal{G}(i_2 \mid i_2') + \zeta\mathcal{G}(i_1 \mid i_2')\mathcal{G}(i_2 \mid i_1') \\ &\quad - \sum\!\!\!\!\!\!\int_{j_1,j_2,j_1',j_2'} \mathcal{G}(i_1 \mid j_1)\mathcal{G}(i_2 \mid j_2)\ \mathrm{Vert}(j_1, j_2 \mid j_1', j_2')\mathcal{G}(j_1' \mid i_1')\mathcal{G}(j_2' \mid i_2')\end{aligned} \tag{15.19}$$

Proof 15.16 Can be concluded from Theorem 16.48.

Remark 15.16.1 Just like the self-energy and the polarization are not quantities that are "easy to identify", the effective interaction Vert is another quantity that needs to be computed. We will learn later how to do it.

15.5. Matsubara-Summations

Without any motivation, we will elucidate how to compute summations of the type

$$S_\zeta = \sum_{\omega_n \in \Omega_\zeta} h(\omega_n). \tag{15.20}$$

since we will encounter summations of this type quite often in the following chapters.

Notation 15.17 For reasons, that will become clear soon, we assume that the function

$$\mathbb{C} - \mathrm{Z} \ni z \mapsto h(-\mathrm{i}z) \in \mathbb{C} \tag{15.21}$$

is complex differentiable in the entire complex plane, with the exception of a finite number of poles of finite order which are no Matsubara-frequencies, which we denote with

$$\mathrm{Z} \equiv \left\{z_1, \ldots, z_N\right\}. \tag{15.22}$$

Lemma 15.18 The complex function

$$\mathbb{C} - \mathrm{i}\Omega_\zeta \ni z \mapsto g_\zeta(z) = \frac{\hbar\beta}{\mathrm{e}^{\hbar\beta z} - \zeta} \in \mathbb{C} \tag{15.23}$$

has simple poles as

$$\forall \mathrm{i}\omega_n \in \mathrm{i}\Omega_\zeta \ : \ \lim_{z \to \mathrm{i}\omega_n} (z - \mathrm{i}\omega_n) g_\zeta(z) = \zeta. \tag{15.24}$$

Proof 15.18 See Appendix, Proofs, page 563

Remark 15.18.1 Notice that now the function

$$\mathbb{C} - \mathrm{P} \ni z \mapsto g_\zeta(z)\, h(-\mathrm{i}z) \equiv f_\zeta(z) \in \mathbb{C} \tag{15.25}$$

is complex differentiable as a product of complex differentiable functions, with the pole-set $\mathrm{P} = \mathrm{i}\Omega_\zeta \cup \mathrm{Z}$.

Remark 15.18.2 Notice further the identity

$$g_\zeta(z) = \frac{\hbar\beta}{\mathrm{e}^{\hbar\beta z} - \zeta} = \hbar\beta \mathrm{n}^\zeta_{\hbar\beta}(z) \tag{15.26}$$

Theorem 15.19 Consider a complex function $f : \mathbb{C} \to \mathbb{C}$, which has poles at the points $\{z_1, \ldots, z_N\} \subset \mathbb{C}$, and is holomorphic on $\mathbb{C} \setminus \{z_1, \ldots, z_N\}$. Let γ be a closed curve in the complex plane. Then the *residue theorem* states that

$$\oint_\gamma dz\, f(z) = 2\pi\mathrm{i} \sum_{z_n} I(\gamma, z_n) \operatorname{Res}(f, z_n),$$

where

$$I(\gamma, z) = \begin{cases} 0, & \text{if } z \text{ is not enclosed by } \gamma, \\ +n, & \text{if } z \text{ is enclosed } n \text{ times counter clockwise by } \gamma, \\ -n, & \text{if } z \text{ is enclosed } n \text{ times clockwise by } \gamma, \end{cases}$$

and the *residue* $\operatorname{Res}(f, z_0)$ of the function f at point z_0 is defined as follows. If f has pole of order n at z_0, meaning that

$$f(z) = \frac{g(z)}{(z - z_0)^n},$$

where $g(z)$ is holomorphic in the vicinity of z_0, then:

$$\operatorname{Res}(f, z_0) = \frac{1}{(n-1)!} \frac{d^{n-1}}{dz^{n-1}} \left((z - z_0)^n f(z) \right) \Big|_{z=z_0}.$$

Proof 15.19 See in the literature, for example [2], Theorem 17 on page 150, or for example [45].

Theorem 15.20 If f decays sufficiently fast[8] at complex infinity, then it follows

$$S_\zeta = \sum_{\omega_n \in \Omega_\zeta} h(\omega_n) \overset{\text{Claim}}{=} -\zeta \sum_{k=1}^{N} \operatorname{Res}\left(f_\zeta(z),\ z = z_k \right) \tag{15.27}$$

[8]This "roughly" that it decays "faster" than $z \to 1/z$, whereas there are exceptions, for example for the free propagator one obtains a regularization through infinitesimal phases, cf. [4].

Proof 15.20 See Appendix, Proofs, page 563

Lemma 15.21 In the case that the complex function can be written as a product of simple poles

$$\mathbb{C} - \mathrm{Z} \ni z \mapsto h(-\mathrm{i}z) \equiv \text{const.} \prod_{k=1}^{N} \frac{1}{\left(z - z_k\right)} \in \mathbb{C} \tag{15.28}$$

one has

$$S_\zeta = \sum_{\omega_n \in \Omega_\zeta} h(\omega_n) \overset{\text{Claim}}{=} -\zeta \hbar\beta \,\text{const} \sum_{k=1}^{N} \mathrm{n}^{\zeta}_{\hbar\beta}(z_k) \prod_{\substack{l=1 \\ l\neq k}}^{N} \frac{1}{z_k - z_l} \tag{15.29}$$

whereas an empty product is as usual defined to be equal to one.

Proof 15.21 Follows immediately by insertion.

Corollary 15.22 For

$$h(\omega_n) = \frac{1}{\hbar\beta} \frac{1}{\mathrm{i}\omega_n - C} \tag{15.30}$$

one finds the identity

$$S_\zeta = \sum_{\omega_n \in \Omega_\zeta} h(\omega_n) \overset{\text{Claim}}{=} -\zeta \mathrm{n}^{\zeta}_{\hbar\beta}(C). \tag{15.31}$$

Proof 15.22 See Appendix, Proofs, page 564

Remark 15.22.1 Notice that this is exactly the type of summation that appears when evaluating Matsubara-sums of the type

$$S_\zeta = \frac{1}{\beta} \sum_{\omega_n \in \Omega_\zeta} \underline{\mathscr{G}}_0 \left(\mathrm{i}\omega_n\right). \tag{15.32}$$

Corollary 15.23 For $\omega_m \in \Omega_{-1}$ and summation-function

$$h(\omega_n) = \frac{1}{\hbar^2\beta} \frac{1}{\mathrm{i}\omega_n - C_1} \frac{-2C_2}{\left(\omega_m - \omega_n\right)^2 + C_2^2} \tag{15.33}$$

one finds the identity

$$S_{-1} = \sum_{\omega_n \in \Omega_{-1}} h(\omega_n) \overset{\text{Claim}}{=} \frac{-1}{\hbar} \left[\frac{\mathrm{B}_{\hbar\beta}(C_2) + \mathrm{F}_{\hbar\beta}(C_1)}{\mathrm{i}\omega_m - C_1 + C_2} + \frac{\mathrm{B}_{\hbar\beta}(C_2) + 1 - \mathrm{F}_{\hbar\beta}(C_1)}{\mathrm{i}\omega_m - C_1 - C_2} \right] \tag{15.34}$$

Proof 15.23 See Appendix, Proofs, page 564

Remark 15.23.1 Notice that this is exactly the type of summation that appears when evaluating Matsubara-sums of the type

$$\frac{1}{\beta} \sum_{\omega_{n_2} \in \Omega_{-1}} \mathscr{G}_{0\ \blacksquare_1}(\mathrm{i}\omega_{n_2})\, \mathscr{D}_{0\ \blacksquare_2}(\mathrm{i}(\omega_n - \omega_{n_2})). \tag{15.35}$$

Part III.

(Thermal) Quantum Field Theory

16. Algebraic Concepts in Quantum Field Theory

"Quantum field theory (QFT) provides an extremely powerful set of computational methods that have yet to find any fundamental limitations. It has led to the most fantastic agreement between theoretical predictions and experimental data in the history of science. It provides deep and profound insights into the nature of our universe, and into the nature of other possible self-consistent universes. On the other hand, the subject is a mess."

M. D. Schwartz in [49], p. xv

"Go for the messes - that's where the action is."

Steven Weinberg in [58], p. 389.

16.1. Quantum Field Theory - Pure Systems

"The formal calculus in Graßmann algebra, which was developed by Berezin in his first book Method of the Second Quantization, made him sure that a nontrivial analogue of analysis exists in which anticommuting variables appear on the same footing as the usual ones."

Felix Berezin in [5].

Supermathematics is a branch of mathematical physics, which (among many other applications) applies algebraic concepts to the study of bosonic and in particular fermionic systems. The mathematical rigorous introduction of these concepts is (at least for the purposes that we have in mind) not very complicated, but it is a lot of simple definitions and theorems.

Since there exists already so much great introductory literature to these concepts we will not prove all the standard-theorems but just list those that we need, referring to the literature[1] for the proofs.

16.1.1. Fundamentals

Definition 16.1 We associate generators $U \cup \overline{U} = \left\{\psi_1, \overline{\psi}_1, \dots, \psi_{\mathrm{D}}, \overline{\psi}_{\mathrm{D}}\right\}$ with annihilation-operators (ψ) and creation-operators ($\overline{\psi}$). Then we define the *algebra of statistical polynomials* $\mathscr{P}_\zeta$ as the associative algebra generated by $\mathbb{C} \oplus U \cup \overline{U}$ with relations

$$\psi_i \psi_j = \zeta \psi_j \psi_i, \qquad \overline{\psi}_i \psi_j = \zeta \psi_j \overline{\psi}_i, \qquad \overline{\psi}_i \overline{\psi}_j = \zeta \overline{\psi}_j \overline{\psi}_i. \tag{16.1}$$

for $i, j \in \{1, \dots, \mathrm{D}\}$.

[1] Cf. [4, 60, 61] etc.

Remark 16.1.1 One distinguishes between two cases:

- For $\zeta = -1$ this algebra is called *Graßmann-algebra* and oftentimes denotes as $\mathscr{P}_{-1} \equiv \mathscr{G}$. The generators $\left\{\psi_i, \overline{\psi}_i\right\}_{i\in\{1,\dots,\mathrm{D}\}}$ are referred to as *Graßmann-numbers*.
- For $\zeta = +1$ this algebra is called *symmetric algebra*. The generators $\left\{\psi_i, \overline{\psi}_i\right\}_{i\in\{1,\dots,\mathrm{D}\}}$ are referred to as *complex-numbers*.

Remark 16.1.2 Notice that these commutation-relations are the same as in Equation (7.7).

Remark 16.1.3 For the moment, we focus on the case $\mathrm{D} = \mathrm{d}_\eta$, such that for each creation- and annihilation-operator there is a Graßmann-variable associated. In the later application, it will be the case that $\mathrm{D} \equiv \mathrm{d}_\eta N$ with $N \to \infty$, such that for each creation- and annihilation-operator, there will be infinitely many Graßmann-variables associated. Typically one has a notation as $\psi_{n\alpha}$ etc. with $\alpha \in \mathscr{A}$ and $n \in \{1, 2, \dots, N\}$. The index n is either associated with an imaginary time $\tau_n \in (0, \hbar\beta)$ (such that $\psi_{n\alpha} \equiv \psi_\alpha(\tau_n)$) or a Matsubara-frequency $\mathrm{i}\omega_n \in \mathrm{i}\Omega_\zeta$ (such that $\psi_{n\alpha} \equiv \psi_\alpha(\mathrm{i}\omega_n)$). When we consider different Graßmann-variables $\left\{\psi_1, \dots, \psi_{\mathrm{d}_\eta}\right\}$ and $\left\{\phi_1, \dots, \phi_{\mathrm{d}_\eta}\right\}$ that anticommute with each other (and correspond to different „timestamps“ or „Matsubara-frequencies“), it is this situation just elucidated that we have in mind.

Lemma 16.2 A basis of the algebra $\mathscr{P}_\zeta$ is given by the monomials

$$\left\{ \psi_1^{n_1} \cdots \psi_D^{n_D} \overline{\psi}_1^{\overline{n}_1} \cdots \overline{\psi}_D^{\overline{n}_D} \quad \middle| \quad n_1, \overline{n}_1 \dots, n_\mathrm{D}, \overline{n}_\mathrm{D} \in \mathbb{N}_\zeta \right\} \quad \subset \quad \mathscr{P}_\zeta \tag{16.2}$$

Proof 16.2 Follows from introductory courses on linear algebra.

Corollary 16.3 Every element $f(\psi, \overline{\psi}) \equiv f \in \mathscr{P}_\zeta$ with $\psi \equiv (\psi_1, \dots, \psi_\mathrm{D})$ can be written as uniquely as

$$f(\psi, \overline{\psi}) = \sum_{\substack{n_1,\dots,n_D \in \mathbb{N}_\zeta \\ \overline{n}_1,\dots,\overline{n}_D \in \mathbb{N}_\zeta}} c_{\substack{n_1,\dots,n_D \\ \overline{n}_1,\dots,\overline{n}_D}} \psi_1^{n_1} \cdots \psi_D^{n_D} \overline{\psi}_1^{\overline{n}_1} \cdots \overline{\psi}_D^{\overline{n}_D} \tag{16.3}$$

with complex numbers $c_{\substack{n_1,\dots,n_D \\ \overline{n}_1,\dots,\overline{n}_D}} \in \mathbb{C}$.

Proof 16.3 Follows from introductory courses on linear algebra.

Remark 16.3.1 We decompose f as

$$\begin{aligned} f(\psi, \overline{\psi}) &= c_{\substack{0,\dots,0 \\ 0,\dots,0}} &&+ \left(f(\psi, \overline{\psi}) - c_{\substack{0,\dots,0 \\ 0,\dots,0}} \right) \\ &\equiv \mathrm{body}_f &&+ \mathrm{soul}_f(\psi, \overline{\psi}) \\ &\equiv f_0 &&+ f_{\mathrm{nil}}(\psi, \overline{\psi}) \end{aligned} \tag{16.4}$$

whereas $c_{\substack{0,\dots,0\\0,\dots,0}} \equiv f_0 \equiv \text{body}_f \in \mathbb{C}$ is called the *body* and $\text{soul}_f \equiv f_{\text{nil}}$ the *soul* of f.

Lemma 16.4 In the case that $\zeta = -1$, one finds that the soul of f is *nilpotent*, i.e.

$$\exists N_f \in \mathbb{N} : f_{\text{nil}}^{N_f}(\psi, \overline{\psi}) = 0. \tag{16.5}$$

whereas we define N_f as the *nilpotency index* of f.

Proof 16.4 The fact that f_{nil} is nilpotent is easily seen by writing down the polynomial expansion and taking the square... The exact value of N_f depends on the structure of the soul.

Remark 16.4.1 Notice that $N_f \leq 2D$.

Definition 16.5 We call a polynomial $f \in \mathscr{P}_\zeta$ *invertible*, if there is another element $f^{-1} \equiv \frac{1}{f} \in \mathscr{P}_\zeta$ such that

$$f f^{-1} = f^{-1} f = 1. \tag{16.6}$$

Remark 16.5.1 We call f^{-1} the *inverse element* of f.

Lemma 16.6 If $\zeta = +1$ a polynomial is always invertibel. If $\zeta = -1$, a polynomial f is invertible, iff $f_0 \neq 0$ and then the inverse element is given by

$$f^{-1}(\psi, \overline{\psi}) = \frac{1}{f_0} \sum_{n=0}^{N_f - 1} \left(-\frac{f_{\text{nil}}(\psi, \overline{\psi})}{f_0} \right)^n. \tag{16.7}$$

Proof 16.6 See Appendix, Proofs, page 567.

Remark 16.6.1 Notice further, that this is "simply" a Graßmann-version of the geometric series, formally

$$f^{-1}(\psi, \overline{\psi}) \equiv \frac{1}{f_0 + f_{\text{nil}}(\psi, \overline{\psi})} \equiv \frac{1}{f_0} \sum_{n=0}^{\infty} \left(-\frac{f_{\text{nil}}(\psi, \overline{\psi})}{f_0} \right)^n. \tag{16.8}$$

Remark 16.6.2 Notice that the inverse element is also again a polynomial.

Definition 16.7 We define derivatives for $\zeta = +1$ in the usual way. For $\zeta = -1$ we define the *left-derivative* for each $j \in \{1, \dots, \text{D}\}$ as

$$f \equiv f_0 + \psi_j f_1 \quad \Rightarrow \quad \frac{\partial}{\partial \psi_j} f := f_1 \tag{16.9}$$

whereas f_1 is independent of ψ_j.

Remark 16.7.1 Something peculiar about Graßmann-derivatives is that one can also define a *right-derivative* as

$$f \equiv f_0 + f_1 \psi_j \quad \Rightarrow \quad \left(\partial f \Big/ \partial \psi_j\right) \equiv f \frac{\overleftarrow{\partial}}{\partial \psi_j} := f_1 \tag{16.10}$$

Remark 16.7.2 The easiest way to see why one can do this, is to realize that derivatives are basically just linear maps on $\mathscr{P}_\zeta$. For $\zeta = 1$ this map is the same, no matter if one defines it as a left- or right-derivative. For $\zeta = -1$ one can define two different maps, which are related to each other.

Definition 16.8 For a monomial expression

$$m \equiv \psi_1^{n_1} \cdots \psi_D^{n_D} \overline{\psi}_1^{\overline{n}_1} \cdots \overline{\psi}_D^{\overline{n}_D} \tag{16.11}$$

we define the *degree* of m as

$$\deg(m) := \sum_{j=1}^{D} \left(n_j + \overline{n}_j\right) \tag{16.12}$$

Theorem 16.9 Let m_1 and m_2 be two monomial expressions in $\mathscr{P}_\zeta$. Then the *graded chain-rule* reads

$$\frac{\partial}{\partial \psi_j}\left(m_1 m_2\right)(\psi, \overline{\psi}) = \left[\left(\frac{\partial m_1}{\partial \psi_j}\right) m_2 + \zeta^{\deg(m_1)} m_1 \left(\frac{\partial m_2}{\partial \psi_j}\right)\right](\psi, \overline{\psi}) \tag{16.13}$$

Proof 16.9 See, for example, [57] Equation (3.5).

Definition 16.10 For a monomial expression

$$m \equiv \psi_1^{n_1} \cdots \psi_D^{n_D} \overline{\psi}_1^{\overline{n}_1} \cdots \overline{\psi}_D^{\overline{n}_D} \tag{16.14}$$

we define[2] *conjugation in the polynomial algebra* as a mapping

$$\begin{aligned} *\equiv \dagger : \mathscr{P}_\zeta &\to \mathscr{P}_\zeta \\ \psi_1^{n_1} \cdots \psi_D^{n_D} \overline{\psi}_1^{\overline{n}_1} \cdots \overline{\psi}_D^{\overline{n}_D} &\mapsto \left(\psi_1^{n_1} \cdots \psi_D^{n_D} \overline{\psi}_1^{\overline{n}_1} \cdots \overline{\psi}_D^{\overline{n}_D}\right)^\dagger \equiv \psi_D^{\overline{n}_D} \cdots \psi_1^{\overline{n}_1} \overline{\psi}_D^{n_D} \cdots \overline{\psi}_1^{n_1} \end{aligned} \tag{16.15}$$

[2] Cf. [38], p. 26.

Lemma 16.11 The *statistics neutral commutation relations* read

$$\left[\frac{\partial}{\partial\psi_i},\,\psi_j\right]_\zeta = \delta_{i,j}, \qquad \left[\frac{\partial}{\partial\psi_i},\,\overline{\psi}_j\right]_\zeta = 0 = \left[\frac{\partial}{\partial\overline{\psi}_i},\,\psi_j\right]_\zeta \tag{16.16}$$

Proof 16.11 See, for example, [57] Equation (3.8)

Lemma 16.12 The *statistics neutral Schwartz-rule* reads

$$0 = \left[\frac{\partial}{\partial\psi_i},\,\frac{\partial}{\partial\psi_j}\right]_\zeta = \left[\frac{\partial}{\partial\psi_i},\,\frac{\partial}{\partial\overline{\psi}_j}\right]_\zeta = \left[\frac{\partial}{\partial\overline{\psi}_i},\,\frac{\partial}{\partial\overline{\psi}_j}\right]_\zeta \tag{16.17}$$

Proof 16.12 See, for example, [57] Equation (3.8)

Remark 16.12.1 Notice that these commutation-relations are the same as in Notation 7.21. In fact, one can introduce the statistical algebra of polynomials and their derivatives as ζ-algebras quite straightforwardly by following the same steps that we did in the previous chapters. It becomes though a little bit difficult to follow on the notation (one needs, for the purposes that we have in mind, eight[3] „copies“ of generators that correspond to creation- and annihilation-operators), and therefore we will not do so here.

Notation 16.13 By inclusion of another set of generators $\left\{j_1, \overline{j}_1, \ldots, j_{\mathrm{D}}, \overline{j}_{\mathrm{D}}\right\}$, which are commonly referred to as *source-terms* we can consider combined polynomial expressions in even another polynomial algebra, which we don't give a name for notational simplicity.

Remark 16.13.1 The introduction of these so-called source-terms is the main trick when it comes to the computation of Green-functions within the framework of "Thermal Quantum Field Theory" (which will be introduced in the next chapter).

Remark 16.13.2 We introduce the notation

$$\overline{\psi}^{\mathrm{T}} \equiv \psi^\dagger \quad \text{and} \quad j^\dagger\psi \equiv \sum_{k=1}^{D} \overline{j}_k\psi_k \tag{16.18}$$

Lemma 16.14 The derivative of a source-term reads

[3] Two copies for polynomials in variables and their conjugates. Two more for their derivatives. And again four more for „source-terms“ and their derivatives (to be introduced soon).

$$\frac{\partial}{\partial \bar{j}_i}\exp\sum_k \bar{j}_k\psi_k = \psi_i \exp\sum_k \bar{j}_k\psi_k$$
$$\frac{\partial}{\partial j_{i'}}\exp\sum_k \overline{\psi}_k j_k = \zeta\,\overline{\psi}_{i'}\exp\sum_k \overline{\psi}_k j_k$$

Proof 16.14 See Appendix, Proofs, page 567.

Corollary 16.15 It holds that

$$\frac{\partial^n}{\partial \bar{j}_{i_1}\cdots\partial \bar{j}_{i_n}}\exp\sum_k \bar{j}_k\psi_k = \psi_{i_1}\cdots\psi_{i_n}\exp\sum_k \bar{j}_k\psi_k$$
$$\frac{\partial^{n'}}{\partial j_{i'_1}\cdots\partial j_{i'_{n'}}}\exp\sum_k \overline{\psi}_k j_k = \zeta^n\overline{\psi}_{i'_1}\cdots\overline{\psi}_{i'_{n'}}\exp\sum_k \overline{\psi}_k j_k$$

Proof 16.15 Using the Lemma above proves the corollary.

Remark 16.15.1 Notice that the commutation-relations imply

$$\frac{\partial^{n+n'}}{\partial \bar{j}_{i_1}\cdots\partial \bar{j}_{i_n}\partial j_{i'_1}\cdots\partial j_{i'_{n'}}}\mathrm{e}^{\sum_k \bar{j}_k\psi_k+\overline{\psi}_k j_k} = \zeta^n\psi_{i_1}\cdots\psi_{i_n}\overline{\psi}_{i'_1}\cdots\overline{\psi}_{i'_{n'}}\mathrm{e}^{\sum_k \bar{j}_k\psi_k+\overline{\psi}_k j_k} \tag{16.19}$$

Definition 16.16 For $\zeta = +1$ we define integration as the usual Riemann- / Lebesgue-integral. For $\zeta = -1$ we define for a function as in Equation (16.3) the *Berezin-integral* as

$$\int \mathrm{d}_\zeta(\psi,\overline{\psi})f(\psi,\overline{\psi}) := \frac{\partial^{2D}}{\partial\psi_1\cdots\partial\psi_D\partial\overline{\psi}_1\cdots\partial\overline{\psi}_D}f \tag{16.20}$$

with integral-measure[4]

$$\mathrm{d}_\zeta(\overline{\psi},\psi) \equiv \prod_{j=1}^{D}\frac{\mathrm{d}\overline{\psi}_j\mathrm{d}\psi_j}{(2\pi\mathrm{i})^{\theta(\zeta)}} \tag{16.22}$$

[4]Notice that in the case $\zeta = +1$, one has

$$\frac{\mathrm{d}\overline{\psi}_j\mathrm{d}\psi_j}{2\pi\mathrm{i}} \equiv \frac{\mathrm{d}\,\mathrm{Re}\,\psi_j\,\mathrm{d}\,\mathrm{Im}\,\psi_j}{\pi} \tag{16.21}$$

16.1.2. Partition-Functions and Expectation-Values for Non-Interacting Models

Notation 16.17 Let $A \in \mathrm{GL}_n(\mathbb{C})$ be an invertible, quadratic matrix. Then we consider *the partition-function corresponding to A with statistics* ζ as

$$Z_0 := \int \mathrm{d}_\zeta(\overline{\psi}, \psi) \exp - \psi^\dagger A \psi \equiv \int \mathrm{d}_\zeta(\overline{\psi}, \psi) \exp - S_0[\psi, \overline{\psi}] \tag{16.23}$$

for complex- or Graßmann-variables.

Remark 16.17.1 Equivalently, we also speak about the *partition-function w.r.t. the action* S.

Remark 16.17.2 Note that we are, following the convention for notational simplicity, surpressing the dependence on ζ in the symbol Z. We will oftentimes surpress this dependence also on other quantities throughout this section (and work).

Lemma 16.18 The partition function can be calculated to

$$Z_0 = \frac{1}{\mathrm{Det}\, A^\zeta}. \tag{16.24}$$

Proof 16.18 For bosons, see [4] Chapter 3 Section 2, for fermions see Chapter 4 Section 1 or, for example for fermions also [63].

Corollary 16.19 It follows also

$$Z_0 = \exp\left(-\zeta\, \mathrm{Tr}\, \mathrm{Log}\, A\right) \tag{16.25}$$

Proof 16.19 Follows from the identity $\mathrm{Tr}\, \mathrm{Log} \bullet = \mathrm{Log}\, \mathrm{Det} \bullet$.

Definition 16.20 We consider a monomial expression in the integration-variables, and define its *expectation value w.r.t. A*

$$\left\langle \psi_{i_1} \cdots \psi_{i_n} \overline{\psi}_{i'_1} \cdots \overline{\psi}_{i'_m} \right\rangle_0 := \frac{1}{Z} \int \mathrm{d}_\zeta(\overline{\psi}, \psi)\, \psi_{i_1} \cdots \psi_{i_n} \overline{\psi}_{i'_1} \cdots \overline{\psi}_{i'_m} \exp - \psi^\dagger A \psi. \tag{16.26}$$

Remark 16.20.1 By $\mathbb{C}$-linearity, one defines *expectation-values w.r.t. A* for polynomial expressions in the integration-variables $\mathrm{P}(\overline{\psi}, \psi)$.

Definition 16.21 We define the *n-body Green-function* $\mathscr{G}_0$ *w.r.t.* A as expectation-value

$$\mathscr{G}_0(i_1,\dots,i_n \mid i'_n,\dots,i'_1) = \left(-\frac{1}{c}\right)^n \left\langle \psi_{i_1}\cdots\psi_{i_n}\overline{\psi}_{i'_1}\cdots\overline{\psi}_{i'_n}\right\rangle_0 \tag{16.27}$$

Remark 16.21.1 The constant c is arbitrary. For the setting that we have in mind later, it is *convention* to set it to $c \equiv \hbar$, such that the dimension of the Green-function becomes $1/\text{Energy}$.

Remark 16.21.2 It is a priori completely unclear, that this definition of the Green-function will turn out to have anything to do with the Green-functions that we defined in earlier chapters. We will however prove in the next chapter, that the Green-functions defined in Equation (14.17) can be re-expressed as correlation-functions of integrals of the type in Equation (16.27).

Theorem 16.22 For monomial expressions, which contain the same number of ψ-variables as $\overline{\psi}$-variables, one finds the *Wick-theorem*

$$\left\langle \psi_{i_1}\cdots\psi_{i_n}\overline{\psi}_{i'_n}\cdots\overline{\psi}_{i'_1}\right\rangle_0 = \sum_{\pi\in \mathrm{S}_n} \mathrm{sign}(\pi)^{1-\theta(\zeta)} \prod_{k=1}^{n} \left\langle \psi_i \overline{\psi}_{i'_{\pi(k)}}\right\rangle_0 = \sum_{\pi\in \mathrm{S}_n} \mathrm{sign}(\pi)^{1-\theta(\zeta)} \prod_{k=1}^{n} A^{-1}_{i_k i'_{\pi(k)}} \tag{16.28}$$

Proof 16.22 See, for example, [61] p. 46.

Remark 16.22.1 Notice the special case for $m = n = 1$

$$-c\mathscr{G}_0(i \mid i') = \left\langle \psi_i \overline{\psi}_{i'}\right\rangle_0 = A^{-1}_{i,i'} \quad\Longleftrightarrow\quad \mathscr{G}_0(i \mid i') = -\frac{1}{c}A^{-1}_{i,i'} \quad\Longleftrightarrow\quad A_{i,i'} = -\frac{1}{c}\mathscr{G}_0^{-1}(i \mid i') \tag{16.29}$$

which allows us to write formally in the non-interacting case

$$Z_0 = \int \mathrm{d}_\zeta(\overline{\psi},\psi)\exp -\psi^\dagger\left(-\frac{1}{c}\mathscr{G}_0^{-1}\right)\psi \equiv \int \mathrm{d}_\zeta(\overline{\psi},\psi)\exp -S_0[\psi,\overline{\psi}] \tag{16.30}$$

Corollary 16.23 The above theorem implies an identity for the calculation of Green-functions as

$$\mathscr{G}_0(i_1,\dots,i_n \mid i'_1,\dots,i'_n) = \left(-\frac{1}{c}\right)^n \left\langle \psi_{i_1}\cdots\psi_{i_n}\overline{\psi}_{i'_n}\cdots\overline{\psi}_{i'_1}\right\rangle_0 = \sum_{\pi\in \mathrm{S}_n} \mathrm{sign}(\pi)^{1-\theta(\zeta)} \prod_{k=1}^{n} \mathscr{G}_0\left(i_k \mid i'_{\pi(k)}\right) \tag{16.31}$$

Proof 16.23 Using the definition, apparently gives the desired result.

Remark 16.23.1 Notice the reversed order in the second argument-series, in contrast to Eq. (16.27).

16.1.3. Partition-Functions and Expectation-Values for Interacting Models

Notation 16.24 Let $A \in \mathrm{GL}_n(\mathbb{C})$ be an invertible, quadratic matrix, and $\mathrm{P}[\overline{\psi}, \psi]$ an arbitrary[5] polynomial expression in the integration-variables. For reasons that are impossible to clarify in advance, we consider the quantity

$$\begin{aligned} Z &\equiv \int \mathrm{d}_\zeta(\overline{\psi}, \psi) \exp - \left(\psi^\dagger A \psi + \mathrm{P}[\psi, \overline{\psi}] \right) \\ &\equiv \int \mathrm{d}_\zeta(\overline{\psi}, \psi) \exp - \left(S_0[\psi, \overline{\psi}] + S_{\mathrm{int}}[\psi, \overline{\psi}] \right) \\ &\equiv \int \mathrm{d}_\zeta(\overline{\psi}, \psi) \exp - S[\psi, \overline{\psi}] \end{aligned}$$

for complex- or Graßmann-variables.

Notation 16.25 We consider a monomial expression in the integration-variables, and define its *expectation value w.r.t. S* as

$$\left\langle \psi_{i_1} \cdots \psi_{i_n} \overline{\psi}_{i'_1} \cdots \overline{\psi}_{i'_m} \right\rangle := \frac{1}{Z} \int \mathrm{d}_\zeta(\overline{\psi}, \psi) \, \psi_{i_1} \cdots \psi_{i_n} \overline{\psi}_{i'_1} \cdots \overline{\psi}_{i'_m} \exp - S[\psi, \overline{\psi}] \tag{16.32}$$

Remark 16.25.1 Accordingly, one also introduces the *n-body-Green-function w.r.t. S* as expectation-value

$$\mathscr{G}(i_1, \ldots, i_n \mid i'_n, \ldots, i'_1) = \left(-\frac{1}{c} \right)^n \left\langle \psi_{i_1} \cdots \psi_{i_n} \overline{\psi}_{i'_1} \cdots \overline{\psi}_{i'_n} \right\rangle . \tag{16.33}$$

Remark 16.25.2 Notice that this allows us to write down a *formal* equation that is *exclusive* for one-body Green-functions

$$\mathscr{G}(i \mid i') \equiv -\frac{1}{c} \frac{1}{Z} \int \mathrm{d}_\zeta(\overline{\psi}, \psi) \, \psi_i \overline{\psi}_{i'} \exp - \psi^\dagger \left(-\frac{1}{c} \mathscr{G}^{-1} \right) \psi . \tag{16.34}$$

Remark 16.25.3 Combining Equations (16.63) and Equation (16.34) yields that we can rewrite correlation functions as functional integrals over the so-called "quadratic part of the effective action $\mathrm{Vert}(i, i') \equiv \mathrm{Vert}$" (which will be introduced later) as

$$\mathscr{G}(i, i') = -\frac{1}{c} \frac{\int \mathscr{D}(\eta, \overline{\eta}) \, \eta(i) \overline{\eta}(i') \exp - \eta^\dagger \left(-\frac{1}{c} \mathrm{Vert}(:, :) \right) \eta}{\int \mathscr{D}(\eta, \overline{\eta}) \exp - \eta^\dagger \left(-\frac{1}{c} \mathrm{Vert}(:, :) \right) \eta} \tag{16.35}$$

[5] Exception: For systems with fermionic statistics (i.e. $\zeta = -1$) we demand that P is even in the fields $\overline{\psi}$ and ψ, meaning that it only contains polynomials with equal number of Graßmann-variables and conjugated Graßmann-variables.

Fact 16.26 In general, there is no possibility to calculate this partition-function or these expectation-values w.r.t. S in closed-form. But it will turn out to be exactly these expectation-values that we need to compute in order to make predictions about the behaviour of non-interacting systems. There are several standard-techniques to evaluate integrals of this kind, for example

- Expanding in the interaction and using the so-called "Wick-theorem" (see below),
- performing a so-called "Hubbard-Stratanovich-transformation" (will be introduced later),
- applying a so-called "saddle-point approximation" (will be introduced later, works only for for $\zeta = 1$).

Assuming strong-convergence[6] one obtains for the expectation-value

$$\left\langle \psi_{i_1} \cdots \psi_{i_n} \overline{\psi}_{i'_1} \cdots \overline{\psi}_{i'_m} \right\rangle = \frac{\sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \left\langle \psi_{i_1} \cdots \psi_{i_n} \overline{\psi}_{i'_1} \cdots \overline{\psi}_{i'_m} \prod_{l=0}^{k} S_{\text{int}}[\psi, \overline{\psi}] \right\rangle_0}{\sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \left\langle \prod_{l=0}^{k} S_{\text{int}}[\psi, \overline{\psi}] \right\rangle_0} \tag{16.36}$$

For the first option (expanding terms) we will see that Feynman-diagrams built a system to efficiently organize the appearing terms.

Remark 16.26.1 For monomial expressions with $n = m = 1$, we introduced the self-energy-concept in order to simplify the computation of one-body Green-functions. For monomial expressions with $n = m = 2$, one can introduce the so-called "Bethe-Salpeter-equation" in order to simplify the computation of two-body Green-functions. For general cases, one can simplify this expression with the so-called linked-cluster-theorem, which leads to the expression in Theorem (15.10).

We conclude with a remark from the literature[7]

> *"One often needs to sum the perturbation expansion up to infinite order. This is done by identifying the most important subset of diagrams and including them in a self-energy. A warning is in place: the correct identification of the most important diagrams can be very tricky, even in the presence of a small parameter. The reason is that some high-order diagrams, which are not included in a particular model, even though formally smaller, may occur in such large numbers that they yield a contribution that must be included. Any perturbation theory may be just an asymptotic series and not converging in the strict mathematical sense. Finally, it is by no means clear that a "good" self-energy always even exists. Strongly interacting systems of this kind need a nonperturbative approach."*

16.1.4. External Sources and Connected Green-Functions

Notation 16.27 We equip the partition-function Z in Notation 16.24 with external sources $j, \overline{j}$, by making the replacement

$$Z \mapsto Z[j, \overline{j}] \equiv \int \mathrm{d}_\zeta(\overline{\psi}, \psi) \exp\Big[- \big(S_0[\psi, \overline{\psi}] + S_{\text{int}}[\psi, \overline{\psi}]\big) + j^\dagger \psi + \psi^\dagger j \Big] \tag{16.37}$$

[6] In the sense, that integral and infinite series can be exchanged without altering the result.
[7] Cf. [23], p. 52.

Remark 16.27.1 We remark, that the sign with which the source-terms enter is convention, which is very error-prone. We emphasize therefore also that even *within* [38] one finds *different* prefactor-conventions, see for example pages 70, 75, 76 with the one convention, and then pages 105 and 107 for the other one.

Theorem 16.28 One finds in the non-interacting case

$$Z_0[j,\overline{j}] = \int \mathrm{d}_\zeta(\overline{\psi},\psi)\exp\left(-\psi^\dagger A\,\psi + j^\dagger\psi + \psi^\dagger j\right) = \frac{\exp\left(-j^\dagger A^{-1}\,j\right)}{\mathrm{Det}\,A^\zeta} \tag{16.38}$$

Proof 16.28 For the bosonic case ($\zeta = +1$) see, for example, [38] page 22 or [4] page 104. For the fermionic case ($\zeta = -1$) see, for example, [38] page 34 or [4] page 165.

Remark 16.28.1 Notice, that this identity can be combined with Equation (16.29) such that one obtains

$$\begin{aligned}\int \mathrm{d}_\zeta(\overline{\psi},\psi)\exp\left(-\psi^\dagger\left(-\frac{1}{c}\mathscr{G}_0^{-1}\right)\psi + j^\dagger\psi + \psi^\dagger j\right) &= \mathrm{Det}\left(-\frac{\mathscr{G}_0^\zeta}{c^{-1}}\right)\exp\left(-\frac{j^\dagger\mathscr{G}_0\,j}{c^{-1}}\right)\\ &= \exp\left(-\zeta\,\mathrm{Tr}\,\mathrm{Log}\left(-\frac{1}{c}\mathscr{G}_0^{-1}\right) \quad - \quad \frac{j^\dagger\mathscr{G}_0\,j}{c^{-1}}\right)\end{aligned}$$

whereas the individual Equation-signs can be advantegous in different situations.

Remark 16.28.2 *Correction note on Theorem 16.28.* The exponent on the right-hand side of the Theorem has to carry a *plus*-sign:

$$Z_0[j,\overline{j}] = \frac{\exp\left(+j^\dagger A^{-1}\,j\right)}{\mathrm{Det}\,A^\zeta}.$$

This follows by completing the square: The shift $\psi_i = \psi'_i + \sum_m (A^{-1})_{i,m} j_m$, $\overline{\psi}_i = \overline{\psi}'_i + \sum_m \overline{j}_m (A^{-1})_{m,i}$ (which leaves the integration-measure invariant, also for Graßmann-valued shifts) gives for both statistics

$$-\psi^\dagger A\,\psi + j^\dagger\psi + \psi^\dagger j = -\psi'^\dagger A\,\psi' + j^\dagger A^{-1}\,j,$$

where no reordering of Graßmann-variables is necessary. This is also the sign of the quoted literature, and the sign of the exponent in Remark 16.28.1 (where $j^\dagger A^{-1} j = -c\,j^\dagger\mathscr{G}_0\,j$). Moreover, it is the only sign compatible with Equation (16.29): Lemma 16.40 gives with the plus-sign

$$\mathscr{G}_0(i \mid i') = -\frac{\zeta}{c}\frac{\partial^2}{\partial\overline{j}_i\,\partial j_{i'}}\mathrm{e}^{j^\dagger A^{-1} j}\Big|_{j=\overline{j}=0} = -\frac{\zeta}{c}\,\zeta\left(A^{-1}\right)_{i,i'} = -\frac{1}{c}\left(A^{-1}\right)_{i,i'},$$

whereas the minus-sign would give $+\frac{1}{c}A^{-1}$. The plus-sign has also been checked by an explicit Berezin-integration for D = 2 (cf. Remark 19.5.2).

Definition 16.29 We introduce the generating functional

$$\frac{Z[\bar{j}, j]}{Z} = \frac{1}{Z} \int \mathscr{D}_{\zeta}(\psi, \overline{\psi})\, \mathrm{e}^{-S[\psi,\overline{\psi}]+j^{\dagger}\psi+\psi^{\dagger}j} = \left\langle \exp\left[j^{\dagger}\psi + \psi^{\dagger}j\right] \right\rangle \tag{16.39}$$

Definition 16.30 We also introduce the *analogue of the Helmholtz free energy / Landau-potential*[8]

$$W[\bar{j}, j] = +\log Z[\bar{j}, j] \tag{16.40}$$

Remark 16.30.1 Notice that this is at zero external sources proportional (with proportionality constant $k_B T$) to the natural energy (a.k.a. grand canonical potential for $\eta = 1$ and free energy for $\eta = 0$) of a system; Cf. Fact 10.4.

Remark 16.30.2 In the literature [42] this quantity is known as "generating functional for connected correlation functions". In the following we will elaborate on what this exactly means. The is also the reason why one omits the factor $k_B T$: This quantity is mostly considered to be an algebraic object, rather than a thermodynamic.

Notation 16.31 We introduce the *field expectation values*

$$\begin{aligned} \phi[\bullet, j, \bar{j}] &= \langle \psi(\bullet) \rangle_{j,\bar{j}} &&= 1 \frac{\partial}{\partial \bar{j}(\bullet)} W[j, \bar{j}], \\ \overline{\phi}[\bullet, j, \bar{j}] &= \langle \overline{\psi}(\bullet) \rangle_{j,\bar{j}} &&= \zeta \frac{\partial}{\partial j(\bullet)} W[j, \bar{j}]. \end{aligned} \tag{16.41}$$

Remark 16.31.1 For $j, \bar{j} \neq 0$ it follows $\phi, \overline{\phi} \overset{\text{in general}}{\neq} 0$.

Lemma 16.32 In the absence of spontaneous symmetry breaking, the field-expectation values $\phi, \overline{\phi}$ are functionals of the sources $j, \bar{j}$, and they are made up of monomials that are *odd* in the sources $j, \bar{j}$.

Proof 16.32 See Appendix, Proofs, page 567.

Lemma 16.33 The mapping $(j, \bar{j}) \mapsto (\phi, \overline{\phi})$ is *invertible*, in the sense that we can find expansions

$$j[\bullet, \phi', \overline{\phi'}], \quad \bar{j}[\bullet, \phi', \overline{\phi'}] \tag{16.42}$$

such that

[8] Notice that we are using a different sign-convention relative to [27].

$$\phi\Big[\bullet, j[\bullet,\phi',\overline{\phi'}],\bar{j}[\bullet,\phi',\overline{\phi'}]\Big]=\phi', \qquad \overline{\phi}\Big[\bullet, j[\bullet,\phi',\overline{\phi'}],\bar{j}[\bullet,\phi',\overline{\phi'}]\Big]=\overline{\phi'}. \tag{16.43}$$

Proof 16.33 See Appendix, Proofs, page 568.

Remark 16.33.1 Notice that in the construction of the inverse, we realized that the expansions for the sources is *odd* in the fields ϕ and $\overline{\phi}$, which implies that the derivatives (w.r.t. to the ϕ-fields) are even in the fields and commute with the fields. This is a crucial observation for the effective action.

Intermezzo: Vectors with Graßmann-Entries and Chain-Rule

Remark 16.33.2

- Definitions ... of a module over a Graßmann-algebra $V_{\mathscr{P}_\zeta} = V \otimes \mathscr{P}_\zeta$
- Derivatives ... at a point $X \in V_{\mathscr{P}_\zeta}$ are defined as linear maps $dF_X : V_{\mathscr{P}_\zeta} \to V_{\mathscr{P}_\zeta}$, so derivatives live in $\mathrm{Hom}_{\mathscr{P}_\zeta}(V_{\mathscr{P}_\zeta}, V_{\mathscr{P}_\zeta})$

Notation 16.34 With the assumption that the mapping $(j,\bar{j}) \mapsto (\phi,\overline{\phi})$ is invertible, and with suppression of the dependencies $j \equiv j[\bullet,\phi,\overline{\phi}]$, we write the fermionic effective action (being the analog of the Gibbs-potential) as a Legendre-transformation of W

$$\Gamma[\phi,\overline{\phi}] = -W[j,\bar{j}] \quad + \quad \phi^\dagger j + j^\dagger \phi. \tag{16.44}$$

Remark 16.34.1 For the Legendre-transformation, there is a diversity in signs throughout the literature... Basically every author seems to be using a different convention.

Lemma 16.35 One immediately concludes that

$$\frac{\partial}{\partial\overline{\phi}(\bullet)}\Gamma[\phi,\overline{\phi}] = 1j[\bullet,\phi,\overline{\phi}],$$
$$\frac{\partial}{\partial\phi(\bullet)}\Gamma[\phi,\overline{\phi}] = \zeta\bar{j}[\bullet,\phi,\overline{\phi}].$$

Proof 16.35.0 See Appendix, Proofs, page 574.

16.1.5. Series-Expansions

Notation 16.36 After one has established an order relation[9] for the generalized indices, one introduces the series-expansions for the functionals

$$\begin{aligned} F[\pi,\overline{\pi}] &\equiv \sum_{n,m=0}^{\infty} \sum_{\substack{i_1<\ldots<i_n \\ i'_1<i'_2<\ldots<i'_m}} \overline{\pi}(i_1)\cdots\overline{\pi}(i_n) f(i_1,\ldots,i_n,i'_1,\ldots i'_m)\,\pi(i'_m)\cdots\pi(i'_1) \\ &= \sum_{n,m=0}^{\infty} \frac{1}{n!\,m!} \sum_{\substack{i_1,\ldots,i_n \\ i'_1,i'_2,\ldots,i'_m}} \overline{\pi}(i_1)\cdots\overline{\pi}(i_n) f(i_1,\ldots,i_n,i'_1,\ldots i'_m)\,\pi(i'_m)\cdots\pi(i'_1) \end{aligned} \tag{16.45}$$

with complex-valued coefficients $f(i_1,\ldots,i_n,i'_1,\ldots i'_m)\in\mathbb{C}$, such that

$$f(i_{\pi(1)},\ldots,i_{\pi(n)},i'_{\sigma(1)},\ldots,i'_{\sigma(m)}) = \mathrm{sgn}(\pi)^{1-\theta(\zeta)}\,\mathrm{sgn}(\sigma)^{1-\theta(\zeta)}\,f(i_1,\ldots,i_n,i'_1,\ldots,i'_m)$$

for $(\pi,\sigma)\in \mathrm{S}_n\times\mathrm{S}_m$.

Remark 16.36.1 Later we will also encounter the situation that the coefficients f take values in an algebra. In this case one has to pay special attention to differentiation-rules TBElaborated.

Remark 16.36.2 Sometimes[10] one might find oneself in the situation that one has access to a series-expansion of the type

$$F[\pi,\overline{\pi}] \equiv \sum_{n,m=0}^{\infty} \sum_{\substack{i_1,\ldots,i_n \\ i'_1,i'_2,\ldots,i'_m}} \overline{\pi}(i_1)\cdots\overline{\pi}(i_n)\widetilde{f}(i_1,\ldots,i_n,i'_1,\ldots i'_m)\,\pi(i'_m)\cdots\pi(i'_1) \tag{16.46}$$

with complex-valued coefficients $\widetilde{f}(i_1,\ldots,i_n,i'_1,\ldots i'_m)\in\mathbb{C}$ that do not obey any symmetry properties. In this case, one has to identify the coefficients f in the expansion in Equation (16.45) as the properly antisymmetrized contributions.

Remark 16.36.3 Sometimes (but not in this work ;-)) the prefactors $(n!m!)^{-1}$ are included in the vertex-functions, such that the definition changes slightly.

Remark 16.36.4 One notates the individual coefficients depending on the functional of consideration, whereas the exact meaning of the word "generate" will be elucidated below.

[9] To avoid double counting.
[10] For example, in the later chapter on electron-phonon-systems.

Functional F	Fields $\pi, \overline{\pi}$	Coefficients f	Purpose
$S[\psi, \overline{\psi}]$	$\psi, \overline{\psi}$	s	Defines the System
$Z[j, \overline{j}]/Z$	$j, \overline{j}$	z	"Generates" Green-functions
$W[j, \overline{j}]$	$j, \overline{j}$	w	"Generates" connected Green-functions
$\Gamma[\phi, \overline{\phi}]$	$\phi, \overline{\phi}$	γ	"Generates" vertex-functions

Table 16.1.: Summary of the functional expansions and their roles.

Lemma 16.37 For $n = m = 2$ one obtains f from $\widetilde{f}$ as

$$f_{1,2,3,4} = \frac{1}{4}\left(\widetilde{f}_{1,2,3,4} + \zeta\,\widetilde{f}_{2,1,3,4} + \zeta\,\widetilde{f}_{1,2,4,3} + \widetilde{f}_{2,1,4,3}\right) \tag{16.47}$$

Proof 16.37 See Appendix, Proofs, page 573.

Remark 16.37.1 Notice that we thous obtain only one surviving contribution is for $\zeta = +1$ given by $f^{\text{sym, sym}}$ and for $\zeta = -1$ it is $f^{\text{as, as}}$.

Fact 16.38 Without proof, we inform the reader that one can apply the same symmetrization-scheme for $n = m = 3$ as

$$f_{1,2,3,4,5,6} = \left(\frac{1}{3!}\right)^2 \sum_{\sigma,\tau \in \mathrm{S}_3} \left[\operatorname{sgn}(\sigma)\operatorname{sgn}(\tau)\right]^{\frac{1-\zeta}{2}} \widetilde{f}_{\sigma(1),\sigma(2),\sigma(3),\tau(4),\tau(5),\tau(6)} \tag{16.48}$$

and generalizations of this formula for the general case.

Remark 16.38.1 *Correction note on Lemma 16.37 and the Fact above.* The prefactors $\frac{1}{4}$ and $\left(\frac{1}{3!}\right)^2$ produce the (anti)symmetric part $f^{(\mathrm{a})\mathrm{s}}$ of $\widetilde{f}$, i.e. the coefficients with $\sum \overline{\pi}\,\overline{\pi}\,\widetilde{f}\,\pi\pi = \sum \overline{\pi}\,\overline{\pi}\,f^{(\mathrm{a})\mathrm{s}}\pi\pi$ *without* factorial prefactor (this is what the proof on page 573 shows). They are *not* the coefficients f of Equation (16.45), which carry the prefactor $\frac{1}{n!\,m!}$. Comparing

$$\sum_{1,2,3,4} \overline{\pi}_1\overline{\pi}_2\,\widetilde{f}_{1,2,3,4}\,\pi_4\pi_3 = \frac{1}{(2!)^2}\sum_{1,2,3,4} \overline{\pi}_1\overline{\pi}_2\,f_{1,2,3,4}\,\pi_4\pi_3$$

gives instead

$$f_{1,2,3,4} = \widetilde{f}_{1,2,3,4} + \zeta\,\widetilde{f}_{2,1,3,4} + \zeta\,\widetilde{f}_{1,2,4,3} + \widetilde{f}_{2,1,4,3} = (2!)^2\,f^{(\mathrm{a})\mathrm{s}}_{1,2,3,4},$$

i.e. the Lemma is off by a factor $(2!)^2 = 4$, and analogously the formula of the Fact is off by a factor $(3!)^2 = 36$ (the correct coefficient is $\sum_{\sigma,\tau\in\mathrm{S}_3}[\operatorname{sgn}(\sigma)\operatorname{sgn}(\tau)]^{(1-\zeta)/2}\widetilde{f}_{\sigma(1),\sigma(2),\sigma(3),\tau(4),\tau(5),\tau(6)}$ without the prefactor). Only these

coefficients are reproduced by the derivatives in Lemma 16.39; this has been checked numerically for both statistics and $n = m = 2, 3$. Cf. also Lemma 19.24.

Lemma 16.39 Notice that we obtain the identity

$$f(i_1, \dots, i_n \mid i'_1, \dots, i'_m) = \zeta^{nm+n(n-1)/2+m(m-1)/2} \frac{\partial^{n+m}}{\partial\overline{\pi}(i_1) \cdots \partial\overline{\pi}(i_n)\partial\pi(i'_m) \cdots \partial\pi(i'_1)} F[\overline{\pi}, \pi]\Big|_{\overline{\pi}=\pi=0} \tag{16.49}$$

Proof 16.39 See Appendix, Proofs, page 574.

Remark 16.39.1 Notice that in the special case that $m = n$ one obtains

$$\zeta^{nm+n(n-1)/2+m(m-1)/2} = \zeta^{n^2+n(n-1)} = \zeta^{n^2} = \zeta^n \tag{16.50}$$

whereas we used in the second last step that the number $n(n-1)$ is even and in the last step, we used that n is even / odd if n^2 is even / odd, which is something that one learns in the first semester of mathematics (usually when one proves that $\sqrt{2}$ is irrational). Thus one finds

$$f(i_1, \dots, i_n \mid i'_1, \dots, i'_n) = \zeta^n \frac{\partial^{2n}}{\partial\overline{\pi}(i_1) \cdots \partial\overline{\pi}(i_n)\partial\pi(i'_n) \cdots \partial\pi(i'_1)} F[\overline{\pi}, \pi]\Big|_{\overline{\pi}=\pi=0} \tag{16.51}$$

Lemma 16.40 The n-body Green-function as functional derivative

$$\mathscr{G}(i_1, \dots, i_n \mid i'_1, \dots, i'_n) = \left(-\frac{\zeta}{c}\right)^n \frac{\partial^{2n}}{\partial\overline{j}(i_1) \cdots \partial\overline{j}(i_n)\partial j(i'_n) \cdots \partial j(i'_1)} \frac{Z[\overline{j}, j]}{Z}\Big|_{\overline{j}=j=0} \tag{16.52}$$

Proof 16.40 See Appendix, Proofs, page 575.

Remark 16.40.1 One obtains thus

$$\mathscr{G}(i_1, \dots, i_n \mid i'_1, \dots, i'_n) = \left(-\frac{1}{c}\right)^n z(i_1, \dots, i_n \mid i'_1, \dots, i'_n) \tag{16.53}$$

and one says that the functional $Z[\overline{j}, j]/Z$ *generates* the Green-functions, since it's expansion coefficients are equal to the Green-functions.

Definition 16.41 We introduce the *[c]onnected Green-functions* as

$$\mathscr{G}_c(i_1, \dots, i_n \mid i'_1, \dots, i'_n) := \left(-\frac{\zeta}{\hbar}\right)^n \frac{\partial^{2n}}{\partial\overline{j}(i_1) \cdots \partial\overline{j}(i_n)\partial j(i'_n) \cdots \partial j(i'_1)} W[\overline{j}, j]\Big|_{\overline{j}=j=0} \tag{16.54}$$

Remark 16.41.1 The fact that this functional generates all connected diagrams is far from trivial. We will come back to this statement in a later chapter.[11].

Remark 16.41.2 One obtains thus

$$\mathcal{G}_c(i_1, \dots, i_n \mid i'_1, \dots, i'_n) = \left(-\frac{1}{\hbar}\right)^n w(i_1, \dots, i_n \mid i'_1, \dots, i'_n) \tag{16.55}$$

and one says that the functional $W[\bar{j}, j]$ *generates* the *connect* Green-functions, since it's expansion coefficients are equal to the Green-functions.

Definition 16.42 We introduce the *vertex-functions* Vert by taking successive derivatives of Γ at the point $\phi = \overline{\phi} = 0$ as

$$\mathrm{Vert}(i_1, \dots, i_n, i'_1, \dots, i'_n) := \left(-\frac{\hbar}{\zeta}\right)^n \frac{\partial^{2n}}{\partial\overline{\phi}(i_1) \cdots \partial\overline{\phi}(i_n)\partial\phi(i'_n) \cdots \partial\phi(i'_1)} \Gamma[\overline{\phi}, \phi]\Big|_{\overline{\phi}=\phi=0} \tag{16.56}$$

Remark 16.42.1 Notice that this implies for the coefficients

$$\mathrm{Vert}(i_1, \dots, i_n, i'_1, \dots, i'_n) = (-\hbar)^n \gamma(i_1, \dots, i_n, i'_1, \dots, i'_n) \tag{16.57}$$

Remark 16.42.2 The particular vertex-function $\gamma(i_1, i_2, i'_1, i'_2)$ is oftentimes [29, 4] referred to as the *effective interaction*. It is said to ...

"describe the true interaction between two particles in the many-body system".

This is however irritating because it doesn't neccessarily have the unit of an energy. Only after appropriate rescaling / change of basis can this vertex-function be interpreted as an interaction (with unit of energy). We will come back to this point in a later chapter.

Remark 16.42.3 One also says that the functional $\Gamma[\phi, \overline{\phi}]$ *generates* the vertex-functions.

Corollary 16.43 It holds

$$\begin{aligned} \mathcal{G}_c(i_1 \mid i'_1) &= \mathcal{G}(i_1 \mid i'_1) \\ \mathcal{G}_c(i_1, i_2 \mid i'_1, i'_2) &= \mathcal{G}(i_1, i_2 \mid i'_1, i'_2) - \left[\mathcal{G}(i_1 \mid i'_1)\mathcal{G}(i_2 \mid i'_2) + \zeta\mathcal{G}(i_1 \mid i'_2)\mathcal{G}(i_2 \mid i'_1)\right] \end{aligned} \tag{16.58}$$

[11] There is a lot about this to read in the literature, with no book proving the identity in the generality in which its circle of applicability is being claimed.

- See, for example, [4] p. 215 for an instruction-manual on how to construct the diagrams.
- See, for example, [38] p. 79 for control-result in first order.
- See, for example [38] p. 97 for the statement itself.
- See, for example [38] p. 107 for more information.

Proof 16.43 See Appendix, Proofs, page 576.

Lemma 16.44 One finds for a functional $F \equiv F[\bar{j}, j]$ the chain-rule

$$\begin{aligned}\frac{\partial}{\partial\phi(\bullet)}F[\bar{j},j] &= \sum_i \zeta\frac{\partial F}{\partial\bar{j}(i)}\frac{\partial^2\Gamma}{\partial\phi(\bullet)\partial\phi(i)} + \frac{\partial F}{\partial j(i)}\frac{\partial^2\Gamma}{\partial\phi(\bullet)\partial\bar{\phi}(i)}\\ \frac{\partial}{\partial\bar{\phi}(\bullet)}F[\bar{j},j] &= \sum_i \zeta\frac{\partial F}{\partial\bar{j}(i)}\frac{\partial^2\Gamma}{\partial\bar{\phi}(\bullet)\partial\phi(i)} + \frac{\partial F}{\partial j(i)}\frac{\partial^2\Gamma}{\partial\bar{\phi}(\bullet)\partial\bar{\phi}(i)}\end{aligned} \tag{16.59}$$

Proof 16.44 See Appendix, Proofs, page 576.

Corollary 16.45 It follows that

$$\sum_{i_2}\begin{pmatrix}\frac{\partial^2 W}{\partial\bar{j}(i_3)\partial j(i_2)} & \zeta\frac{\partial^2 W}{\partial\bar{j}(i_3)\partial\bar{j}(i_2)}\\ \zeta\frac{\partial^2 W}{\partial j(i_3)\partial j(i_2)} & \frac{\partial^2 W}{\partial j(i_3)\partial\bar{j}(i_2)}\end{pmatrix}\begin{pmatrix}\frac{\partial^2\Gamma}{\partial\bar{\phi}(i_2)\partial\phi(i_1)} & \frac{\partial^2\Gamma}{\partial\bar{\phi}(i_2)\partial\bar{\phi}(i_1)}\\ \frac{\partial^2\Gamma}{\partial\phi(i_2)\partial\phi(i_1)} & \frac{\partial^2\Gamma}{\partial\phi(i_2)\partial\bar{\phi}(i_1)}\end{pmatrix} = \delta_{i_1,i_3}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} \tag{16.60}$$

Proof 16.45 See Appendix, Proofs, page 577.

Lemma 16.46 In the absense of "spontaneous symmetry breaking"[12], we can write down the quadratic part of the effective action $\mathrm{Vert}(:,:)$ by simple inversion of a matrix:

$$\mathrm{Vert}(:,:) = \mathscr{G}_{\mathrm{c}}^{-1}(:,:) = \mathscr{G}^{-1}(:,:) \tag{16.61}$$

Proof 16.46 Using that the effective action has the same symmetries as the original action (cf. TBReferenced) we obtain from Equation (34.30) the simplified identity

$$\delta_{1,3} = \sum_2\left(-\frac{c}{\zeta}\mathscr{G}(2|3)\left(-\frac{\zeta}{c}\frac{\partial^2\Gamma}{\partial\bar{\phi}(1)\partial\phi(2)}\right)\right) = \sum_2\mathscr{G}(2|3)\,\mathrm{Vert}(1|2) = \sum_2\mathrm{Vert}(1|2)\mathscr{G}(2|3) \tag{16.62}$$

Thus we obtain

$$\Big[\mathrm{Vert}(:,:)\cdot\mathscr{G}(:,:)\Big]_{n,m} = \delta_{n,m} \quad\Longleftrightarrow\quad \mathrm{Vert} = \mathscr{G}^{-1} \tag{16.63}$$

which yields in matrix-notation the desired result.

[12] This will be introduced later.

Remark 16.46.1 Notice that from here, we can easily obtain the generic version of the Dyson-equation (cf. Equation (15.16))

$$\mathscr{G}^{-1} = \mathscr{G}_0^{-1} - \Sigma \tag{16.64}$$

by introducing the self-energy Σ as the difference between the inverse of the free Green-function and the inverse of the full Green-function. This result alone is already quite nice, but we will see (in the next chapter) that one can conclude the explicit shape of the self-energy as well from symmetry-principles which will be quite a revealing moment for the interested reader.

Remark 16.46.2 One can[13] also rewrite this equation in a more general way for system that have a broken symmetry, but we will not do this here for pedagogical purposes.

Theorem 16.47 In the absence of spontaneous symmetry breaking, another useful identity[14]. is

$$\mathscr{G}_{\mathrm{c}}(i_1, i_2 \mid i_1', i_2') = -\sum_{l_1, l_2, l_1', l_2'} \mathscr{G}_{\mathrm{c}}(i_1 \mid l_1)\mathscr{G}_{\mathrm{c}}(i_2 \mid l_2)\ \mathrm{Vert}(l_1, l_2 \mid l_1', l_2')\mathscr{G}_{\mathrm{c}}(l_1' \mid i_1')\mathscr{G}_{\mathrm{c}}(l_2' \mid i_2') \tag{16.65}$$

Proof 16.47 See Appendix, Proofs, page 578.

Remark 16.47.1 In a later chapter we will see how this can be rewritten diagrammatically[15].

Theorem 16.48 In the absence of spontaneous symmetry breaking, one concludes the *Bethe-Salpeter-equation for the two-body Green-function* as

$$\begin{aligned}\mathscr{G}(i_1, i_2 \mid i_1', i_2') = {} & \mathscr{G}(i_1 \mid i_1')\mathscr{G}(i_2 \mid i_2') + \zeta\mathscr{G}(i_1 \mid i_2')\mathscr{G}(i_2 \mid i_1') \\ & - \sum_{l_1, l_2, l_1', l_2'} \mathscr{G}(i_1 \mid l_1)\mathscr{G}(i_2 \mid l_2)\ \mathrm{Vert}(l_1, l_2 \mid l_1', l_2')\mathscr{G}(l_1' \mid i_1')\mathscr{G}(l_2' \mid i_2')\end{aligned} \tag{16.66}$$

Proof 16.48 Combining Corollary 16.43 and Theorem 16.47 and rearranging terms gives the desired result.

Hypothesis 16.49 With induction, one sees that the following three problems are equivalent, in the sense that if one of them is solved, the other two are solved as well:

[13] Cf. [38] Equation (7.52).

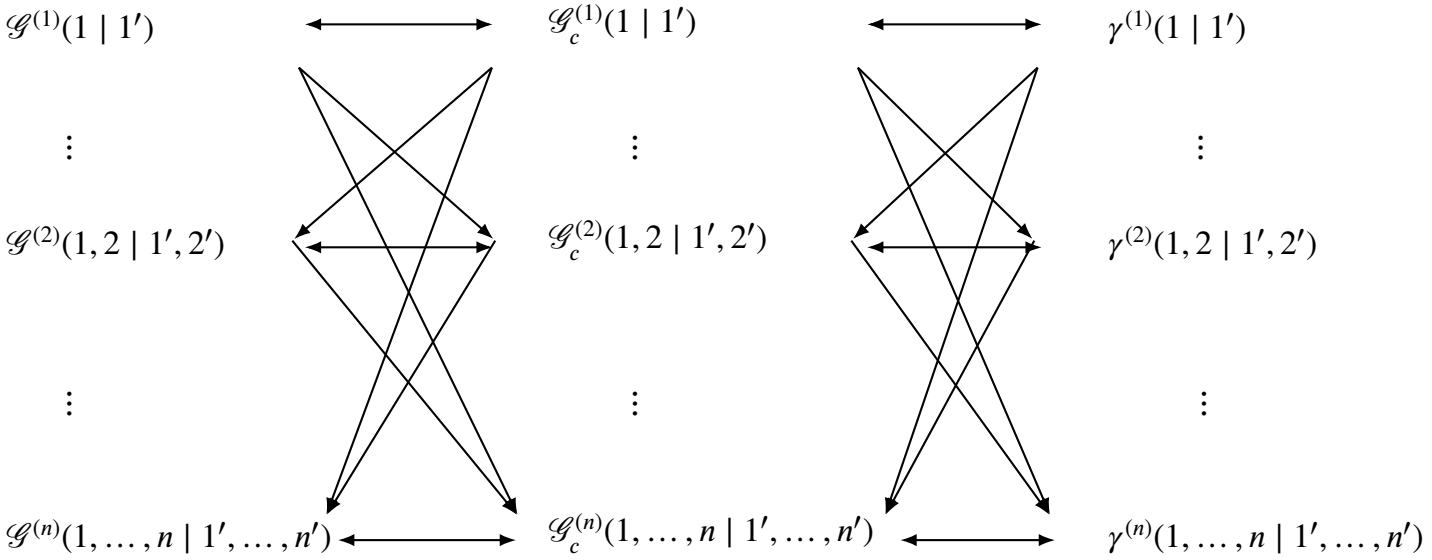
[14] Other identities that are relevant in this context are given in the literature. Cf. for example
- [38]. Negele p. 108.
- [38] Equation (6.79 a,b) Identity for quartic green-function as correlation-functions
- For the relations between $\mathscr{G}^{(6)}$ and $\Gamma^{(6)}$: see, for example, [36] Equation (12).

[15] See also [38] p. 118.

• *Finding all many-body Green-Functions*	$\mathcal{G}^{(1)}(i_1, i_1')$,	$\mathcal{G}^{(2)}(i_1, i_2, i_1', i_2')$, … ,	$\mathcal{G}^{(n)}(i_1, \dots, i_n, i_1', \dots, i_n')$
• *Finding all connected many-body Green-Functions*	$\mathcal{G}_c^{(1)}(i_1, i_1')$,	$\mathcal{G}_c^{(2)}(i_1, i_2, i_1', i_2')$, … ,	$\mathcal{G}_c^{(n)}(i_1, \dots, i_n, i_1', \dots, i_n')$
• *Finding all many-body vertex-Functions*	$\gamma^{(1)}(i_1, i_1')$,	$\gamma^{(2)}(i_1, i_2, i_1', i_2')$, … ,	$\gamma^{(n)}(i_1, \dots, i_n, i_1', \dots, i_n')$

Remark 16.49.1 For the lowest orders, this follows from the Equations derived in this section. It is a standard-folklore-statement that this is a general theorem (see, for example, [38]).

Remark 16.49.2 The picture visualizes the equivalence of the three problems.



16.1.6. Change of Coordinates

Notation 16.50 We consider an invertible linear mapping M (with complex conjugate $\overline{M}$) between integration-variables („coordinate-change“)

$$\psi_i \mapsto (M \cdot \psi)_i \equiv \sum_{i'} M_{i,i'}\, \psi_{i'}, \qquad \overline{\psi}_i \mapsto (\overline{M} \cdot \overline{\psi})_i \equiv \sum_{i'} \overline{M}_{i,i'}\, \overline{\psi}_{i'}$$

Remark 16.50.1 Notice that in the notation of physicists, this would be written as

$$\psi_i' = \psi_i'(\psi) = \sum_i M_{i',i}\psi_i, \qquad \overline{\psi}_i{}' = \overline{\psi}_i{}'(\psi) = \sum_i \overline{M}_{i',i}\overline{\psi}_i \tag{16.67}$$

Remark 16.50.2 Notice that this mapping changes a monomial expression in the integration-variables according to

$$\psi_{i_1}\cdots\psi_{i_n}\overline{\psi}_{i'_1}\cdots\overline{\psi}_{i'_m}\mapsto\sum_{\substack{j_1,\ldots,j_n\\ j'_1,j'_2,\ldots,j'_{m-1},j'_m}}\left(\prod_{l=1}^{n}M_{i_l,j_l}\right)\left(\prod_{l=1}^{m}\overline{M}_{i'_l j'_l}\right)\psi_{j_1}\cdots\psi_{j_n}\overline{\psi}_{j'_1}\cdots\overline{\psi}_{j'_m}\tag{16.68}$$

Remark 16.50.3 The most important transformation will turn out to be the Fourier-series. It removes the derivatives (if one concatenates the variable-transformation with a standard-approximation) s.t. we can simply invert the matrix appearing in the action.

Lemma 16.51 Changing the coordinates according to Equation (16.67) yields for the derivatives

$$\frac{\partial}{\partial\psi'_i}=\sum_i\frac{\partial\psi_i}{\partial\psi'_i}\frac{\partial}{\partial\psi_i},\qquad\frac{\partial}{\partial\overline{\psi}_i{}'}=\sum_i\frac{\partial\overline{\psi}_i}{\partial\overline{\psi}_i{}'}\frac{\partial}{\partial\overline{\psi}_i}\tag{16.69}$$

Proof 16.51 See, for example, [60] p. 11.

Lemma 16.52 Changing the coordinates according to Equation (16.67) changes the integration-measure as

$$\mathrm{d}_\zeta(\overline{\psi}',\psi')\equiv\mathrm{Det}\left(\frac{\partial\psi'_i}{\partial\psi_j}\right)^{\zeta}\mathrm{Det}\left(\frac{\partial\overline{\psi}_i{}'}{\partial\overline{\psi}_j}\right)^{\zeta}\mathrm{d}_\zeta(\overline{\psi},\psi)\tag{16.70}$$

Proof 16.52 TBDone.

Theorem 16.53 Assuming that one has statistical variables

$$\phi=\phi(\eta,\overline{\eta}),\qquad\overline{\phi}=\overline{\phi}(\eta,\overline{\eta})\tag{16.71}$$

we introduce the jacobian J as

$$J=\frac{\partial(\phi,\overline{\phi})}{\partial(\eta,\overline{\eta})}\tag{16.72}$$

then we obtain the *transformation-formula* as

$$\int\mathrm{d}(\overline{\phi},\phi)F(\overline{\phi},\phi)=(\det J)^{\zeta}\int\mathrm{d}(\overline{\eta},\eta)F\left(\overline{\phi}(\overline{\eta},\eta),\phi(\overline{\eta},\eta)\right)\tag{16.73}$$

Proof 16.53 See in the literature [TBReferenced]

Corollary 16.54 Emphasizing the role of the matrices A and $M(A) \equiv M^\dagger A M$ into the notation, we obtain the important result

$$\langle \psi_{i_1} \cdots \psi_{i_n} \overline{\psi}_{i'_1} \cdots \overline{\psi}_{i'_m} \rangle_\zeta[A] = \sum_{\substack{j_1,\ldots,j_n \\ j'_1,j'_2,\ldots,j'_{m-1},j'_m}} \left(\prod_{l=1}^{n} M_{i_l,j_l} \right) \left(\prod_{l=1}^{m} \overline{M}_{i'_l j'_l} \right) \langle \psi_{j_1} \cdots \psi_{j_n} \overline{\psi}_{j'_1} \cdots \overline{\psi}_{j'_m} \rangle_\zeta[M(A)]$$

Proof 16.54 See Appendix, Proofs, page **??**.

Using this mapping as transformation-matrix, we obtain for the partition-function the scaling-factor

$$Z_\zeta[A] \equiv \int \mathrm{d}_\zeta(\overline{\psi}, \psi)\, \mathrm{e}^{-\psi^\dagger A \psi} \equiv \mathrm{Det}\, M^{-\zeta} \int \mathrm{d}_\zeta(\overline{\psi}, \psi)\, \mathrm{e}^{-\psi^\dagger M^\dagger A M \psi} \equiv \mathrm{Det}\, M^{-\zeta} \cdot Z_\zeta[\widetilde{A}]$$

and equally we obtain another scaling-factor for the numerator in the expression of the expectation-value.

Remark 16.54.1 Notice that in the case of a simple transformation as

$$\begin{pmatrix} \phi \\ \overline{\phi} \end{pmatrix} = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} \begin{pmatrix} \eta \\ \overline{\eta} \end{pmatrix} \tag{16.74}$$

such that one has

$$\det J = \det A \det B. \tag{16.75}$$

16.1.7. The Tree-Level-Approximation for the Effective Action

Approximation 16.55 In the so-called Tree-Level-Approximation, one obtains for the fermionic effective action

$$\Gamma[\phi, \overline{\phi}] \quad \approx \quad S[\phi, \overline{\phi}]. \tag{16.76}$$

Proof 16.55 See Appendix, Proofs, page 582.

Remark 16.55.1 This approximation is usually depicted with Feynman-diagrams as in the figure

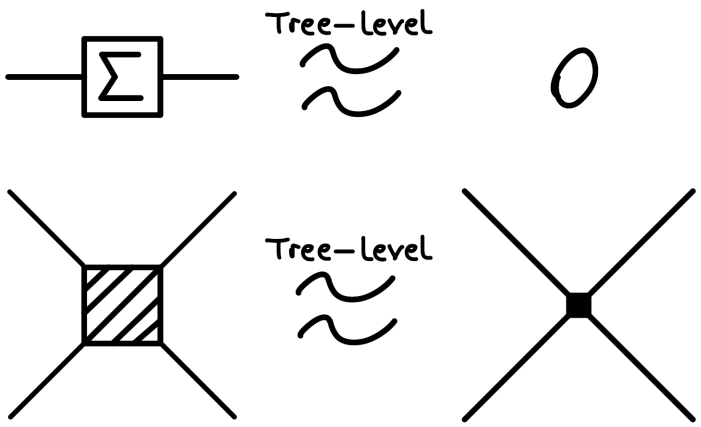


Figure 16.1.: Feynman-Diagrams (schematically) for the Tree-Level-Approximation.

Corollary 16.56 Within the Tree-Level-Approximation, equations (16.44) and (16.76) can be combined, which gives

$$\frac{\partial}{\partial \phi} S[\phi, \overline{\phi}] = \overline{j} \qquad \text{and} \qquad \frac{\partial}{\partial \overline{\phi}} S[\phi, \overline{\phi}] = -j. \tag{16.77}$$

Proof 16.56 Follows immediately from the approximation and Remark 16.35.

16.1.8. The One-Loop-Approximation for the Effective Action

Approximation 16.57 In the so-called One-Loop-Approximation, one obtains for the fermionic effective action

$$\Gamma[\phi, \overline{\phi}] \approx S[\phi, \overline{\phi}] - \frac{1}{2} \operatorname{Tr} \log \begin{pmatrix} \frac{\partial^2}{\partial \phi \, \partial \phi} S[\phi, \overline{\phi}] & \frac{\partial^2}{\partial \phi \, \partial \overline{\phi}} S[\phi, \overline{\phi}] \\ \frac{\partial^2}{\partial \overline{\phi} \, \partial \phi} S[\phi, \overline{\phi}] & \frac{\partial^2}{\partial \overline{\phi} \, \partial \overline{\phi}} S[\phi, \overline{\phi}] \end{pmatrix}, \tag{16.78}$$

where

$$\left(\frac{\partial^2}{\partial \phi \, \partial \phi} S[\phi, \overline{\phi}] \right) \equiv \left(\frac{\partial^2}{\partial \phi \, \partial \phi} S[\phi, \overline{\phi}] \right) (i, j) \equiv \frac{\partial^2}{\partial \phi(i) \, \partial \phi(j)} S[\phi, \overline{\phi}], \quad \text{etc.}$$

Proof 16.57 See Appendix, Proofs, page 584.

Approximation 16.58 Expanding the r.h.s. of eq. (16.78) up to quartic order in the Graßmann-fields and neglecting higher order terms yields

$$\begin{aligned}\Gamma[\phi,\overline{\phi}] \quad \approx \quad S[\phi,\overline{\phi}] \quad - \quad & \mathrm{Tr}\left[G_0 \cdot \frac{\partial^2}{\partial\overline{\phi}\,\partial\phi} S_{\mathrm{int}}[\phi,\overline{\phi}]\right] \\ - \quad \frac{1}{2} \quad & \mathrm{Tr}\left[G_0 \cdot \frac{\partial^2}{\partial\overline{\phi}\,\partial\overline{\phi}} S_{\mathrm{int}}[\phi,\overline{\phi}] \cdot G_0^{\mathrm{T}} \cdot \frac{\partial^2}{\partial\phi\,\partial\phi} S_{\mathrm{int}}[\phi,\overline{\phi}]\right] \\ + \quad \frac{1}{2} \quad & \mathrm{Tr}\left[G_0 \cdot \frac{\partial^2}{\partial\overline{\phi}\,\partial\phi} S_{\mathrm{int}}[\phi,\overline{\phi}] \cdot G_0 \cdot \frac{\partial^2}{\partial\overline{\phi}\,\partial\phi} S_{\mathrm{int}}[\phi,\overline{\phi}]\right]\end{aligned} \tag{16.79}$$

Proof 16.58 See Appendix, Proofs, page 585.

Remark 16.58.1 This approximation is usually depicted with Feynman-diagrams as in the figure. The corrections to the Tree-Level contribution of the effective interaction $\gamma(x_1, x_2, x_3, x_4)$ are the particle-particle- and particle-hole-diagrams respectively.

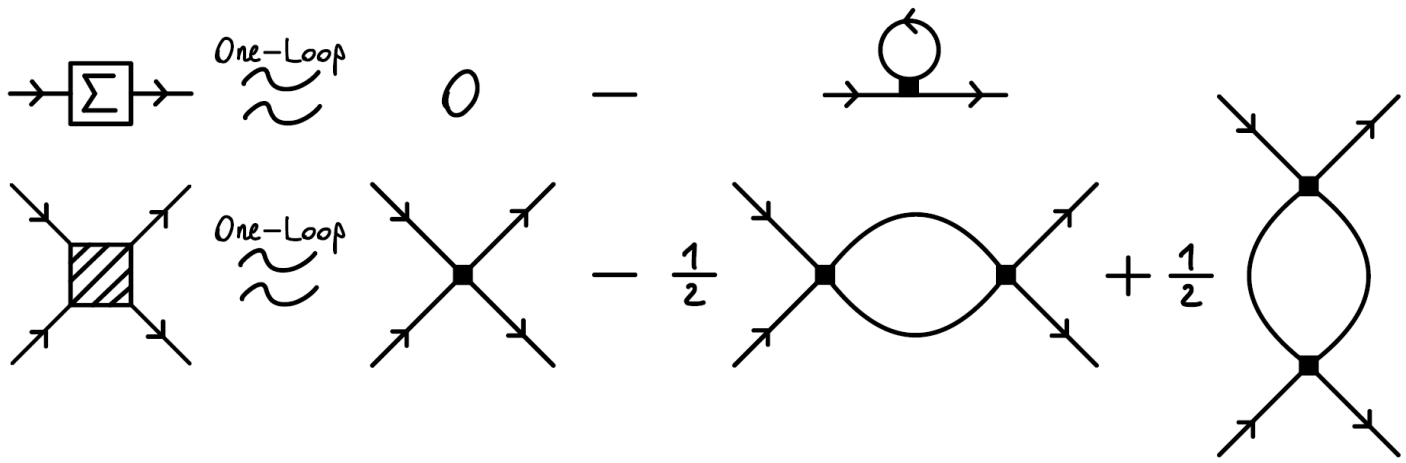


Figure 16.2.: Feynman-Diagrams (schematically) for the One-Loop-Approximation.

16.2. Quantum Field Theory - Mixed Systems

16.2.1. Fundamentals

TBCopied (a lot from Zinn-Justin).

16.2.2. Partition-Functions and Expectation-Values for Non-Interacting Models

TBD

16.2.3. Partition-Functions and Expectation-Values for Interacting Models

TBD

16.2.4. Gauss-Identities

TBD

16.2.5. External Sources, Connected Green-Functions and Vertex-Functions

TBD

17. More Algebraic Concepts in Quantum Field Theory

17.1. A General Comment

Definition 17.1 We call a polynomial expression in statistical variables X to be *self-conjugated* iff $X^\dagger = X$.

Fact 17.2 If a quartic interaction ... can be rewritten as a bilinear with ...

- a self-conjugated expression, one decouples it with a "real auxiliary-field".
- a not-self-conjugated expression, one decouples it with a "complex auxiliary-field".

Remark 17.2.1 Since the notation is weird inside the literature, we will not speak about the different channels, except for the "Cooper-channel". Whereas all words that are written in quotation-marks will be introduced in the course of this chapter.

17.2. The "Complex" Hubbard-Stratonovich Transformations for Quartic Interactions

17.2.1. The Fundamental Identities

Definition 17.3 Let V be Hermitian and positive definite on $\mathbb{C}^N$. For a complex auxiliary field $\Delta \in \mathbb{C}^N$, we introduce the *Normalized complex Gaussian measure*

$$\int \mathrm{d}\mu_V(\Delta, \overline{\Delta}) F(\Delta, \overline{\Delta}) \equiv \det\left(V^{-1}\right) \int \mathrm{d}_{+1}(\Delta, \overline{\Delta}) \exp\left(-\Delta^\dagger V^{-1} \Delta\right) F(\Delta, \overline{\Delta}). \tag{17.1}$$

Lemma 17.4 The measure $\mathrm{d}\mu_V$ is *normalized*, i.e. $\int \mathrm{d}\mu_V(\Delta, \overline{\Delta}) = 1$.

Proof 17.4 Apply Lemma 16.18 for bosons ($\zeta = +1$) with $A = V^{-1}$, which is invertible, since V is positive definite. This gives $\int \mathrm{d}_{+1}(\Delta, \overline{\Delta}) \exp\left(-\Delta^\dagger V^{-1} \Delta\right) = 1/\det\left(V^{-1}\right)$, which cancels the prefactor $\det\left(V^{-1}\right)$ in the definition of $\mathrm{d}\mu_V$.

Lemma 17.5 For every $j \in \mathbb{C}^N$ we introduce the *complex Gaussian generating function with conjugate sources* as

$$\int \mathrm{d}\mu_V(\Delta, \overline{\Delta}) \exp\left(\Delta^\dagger j + j^\dagger \Delta\right) = \exp\left(j^\dagger V j\right). \tag{17.2}$$

Proof 17.5 See Appendix, Proofs, page 587.

Notation 17.6 We introduce the auxiliary functions

$$\begin{aligned} G(j,K) &\equiv \int \mathrm{d}\mu_V(\Delta, \overline{\Delta}) \quad \exp\left(\Delta^\dagger j + K^\mathsf{T} \Delta\right) \\ E(j,K) &\equiv \qquad\qquad\qquad\quad \exp\left(K^\mathsf{T} V j\right) \end{aligned} \tag{17.3}$$

Something is wrong here with the order of logic...

Lemma 17.7 For all $j, K \in \mathbb{C}^N$ which represent *independent sources*[1], we introduce and prove

$$G(j,K) \equiv \int \mathrm{d}\mu_V(\Delta, \overline{\Delta}) \exp\left(\Delta^\dagger j + K^\mathsf{T} \Delta\right) \overset{\text{Claim}}{=} \exp\left(K^\mathsf{T} V j\right) \equiv E(j,K). \tag{17.4}$$

Proof 17.7 See Appendix, Proofs, page 587.

Lemma 17.8 For multi-indices $\alpha, \beta \in \mathbb{N}_0^N$ write $j^\alpha = \prod_a j_a^{\alpha_a}$, $\alpha! = \prod_a \alpha_a!$, and expand the entire function

$$E(j,K) = \exp\left(K^\mathsf{T} V j\right) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(K^\mathsf{T} V j\right)^n = \sum_{\alpha,\beta} c_{\alpha\beta}\, j^\alpha K^\beta.$$

Then we have the *moments*

$$\int \mathrm{d}\mu_V(\Delta, \overline{\Delta})\, \overline{\Delta}^\alpha \Delta^\beta = \alpha!\, \beta!\, c_{\alpha\beta}. \tag{17.5}$$

Proof 17.8 See Appendix, Proofs, page 587.

Lemma 17.9 Let $j_1, \ldots, j_N, K_1, \ldots, K_N$ be *Grassmann-even sources* without body. Then Equation (17.4) still holds,

[1] I.e. they are *not* necessarily related by e.g. $K = \overline{j}$.

$$\int \mathrm{d}\mu_V(\Delta, \overline{\Delta}) \, \exp\left(\Delta^\dagger j + K^\mathsf{T} \Delta\right) = \exp\left(K^\mathsf{T} V j\right),$$

where the integral of a Grassmann-valued integrand is taken coefficient by coefficient in a basis of the Grassmann algebra.

Proof 17.9 See Appendix, Proofs, page 588.

Theorem 17.10 Assume the following.

1. $V \in \mathrm{Mat}_{N\times N}(\mathbb{C})$ is *Hermitian*, $V^\dagger = V$.
2. V is *positive definite*[2].
3. $P = (P_1, \ldots, P_N)$ and $\overline{\mathrm{Q}} = (\overline{\mathrm{Q}}_1, \ldots, \overline{\mathrm{Q}}_N)$ are Grassmann-even elements without body[3] $\overline{\mathrm{Q}}$ is *entirely independent* of P: it may, but need not, be the conjugate partner $\overline{P}$ of P.

Then the *complex Hubbard-Stratonovich-transformation* holds in both sign versions,

$$\begin{aligned} \exp\left(-\overline{\mathrm{Q}}^\mathsf{T} V P\right) &= \int \mathrm{d}\mu_V(\Delta, \overline{\Delta}) \exp \mathrm{i} \left[\Delta^\dagger P + \overline{\mathrm{Q}}^\mathsf{T} \Delta\right], \\ \exp\left(+\overline{\mathrm{Q}}^\mathsf{T} V P\right) &= \int \mathrm{d}\mu_V(\Delta, \overline{\Delta}) \exp 1 \left[\Delta^\dagger P + \overline{\mathrm{Q}}^\mathsf{T} \Delta\right]. \end{aligned} \tag{17.6}$$

Proof 17.10 See Appendix, Proofs, page 588.

If something is not hermitian, one might be able to use some trixxx... Maybe this will be important soon...

[2] Recall that this means that $x^\dagger V x > 0$ for all $0 \neq x \in \mathbb{C}^N$, or (equivalently) that all (real) eigenvalues of V are strictly positive.
[3] Notice that this represents, for example, bilinears in finitely many Grassmann generators.

17.3. The "Real" Hubbard-Stratonovich Transformations for Quartic Interactions

17.3.1. The finite-dimensional Hubbard–Stratonovich identity

Definition 17.11 Let $V \in \mathrm{Mat}_{N\times N}(\mathbb{R})$ be real, symmetric, and positive definite. For a commuting vector $\varphi \in \mathbb{R}^N$, define the *expectation-value of* F *relative to* V as

$$\int \mathrm{d}\mu_V(\varphi)\, F(\varphi) \equiv \frac{1}{\sqrt{\det(2\pi V)}} \int_{\mathbb{R}^N} \mathrm{d}^N\varphi\, \exp\left(-\frac{1}{2}\varphi^{\mathsf{T}} V^{-1}\varphi\right) F(\varphi). \tag{17.7}$$

Thus $\int \mathrm{d}\mu_V = 1$.

Lemma 17.12 For every commuting source $j \in \mathbb{C}^N$, we obtain *the ordinary Gaussian generating function*

$$\int \mathrm{d}\mu_V(\varphi)\, \exp\left(j^{\mathsf{T}}\varphi\right) = \exp\left(\frac{1}{2} j^{\mathsf{T}} V j\right). \tag{17.8}$$

Proof 17.12 See Appendix, Proofs, page 588.

Theorem 17.13 Let $V \in \mathrm{Mat}_{N\times N}(\mathbb{R})$ be real, symmetric, and positive definite and let $\rho \in \mathbb{C}^N$ be a vector of mutually commuting quantities. Then *the Real Hubbard–Stratonovich transformation* holds in both sign versions,

$$\begin{aligned}
\exp\left(-\frac{1}{2}\rho^{\mathsf{T}} V \rho\right) &= \int \mathrm{d}\mu_V(\varphi) \exp\left(-\mathrm{i}\,\varphi^{\mathsf{T}}\rho\right) = \frac{1}{\sqrt{\det(2\pi V)}} \int_{\mathbb{R}^N} \mathrm{d}^N\varphi\, \exp\left(-\frac{1}{2}\varphi^{\mathsf{T}} V^{-1}\varphi - \mathrm{i}\,\varphi^{\mathsf{T}}\rho\right), \\
\exp\left(+\frac{1}{2}\rho^{\mathsf{T}} V \rho\right) &= \int \mathrm{d}\mu_V(\varphi) \exp\left(+1\varphi^{\mathsf{T}}\rho\right) = \frac{1}{\sqrt{\det(2\pi V)}} \int_{\mathbb{R}^N} \mathrm{d}^N\varphi\, \exp\left(-\frac{1}{2}\varphi^{\mathsf{T}} V^{-1}\varphi + 1\varphi^{\mathsf{T}}\rho\right).
\end{aligned} \tag{17.9}$$

Proof 17.13 See Appendix, Proofs, page 589.

18. Symmetry-Transformations

18.1. Pure Systems

18.1.1. Introduction

In this section we will see how symmetry considerations will constrain the shape of the coefficients γ.

Definition 18.1 We call an invertible linear mapping M (with complex conjugate $\overline{M}$) between Graßmann-fields

$$\psi(x) \mapsto (M \cdot \psi)(i) \equiv \sum_y M(i,j)\,\psi(j), \qquad \overline{\psi}(i) \mapsto (\overline{M} \cdot \overline{\psi})(i) \equiv \sum_y \overline{M}(i,j)\,\overline{\psi}(j)$$

a *symmetry transformation* if both, the integration measure and the action remain unchanged under the action of the mapping M (and $\overline{M}$):

$$\mathscr{D}(\psi,\overline{\psi}) = \mathscr{D}(M \cdot \psi, \overline{M} \cdot \overline{\psi}) \quad \text{and} \quad S[\psi,\overline{\psi}] = S[M \cdot \psi, \overline{M} \cdot \overline{\psi}]. \tag{18.1}$$

Remark 18.1.1 The set of all symmetry transformations, equipped with composition as binary-operation, is a group. For each action and integration measure one refers to this group as the "symmetry group" of the problem [29].

Lemma 18.2 For a symmetry transformation M one has

$$W[j,\bar{j}] = W[\overline{M}^{\mathrm{T}} \cdot j, M^{\mathrm{T}} \cdot \bar{j}]. \tag{18.2}$$

implying the equations

$$\phi[\bullet, \overline{M}^{\mathrm{T}} \cdot j, M^{\mathrm{T}} \cdot \bar{j}] = (M^{-1} \cdot \phi)[\bullet, j, \bar{j}],$$
$$\overline{\phi}[\bullet, \overline{M}^{\mathrm{T}} \cdot j, M^{\mathrm{T}} \cdot \bar{j}] = (\overline{M}^{-1} \cdot \overline{\phi})[\bullet, j, \bar{j}].$$

Proof 18.2 See Appendix, Proofs, page 594.

Theorem 18.3 With the above preparations one obtains for a symmetry transformation M the equation

$$\Gamma[\phi, \overline{\phi}] = \Gamma[M^{-1} \cdot \phi, \overline{M}^{-1} \cdot \overline{\phi}]. \tag{18.3}$$

Proof 18.3 See Appendix, Proofs, page 595.

Remark 18.3.1 Thus, by equation (18.3) we obtain for each symmetry transformation M (respectively its inverse M^{-1}), by comparing coefficients, restricting conditions for the vertex-functions:

$$\gamma(i_1, \dots, i_n, j_1, \dots, j_m) = \sum_{\substack{\tilde{i}_1, \dots, \tilde{i}_n \\ \tilde{j}_1, \tilde{j}_2, \dots, \tilde{j}_{m-1}, \tilde{j}_m}} \left(\prod_{l=1}^{n} \overline{M}(i_l, \tilde{i}_l) \right) \left(\prod_{l=1}^{m} M(j_l, \tilde{j}_l) \right) \gamma(\tilde{i}_1, \dots, \tilde{i}_n, \tilde{j}_1, \dots, \tilde{j}_m)$$

The shape of the coefficients is therefore dictated by the symmetries of the underlying physical system. This realization will simplify concrete calculations later.

Remark 18.3.2 The above results can be memorized by the following sentence from [10]:

The effective action Γ *shares all the symmetries of the action* S.

Remark 18.3.3 Equation (18.2) gives analogous results for the free energy W.

Remark 18.3.4 The figure summarizes the results pictographically.

$$\left.\begin{array}{l} S[\varphi,\overline{\varphi}] = S[M\cdot\varphi, \overline{M}\cdot\overline{\varphi}] \\ \mathcal{Q}(\varphi,\overline{\varphi}) = \mathcal{Q}(M\cdot\varphi, \overline{M}\cdot\overline{\varphi}) \end{array}\right\} \Longleftrightarrow W[j,\overline{j}] = W[\overline{M}^{\mathsf{T}}\cdot j, M^{\mathsf{T}}\cdot\overline{j}] \Longleftrightarrow \Gamma[\phi,\overline{\phi}] = \Gamma[M^{-1}\cdot\phi, \overline{M}^{-1}\cdot\overline{\phi}]$$

Figure 18.1.: Summary for Symmetry Transformations.

18.1.2. Implications

TBCopied from [27, 43].

18.2. Mixed Systems

TBD.

18.2.1. Introduction

TBD.

18.2.2. Implications

TBD.

19. Functional Renormalization

In this chapter we formulate the functional renormalization group (FRG) in the conventions of these notes. The presentation follows [27], where everything was formulated for fermionic systems only, with continuous "generalized indices" and with a different sign-convention for the free energy. In comparison to [27] ...

- we treat bosonic ($\zeta = +1$) and fermionic ($\zeta = -1$) systems simultaneously,
- we use the conventions of Chapter 16, i.e.

$$W[\bar{j}, j] = +\log Z[\bar{j}, j], \qquad \phi_i = \frac{\partial W}{\partial \bar{j}_i}, \qquad \bar{\phi}_i = \zeta \frac{\partial W}{\partial j_i}, \qquad \Gamma[\phi, \bar{\phi}] = -W[\bar{j}, j] + \phi^\dagger j + j^\dagger \phi,$$

  whereas *all* derivatives are left-derivatives,
- we use exclusively discrete indices, such that all "functional integrals" are finite-dimensional integrals, all "functional derivatives" are partial derivatives and all Dirac-deltas are replaced by Kronecker-deltas,
- we keep the feedback of the self-energy into the flow-equations of the vertex-functions.

All derivations are kept in the main text (and not in the appendix), such that every single sign can be checked directly. We write $\phi_i \equiv \phi(i)$, $j_i \equiv j(i)$, etc. and for second derivatives

$$\frac{\partial^2 F}{\partial \pi_x \, \partial \pi'_y} \equiv \frac{\partial}{\partial \pi_x} \frac{\partial}{\partial \pi'_y} F,$$

i.e. the right-most derivative acts first.

19.1. Functional Differential Equation for the Free Energy

Notation 19.1 We consider the setting of Notation 16.24 and Notation 16.27: Statistical variables $\psi_i, \overline{\psi}_i$ with discrete indices $i \in \{1, \dots, D\}$, the action

$$S[\psi, \overline{\psi}] = \underbrace{\sum_{i,i'} \overline{\psi}_i \, A_{i,i'} \, \psi_{i'}}_{= \psi^\dagger A \, \psi \equiv S_0[\psi, \overline{\psi}]} + S_{\text{int}}[\psi, \overline{\psi}], \qquad A = -\frac{1}{\hbar} \mathscr{G}_0^{-1}, \tag{19.1}$$

(cf. Equation (16.29), where we use the convention $c \equiv \hbar$ throughout this chapter) and the source-dependent partition-function

$$Z[\bar{j}, j] = \int \mathrm{d}_\zeta(\overline{\psi}, \psi) \, \mathrm{e}^{X[\psi, \overline{\psi}, j, \bar{j}]}, \qquad X[\psi, \overline{\psi}, j, \bar{j}] := -S[\psi, \overline{\psi}] + \sum_k \left(\bar{j}_k \psi_k + \overline{\psi}_k j_k \right). \tag{19.2}$$

As in Notation 16.24 we demand that the interaction S_{int} contains only monomials with equally many variables ψ and $\overline{\psi}$ ("U(1)-invariance"). For $\zeta = -1$ this implies in particular that S (and thus X) is *even*, i.e. it commutes with every element of the algebra.

Remark 19.1.1 Up to (and including) Theorem 19.11 we only need that X is even. The U(1)-invariance (and the absence of spontaneous symmetry breaking) will only be used from Lemma 19.13 onwards.

Notation 19.2 We introduce a parameter $\Lambda \in [0, \Lambda_0]$ (where $\Lambda_0 = \infty$ is allowed) and modify the free Green-function according to

$$\mathscr{G}_0 \mapsto \mathscr{G}_{0,\Lambda}, \qquad A \mapsto A_\Lambda = -\frac{1}{\hbar}\mathscr{G}_{0,\Lambda}^{-1}, \tag{19.3}$$

whereas the Λ-dependence is chosen such that

$$\mathscr{G}_{0,\Lambda}^{-1} \longrightarrow \begin{cases} \mathscr{G}_0^{-1} & \text{for } \Lambda \to 0, \\ \infty \quad (\text{i.e. } \mathscr{G}_{0,\Lambda} \to 0) & \text{for } \Lambda \to \Lambda_0. \end{cases} \tag{19.4}$$

The interaction S_{int} remains Λ-independent. The Λ-dependence is inherited by all quantities of Chapter 16, which we mark by a subscript: S_Λ, X_Λ, $Z_\Lambda[\bar{j}, j]$, $W_\Lambda[\bar{j}, j]$, $\phi_\Lambda[\bullet, j, \bar{j}]$, $j_\Lambda[\bullet, \phi, \overline{\phi}]$, $\Gamma_\Lambda[\phi, \overline{\phi}]$, etc. Further, we abbreviate the *free propagator in field-normalization*

$$G_{0,\Lambda} := A_\Lambda^{-1} = -\hbar\,\mathscr{G}_{0,\Lambda}, \qquad \text{such that} \qquad G_{0,\Lambda}(i \mid i') = \left\langle \psi_i \overline{\psi}_{i'} \right\rangle_{0,\Lambda} \qquad \text{(cf. Equation (16.29))}. \tag{19.5}$$

Remark 19.2.1 We write ∂_Λ for the derivative w.r.t. Λ at *fixed sources* when it acts on Z_Λ and W_Λ, and at *fixed fields* when it acts on Γ_Λ. When the distinction is important, we write $(\partial_\Lambda W_\Lambda)[\bar{j}, j]$ for the former.

Remark 19.2.2 The philosophy of this scheme is the following: For $\Lambda \to \Lambda_0$ the Gaussian weight $\mathrm{e}^{-\psi^\dagger A_\Lambda \psi}$ suppresses all fluctuations, such that the Tree-Level-Approximation (Approximation 16.55) becomes exact, $\Gamma_{\Lambda_0} = S_{\Lambda_0} + \text{const.}$ (see Remark 19.19.1). For $\Lambda \to 0$ one recovers the original problem. The flow-equations derived below interpolate between these two limits by successively "switching on" the fluctuations. Equivalently, one can write $A_\Lambda = A + R_\Lambda$ with an (additive) *regulator* $R_\Lambda := A_\Lambda - A$, which vanishes for $\Lambda \to 0$. A concrete choice is presented in Section 19.3.

Lemma 19.3 ("Source-trick" [29].) For all $k, l \in \{1, \dots, \mathrm{D}\}$ one has

$$\overline{\psi}_k \psi_l\, \mathrm{e}^{X_\Lambda} = \zeta \frac{\partial^2}{\partial j_k\, \partial \bar{j}_l} \mathrm{e}^{X_\Lambda} \qquad \text{and therefore} \qquad \partial_\Lambda Z_\Lambda[\bar{j}, j] = -\zeta \sum_{k,l} \left(\partial_\Lambda A_\Lambda\right)_{k,l} \frac{\partial^2 Z_\Lambda[\bar{j}, j]}{\partial j_k\, \partial \bar{j}_l}. \tag{19.6}$$

Proof 19.3 All three factors in $\mathrm{e}^{X_\Lambda} = \mathrm{e}^{-S_\Lambda}\, \mathrm{e}^{\sum_k \bar{j}_k \psi_k}\, \mathrm{e}^{\sum_k \overline{\psi}_k j_k}$ have even exponents and therefore commute with each other. With Lemma 16.14 (and since e^{-S_Λ} is independent of the sources and even) we obtain

$$\frac{\partial}{\partial \bar{j}_l} e^{X_\Lambda} = \psi_l \, e^{X_\Lambda}, \qquad \frac{\partial}{\partial j_k} e^{X_\Lambda} = \zeta \, \overline{\psi}_k \, e^{X_\Lambda}.$$

The variable ψ_l is independent of the sources and of degree one, such that the graded chain-rule (Theorem 16.9) and the relations (16.1) give

$$\begin{aligned} \frac{\partial^2}{\partial j_k \, \partial \bar{j}_l} e^{X_\Lambda} &= \frac{\partial}{\partial j_k} \left(\psi_l \, e^{X_\Lambda} \right) = \zeta \, \psi_l \frac{\partial}{\partial j_k} e^{X_\Lambda} \\ &= \zeta^2 \, \psi_l \overline{\psi}_k \, e^{X_\Lambda} = \psi_l \overline{\psi}_k \, e^{X_\Lambda} = \zeta \, \overline{\psi}_k \psi_l \, e^{X_\Lambda}. \end{aligned}$$

Multiplication with ζ (and $\zeta^2 = 1$) gives the first identity. For the second identity we use that

$$\partial_\Lambda X_\Lambda = - \sum_{k,l} \overline{\psi}_k \left(\partial_\Lambda A_\Lambda \right)_{k,l} \psi_l$$

is even and commutes with X_Λ, such that

$$\begin{aligned} \partial_\Lambda Z_\Lambda[\bar{j}, j] &= \int \mathrm{d}_\zeta(\overline{\psi}, \psi) \, \left(\partial_\Lambda X_\Lambda \right) e^{X_\Lambda} = - \sum_{k,l} \left(\partial_\Lambda A_\Lambda \right)_{k,l} \int \mathrm{d}_\zeta(\overline{\psi}, \psi) \, \overline{\psi}_k \psi_l \, e^{X_\Lambda} \\ &= -\zeta \sum_{k,l} \left(\partial_\Lambda A_\Lambda \right)_{k,l} \frac{\partial^2}{\partial j_k \, \partial \bar{j}_l} \int \mathrm{d}_\zeta(\overline{\psi}, \psi) \, e^{X_\Lambda}. \end{aligned}$$

In the last step we used that a derivative w.r.t. a source commutes with the Berezin-integral (Definition 16.16), since passing the 2D derivatives w.r.t. the integration-variables gives the sign $\zeta^{2\mathrm{D}} = 1$ (Lemma 16.12). For $\zeta = +1$ we assume (as in Fact 16.26) that differentiation and integration can be interchanged.

Lemma 19.4 With the expectation-value in the presence of sources $\langle \bullet \rangle_{j,\Lambda} := Z_\Lambda[\bar{j}, j]^{-1} \int \mathrm{d}_\zeta(\overline{\psi}, \psi) \, \bullet \, e^{X_\Lambda}$ one has

$$\frac{1}{Z_\Lambda[\bar{j}, j]} \frac{\partial^2 Z_\Lambda[\bar{j}, j]}{\partial j_k \, \partial \bar{j}_l} = \left\langle \psi_l \overline{\psi}_k \right\rangle_{j,\Lambda} = \frac{\partial^2 W_\Lambda[\bar{j}, j]}{\partial j_k \, \partial \bar{j}_l} + \phi_l \overline{\phi}_k, \tag{19.7}$$

where $\phi_l \equiv \phi_\Lambda[l, j, \bar{j}]$ and $\overline{\phi}_k \equiv \overline{\phi}_\Lambda[k, j, \bar{j}]$.

Proof 19.4 The first equality follows from the proof of Lemma 19.3, since $\frac{\partial^2}{\partial j_k \, \partial \bar{j}_l} e^{X_\Lambda} = \psi_l \overline{\psi}_k \, e^{X_\Lambda}$. For the second equality we write $Z_\Lambda = e^{W_\Lambda}$. Since Z_Λ is even (with non-vanishing body), W_Λ is even as well (cf. the proof of Lemma 16.32) and commutes with its own derivatives, such that

$$\frac{\partial Z_\Lambda}{\partial \bar{j}_l} = \frac{\partial W_\Lambda}{\partial \bar{j}_l} \, e^{W_\Lambda} = \phi_l \, e^{W_\Lambda} \qquad \text{(Notation 16.31)}.$$

The field ϕ_l consists of monomials which are odd in the sources (Lemma 16.32), i.e. it has the same parity as ψ_l. The graded chain-rule (Theorem 16.9) thus gives

$$\frac{\partial}{\partial j_k}\left(\phi_l\, \mathrm{e}^{W_\Lambda}\right) = \left(\frac{\partial \phi_l}{\partial j_k} + \zeta\, \phi_l \frac{\partial W_\Lambda}{\partial j_k}\right) \mathrm{e}^{W_\Lambda} = \left(\frac{\partial^2 W_\Lambda}{\partial j_k\, \partial \bar{j}_l} + \zeta\, \phi_l\, \zeta\, \bar{\phi}_k\right) \mathrm{e}^{W_\Lambda},$$

where we used $\frac{\partial W_\Lambda}{\partial j_k} = \zeta\, \bar{\phi}_k$ (Notation 16.31). With $\zeta^2 = 1$ the claim follows.

Theorem 19.5 The free energy (in the sense of Definition 16.30) obeys the functional differential equation

$$\left(\partial_\Lambda W_\Lambda\right)[\bar{j}, j] = -\zeta \sum_{k,l} \left(\partial_\Lambda A_\Lambda\right)_{k,l} \frac{\partial^2 W_\Lambda[\bar{j}, j]}{\partial j_k\, \partial \bar{j}_l} - \sum_{k,l} \bar{\phi}_k \left(\partial_\Lambda A_\Lambda\right)_{k,l} \phi_l. \tag{19.8}$$

In terms of the free Green-function, $\partial_\Lambda A_\Lambda = -\frac{1}{\hbar}\partial_\Lambda \mathscr{G}_{0,\Lambda}^{-1}$, this reads

$$\left(\partial_\Lambda W_\Lambda\right)[\bar{j}, j] = \frac{\zeta}{\hbar} \sum_{k,l} \left(\partial_\Lambda \mathscr{G}_{0,\Lambda}^{-1}\right)(k \mid l) \frac{\partial^2 W_\Lambda[\bar{j}, j]}{\partial j_k\, \partial \bar{j}_l} + \frac{1}{\hbar} \sum_{k,l} \bar{\phi}_k \left(\partial_\Lambda \mathscr{G}_{0,\Lambda}^{-1}\right)(k \mid l) \phi_l. \tag{19.9}$$

Proof 19.5 Since Z_Λ is even, we have $\partial_\Lambda W_\Lambda = \partial_\Lambda \log Z_\Lambda = Z_\Lambda^{-1} \partial_\Lambda Z_\Lambda$. With Lemma 19.3 and Lemma 19.4 we obtain

$$\left(\partial_\Lambda W_\Lambda\right)[\bar{j}, j] = -\zeta \sum_{k,l} \left(\partial_\Lambda A_\Lambda\right)_{k,l} \frac{1}{Z_\Lambda} \frac{\partial^2 Z_\Lambda}{\partial j_k\, \partial \bar{j}_l} = -\zeta \sum_{k,l} \left(\partial_\Lambda A_\Lambda\right)_{k,l} \left(\frac{\partial^2 W_\Lambda}{\partial j_k\, \partial \bar{j}_l} + \phi_l \bar{\phi}_k\right).$$

Since ϕ_l and $\bar{\phi}_k$ have the same parity as ψ, one has $\zeta\, \phi_l \bar{\phi}_k = \bar{\phi}_k \phi_l$, which gives the second term. Equation (19.9) follows by inserting $A_\Lambda = -\frac{1}{\hbar}\mathscr{G}_{0,\Lambda}^{-1}$.

Remark 19.5.1 Equation (19.8) is nothing but the statement

$$\partial_\Lambda W_\Lambda = -\left\langle \partial_\Lambda S_{0,\Lambda}[\psi, \bar{\psi}] \right\rangle_{j,\Lambda} = -\sum_{k,l} \left(\partial_\Lambda A_\Lambda\right)_{k,l} \left\langle \bar{\psi}_k \psi_l \right\rangle_{j,\Lambda},$$

where the expectation-value $\langle \bar{\psi}_k \psi_l \rangle_{j,\Lambda} = \zeta \langle \psi_l \bar{\psi}_k \rangle_{j,\Lambda}$ has been split into its connected part (first term) and its disconnected part $\bar{\phi}_k \phi_l$ (second term).

Remark 19.5.2 (Consistency check.) For $S_{\mathrm{int}} = 0$ one obtains by completing the square

$$Z_{0,\Lambda}[\bar{j}, j] = Z_{0,\Lambda} \exp\left(+ \sum_{k,l} \bar{j}_k \left(A_\Lambda^{-1}\right)_{k,l} j_l\right), \qquad Z_{0,\Lambda} \propto \mathrm{e}^{-\zeta\, \mathrm{Tr\,Log}\, A_\Lambda},$$

where the proportionality constant (which depends on the ordering of the integration-measure) is independent of Λ. Notice the *plus*-sign in the exponent, which is in accordance with Remark 16.28.1 (it has been checked

by an explicit Berezin-integration for D = 2), but not with Theorem 16.28 (cf. Remark 16.28.2). Thus $W_{0,\Lambda} = \log Z_{0,\Lambda} + \sum_{k,l} \bar{j}_k (A_\Lambda^{-1})_{k,l} j_l$, and with $\partial_\Lambda A_\Lambda^{-1} = -A_\Lambda^{-1}(\partial_\Lambda A_\Lambda)A_\Lambda^{-1}$ the left-hand side of Equation (19.8) is

$$\left(\partial_\Lambda W_{0,\Lambda}\right)[\bar{j}, j] = -\zeta \operatorname{Tr}\left(A_\Lambda^{-1}\partial_\Lambda A_\Lambda\right) - \sum_{k,l} \bar{j}_k \left(A_\Lambda^{-1}(\partial_\Lambda A_\Lambda)A_\Lambda^{-1}\right)_{k,l} j_l.$$

On the right-hand side we need $\phi_l = \sum_m (A_\Lambda^{-1})_{l,m} j_m$, $\bar{\phi}_k = \sum_m \bar{j}_m (A_\Lambda^{-1})_{m,k}$ and $\frac{\partial^2 W_{0,\Lambda}}{\partial j_k \partial \bar{j}_l} = (A_\Lambda^{-1})_{l,k}$. Inserting this into Equation (19.8) reproduces the left-hand side term by term.

Remark 19.5.3 Compared to Lemma 3.22 in [27] (quantities in the conventions of [27] are marked by a superscript "MT") the overall sign is reversed, since $W^{\mathrm{MT}} = -W$ (cf. Definition 16.30), whereas ϕ, $\bar{\phi}$ and Γ coincide in both conventions. For $\zeta = -1$ and $G_{0,\Lambda}^{-1}\Big|_{\mathrm{MT}} = A_\Lambda$ the two equations agree, once the different derivative-conventions (derivatives "from the right" in [27]) are taken into account. Also the "trivial identity" of [27] now reads $\left(\partial_\Lambda W_\Lambda\right)[\bar{j}, j] = \left(\partial_\Lambda Z_\Lambda / Z_\Lambda\right)[\bar{j}, j]$, i.e. without a minus sign.

Remark 19.5.4 For reasons that are explained at length in the literature [43, 29] this is not the flow-equation that we seek to work with: The expansion-coefficients of W_Λ are connected Green-functions (Definition 16.41), which still contain one-particle-reducible parts, and truncations of the corresponding hierarchy are much harder to control than truncations of the hierarchy for the vertex-functions (see below).

19.2. Functional Differential Equation for the Effective Action

This section is dedicated to the derivation of the Wetterich-equation for bosonic and fermionic systems.

Lemma 19.6 The flow of the effective action at fixed fields is given by the flow of the free energy at fixed sources:

$$\partial_\Lambda \Gamma_\Lambda[\phi, \bar{\phi}] = -\left(\partial_\Lambda W_\Lambda\right)[\bar{j}, j]\Big|_{j = j_\Lambda[\bullet, \phi, \bar{\phi}],\ \bar{j} = \bar{j}_\Lambda[\bullet, \phi, \bar{\phi}]}. \tag{19.10}$$

Proof 19.6 The important thing in this calculation is to consider the Λ-dependence of the sources $j_\Lambda \equiv j_\Lambda[\bullet, \phi, \bar{\phi}]$ and $\bar{j}_\Lambda \equiv \bar{j}_\Lambda[\bullet, \phi, \bar{\phi}]$ at fixed fields. With Notation 16.34 we have

$$\Gamma_\Lambda[\phi, \bar{\phi}] = -W_\Lambda[\bar{j}_\Lambda, j_\Lambda] + \sum_k \left(\bar{\phi}_k\, j_{\Lambda,k} + \bar{j}_{\Lambda,k}\, \phi_k\right).$$

Since Λ is an even parameter, the chain-rule (with the inner derivative to the left, cf. the definition of the left-derivative) gives

$$\begin{aligned}
\partial_\Lambda\Big(W_\Lambda[\bar{j}_\Lambda, j_\Lambda]\Big) &= \left(\partial_\Lambda W_\Lambda\right)[\bar{j}, j] + \sum_k \left(\left(\partial_\Lambda \bar{j}_{\Lambda,k}\right)\frac{\partial W_\Lambda}{\partial \bar{j}_k} + \left(\partial_\Lambda j_{\Lambda,k}\right)\frac{\partial W_\Lambda}{\partial j_k}\right) \\
&= \left(\partial_\Lambda W_\Lambda\right)[\bar{j}, j] + \sum_k \left(\left(\partial_\Lambda \bar{j}_{\Lambda,k}\right)\phi_k + \zeta\left(\partial_\Lambda j_{\Lambda,k}\right)\bar{\phi}_k\right),
\end{aligned}$$

where we used Notation 16.31. Since $\partial_\Lambda j_{\Lambda,k}$ and $\overline{\phi}_k$ both have the parity of ψ, one has $\zeta\,(\partial_\Lambda j_{\Lambda,k})\,\overline{\phi}_k = \overline{\phi}_k\,\partial_\Lambda j_{\Lambda,k}$. On the other hand, the source-terms give

$$\partial_\Lambda \sum_k \left(\overline{\phi}_k\, j_{\Lambda,k} + \bar{j}_{\Lambda,k}\,\phi_k\right) = \sum_k \left(\overline{\phi}_k\,\partial_\Lambda j_{\Lambda,k} + \left(\partial_\Lambda \bar{j}_{\Lambda,k}\right)\phi_k\right),$$

such that all derivatives of the sources cancel and only $-\left(\partial_\Lambda W_\Lambda\right)[\bar{j}, j]$ survives.

Notation 19.7 For a functional $F[\phi, \overline{\phi}]$ we introduce the 2D×2D-matrix of second derivatives (rows labelled by $(\overline{\phi}_x, \phi_x)$, columns labelled by $(\phi_y, \overline{\phi}_y)$)

$$\boldsymbol{F}^{(2)}[\phi, \overline{\phi}] := \begin{pmatrix} \dfrac{\partial^2 F}{\partial\overline{\phi}\,\partial\phi} & \dfrac{\partial^2 F}{\partial\overline{\phi}\,\partial\overline{\phi}} \\ \dfrac{\partial^2 F}{\partial\phi\,\partial\phi} & \dfrac{\partial^2 F}{\partial\phi\,\partial\overline{\phi}} \end{pmatrix}, \qquad \left(\frac{\partial^2 F}{\partial\overline{\phi}\,\partial\phi}\right)(x,y) \equiv \frac{\partial^2 F}{\partial\overline{\phi}_x\,\partial\phi_y}, \quad \text{etc.} \tag{19.11}$$

In particular we write $\boldsymbol{\Gamma}^{(2)}_\Lambda[\phi, \overline{\phi}]$ for the effective action. Correspondingly, we introduce for the free energy the matrix

$$\mathbf{W}_\Lambda[\bar{j}, j] := \begin{pmatrix} \dfrac{\partial^2 W_\Lambda}{\partial\bar{j}\,\partial j} & \zeta\dfrac{\partial^2 W_\Lambda}{\partial\bar{j}\,\partial\bar{j}} \\ \zeta\dfrac{\partial^2 W_\Lambda}{\partial j\,\partial j} & \dfrac{\partial^2 W_\Lambda}{\partial j\,\partial\bar{j}} \end{pmatrix}, \qquad \left(\frac{\partial^2 W_\Lambda}{\partial\bar{j}\,\partial j}\right)(x,y) \equiv \frac{\partial^2 W_\Lambda}{\partial\bar{j}_x\,\partial j_y}, \quad \text{etc.} \tag{19.12}$$

These are exactly the matrices of Corollary 16.45. We denote the blocks by $\mathbf{W}_{11}, \mathbf{W}_{12}, \mathbf{W}_{21}, \mathbf{W}_{22}$, and analogously for $\boldsymbol{F}^{(2)}$.

Lemma 19.8 For $\pi, \pi' \in \{\phi, \overline{\phi}\}$ one has $\frac{\partial^2 F}{\partial\pi_x\,\partial\pi'_y} = \zeta\frac{\partial^2 F}{\partial\pi'_y\,\partial\pi_x}$, which implies for the blocks of $\boldsymbol{F}^{(2)}$

$$\frac{\partial^2 F}{\partial\phi\,\partial\overline{\phi}} = \zeta\left(\frac{\partial^2 F}{\partial\overline{\phi}\,\partial\phi}\right)^{\mathrm{T}}, \qquad \left(\frac{\partial^2 F}{\partial\overline{\phi}\,\partial\overline{\phi}}\right)^{\mathrm{T}} = \zeta\frac{\partial^2 F}{\partial\overline{\phi}\,\partial\overline{\phi}}, \qquad \left(\frac{\partial^2 F}{\partial\phi\,\partial\phi}\right)^{\mathrm{T}} = \zeta\frac{\partial^2 F}{\partial\phi\,\partial\phi}. \tag{19.13}$$

Analogously, one has for the free energy $\mathbf{W}_{11} = \zeta\,\mathbf{W}_{22}^{\mathrm{T}}$, i.e. $\frac{\partial^2 W_\Lambda}{\partial\bar{j}_l\,\partial j_k} = \zeta\frac{\partial^2 W_\Lambda}{\partial j_k\,\partial\bar{j}_l}$.

Proof 19.8 This is the statistics neutral Schwartz-rule (Lemma 16.12), applied to the fields (or sources) instead of the integration-variables. For $\zeta = -1$, $\pi = \pi'$ and $x = y$ both sides vanish.

Lemma 19.9 For a bilinear functional $F[\phi, \overline{\phi}] = \sum_{k,l}\overline{\phi}_k M_{k,l}\phi_l$ with even (e.g. complex) coefficients $M_{k,l}$ one has

$$\boldsymbol{F}^{(2)} = \begin{pmatrix} \zeta M & 0 \\ 0 & M^{\mathrm{T}} \end{pmatrix}. \tag{19.14}$$

In particular, for $S_{0,\Lambda}[\phi,\bar\phi] = \sum_{k,l}\bar\phi_k (A_\Lambda)_{k,l}\phi_l$ we obtain $\boldsymbol{S}^{(2)}_{0,\Lambda} = \mathrm{diag}(\zeta A_\Lambda, A_\Lambda^{\mathrm{T}})$.

Proof 19.9 Moving ϕ_y to the front (past $\bar\phi_k$) gives $\frac{\partial F}{\partial \phi_y} = \zeta \sum_k \bar\phi_k M_{k,y}$, hence $\frac{\partial^2 F}{\partial\bar\phi_x\,\partial\phi_y} = \zeta M_{x,y}$. Further, $\frac{\partial F}{\partial\bar\phi_y} = \sum_l M_{y,l}\phi_l$, hence $\frac{\partial^2 F}{\partial\phi_x\,\partial\bar\phi_y} = M_{y,x} = (M^{\mathrm{T}})_{x,y}$. The two remaining blocks vanish, since F contains no monomials with two ϕ's or two $\bar\phi$'s.

Lemma 19.10 (Inverse-rule, cf. Corollary 16.45.) On the domain where the mapping $(\bar j, j)\mapsto(\phi,\bar\phi)$ is invertible, one has (with $\mathbf{W}_\Lambda$ evaluated at $j = j_\Lambda[\bullet,\phi,\bar\phi]$, $\bar j = \bar j_\Lambda[\bullet,\phi,\bar\phi]$)

$$\sum_y \mathbf{W}_\Lambda(x,y)\,\boldsymbol{\Gamma}^{(2)}_\Lambda(y,z) = \delta_{x,z}\begin{pmatrix}1&0\\0&1\end{pmatrix} \qquad\Longleftrightarrow\qquad \mathbf{W}_\Lambda = \left(\boldsymbol{\Gamma}^{(2)}_\Lambda\right)^{-1}. \tag{19.15}$$

Proof 19.10 We repeat the proof of Corollary 16.45 in a compact form. A functional F of the fields can be considered as a functional of the sources via $\phi = \phi[\bullet, j, \bar j]$. The chain-rule (the counterpart of Lemma 16.44) reads

$$\frac{\partial F}{\partial j_x} = \sum_y\left(\frac{\partial\phi_y}{\partial j_x}\frac{\partial F}{\partial\phi_y} + \frac{\partial\bar\phi_y}{\partial j_x}\frac{\partial F}{\partial\bar\phi_y}\right), \qquad \frac{\partial F}{\partial \bar j_x} = \sum_y\left(\frac{\partial\phi_y}{\partial \bar j_x}\frac{\partial F}{\partial\phi_y} + \frac{\partial\bar\phi_y}{\partial \bar j_x}\frac{\partial F}{\partial\bar\phi_y}\right),$$

with the inner derivatives (Notation 16.31)

$$\frac{\partial\phi_y}{\partial j_x} = \frac{\partial^2 W}{\partial j_x\,\partial\bar j_y}, \qquad \frac{\partial\bar\phi_y}{\partial j_x} = \zeta\frac{\partial^2 W}{\partial j_x\,\partial j_y}, \qquad \frac{\partial\phi_y}{\partial\bar j_x} = \frac{\partial^2 W}{\partial\bar j_x\,\partial\bar j_y}, \qquad \frac{\partial\bar\phi_y}{\partial\bar j_x} = \zeta\frac{\partial^2 W}{\partial\bar j_x\,\partial j_y}.$$

These inner derivatives are even, such that the order of the factors is irrelevant. We apply the chain-rule to $j_z = \frac{\partial\Gamma}{\partial\bar\phi_z}$ and $\bar j_z = \zeta\frac{\partial\Gamma}{\partial\phi_z}$ (Lemma 16.35) and suppress the index Λ:

$$\begin{aligned}
\delta_{x,z} = \frac{\partial j_z}{\partial j_x} &= \sum_y\left(\frac{\partial^2 W}{\partial j_x\,\partial\bar j_y}\frac{\partial^2\Gamma}{\partial\phi_y\,\partial\bar\phi_z} + \zeta\frac{\partial^2 W}{\partial j_x\,\partial j_y}\frac{\partial^2\Gamma}{\partial\bar\phi_y\,\partial\bar\phi_z}\right) = \sum_y\Big(\mathbf{W}_{22}(x,y)\boldsymbol{\Gamma}^{(2)}_{22}(y,z) + \mathbf{W}_{21}(x,y)\boldsymbol{\Gamma}^{(2)}_{12}(y,z)\Big),\\
0 = \frac{\partial j_z}{\partial\bar j_x} &= \sum_y\left(\frac{\partial^2 W}{\partial\bar j_x\,\partial\bar j_y}\frac{\partial^2\Gamma}{\partial\phi_y\,\partial\bar\phi_z} + \zeta\frac{\partial^2 W}{\partial\bar j_x\,\partial j_y}\frac{\partial^2\Gamma}{\partial\bar\phi_y\,\partial\bar\phi_z}\right) = \zeta\sum_y\Big(\mathbf{W}_{12}(x,y)\boldsymbol{\Gamma}^{(2)}_{22}(y,z) + \mathbf{W}_{11}(x,y)\boldsymbol{\Gamma}^{(2)}_{12}(y,z)\Big),\\
\delta_{x,z} = \frac{\partial\bar j_z}{\partial\bar j_x} &= \zeta\sum_y\left(\frac{\partial^2 W}{\partial\bar j_x\,\partial\bar j_y}\frac{\partial^2\Gamma}{\partial\phi_y\,\partial\phi_z} + \zeta\frac{\partial^2 W}{\partial\bar j_x\,\partial j_y}\frac{\partial^2\Gamma}{\partial\bar\phi_y\,\partial\phi_z}\right) = \sum_y\Big(\mathbf{W}_{12}(x,y)\boldsymbol{\Gamma}^{(2)}_{21}(y,z) + \mathbf{W}_{11}(x,y)\boldsymbol{\Gamma}^{(2)}_{11}(y,z)\Big),\\
0 = \frac{\partial\bar j_z}{\partial j_x} &= \zeta\sum_y\left(\frac{\partial^2 W}{\partial j_x\,\partial\bar j_y}\frac{\partial^2\Gamma}{\partial\phi_y\,\partial\phi_z} + \zeta\frac{\partial^2 W}{\partial j_x\,\partial j_y}\frac{\partial^2\Gamma}{\partial\bar\phi_y\,\partial\phi_z}\right) = \zeta\sum_y\Big(\mathbf{W}_{22}(x,y)\boldsymbol{\Gamma}^{(2)}_{21}(y,z) + \mathbf{W}_{21}(x,y)\boldsymbol{\Gamma}^{(2)}_{11}(y,z)\Big).
\end{aligned}$$

These four equations are the $(2,2)$-, $(1,2)$-, $(1,1)$- and $(2,1)$-block of Equation (19.15). Since the entries of both matrices are even (and thus commute), a left-inverse is also a right-inverse.

Theorem 19.11 The Wetterich-equation for the effective action with statistics ζ reads

$$\partial_\Lambda \Gamma_\Lambda[\phi,\overline{\phi}] \quad = \quad \frac{\zeta}{2}\,\mathrm{Tr}\left(\frac{\begin{pmatrix}\zeta\,\partial_\Lambda A_\Lambda & 0\\ 0 & \partial_\Lambda A_\Lambda^{\mathrm{T}}\end{pmatrix}}{\boldsymbol{\Gamma}^{(2)}_\Lambda[\phi,\overline{\phi}]}\right) \quad + \quad \sum_{k,l}\overline{\phi}_k\left(\partial_\Lambda A_\Lambda\right)_{k,l}\phi_l, \tag{19.16}$$

where the numerator is $\partial_\Lambda \boldsymbol{S}^{(2)}_{0,\Lambda}$ (Lemma 19.9) and the quotient means $\mathrm{Tr}(X/Y) \equiv \mathrm{Tr}(X\cdot Y^{-1})$. In terms of the free Green-function this reads

$$\partial_\Lambda \Gamma_\Lambda[\phi,\overline{\phi}] \quad = \quad -\frac{1}{2\hbar}\,\mathrm{Tr}\left(\frac{\begin{pmatrix}\partial_\Lambda \mathscr{G}^{-1}_{0,\Lambda} & 0\\ 0 & \zeta\,\partial_\Lambda \mathscr{G}^{-\mathrm{T}}_{0,\Lambda}\end{pmatrix}}{\boldsymbol{\Gamma}^{(2)}_\Lambda[\phi,\overline{\phi}]}\right) \quad - \quad \frac{1}{\hbar}\sum_{k,l}\overline{\phi}_k\left(\partial_\Lambda \mathscr{G}^{-1}_{0,\Lambda}\right)(k\,|\,l)\phi_l. \tag{19.17}$$

Proof 19.11 Combining Lemma 19.6 with Theorem 19.5 gives

$$\partial_\Lambda \Gamma_\Lambda[\phi,\overline{\phi}] = \zeta\sum_{k,l}\left(\partial_\Lambda A_\Lambda\right)_{k,l}\frac{\partial^2 W_\Lambda}{\partial j_k\,\partial\bar{j}_l} + \sum_{k,l}\overline{\phi}_k\left(\partial_\Lambda A_\Lambda\right)_{k,l}\phi_l.$$

For the first term we use $\frac{\partial^2 W_\Lambda}{\partial j_k\,\partial\bar{j}_l} = \mathbf{W}_{22}(k,l) = \zeta\,\mathbf{W}_{11}(l,k)$ (Lemma 19.8) to write it in a symmetric way:

$$\begin{aligned}\sum_{k,l}\left(\partial_\Lambda A_\Lambda\right)_{k,l}\mathbf{W}_{22}(k,l) &= \frac{1}{2}\sum_{k,l}\left(\left(\partial_\Lambda A_\Lambda^{\mathrm{T}}\right)_{l,k}\mathbf{W}_{22}(k,l) + \zeta\left(\partial_\Lambda A_\Lambda\right)_{k,l}\mathbf{W}_{11}(l,k)\right)\\ &= \frac{1}{2}\left(\mathrm{Tr}\left(\partial_\Lambda A_\Lambda^{\mathrm{T}}\cdot\mathbf{W}_{22}\right) + \mathrm{Tr}\left(\zeta\,\partial_\Lambda A_\Lambda\cdot\mathbf{W}_{11}\right)\right)\\ &= \frac{1}{2}\,\mathrm{Tr}\left(\begin{pmatrix}\zeta\,\partial_\Lambda A_\Lambda & 0\\ 0 & \partial_\Lambda A_\Lambda^{\mathrm{T}}\end{pmatrix}\cdot\mathbf{W}_\Lambda\right).\end{aligned}$$

With the inverse-rule $\mathbf{W}_\Lambda = (\boldsymbol{\Gamma}^{(2)}_\Lambda)^{-1}$ (Lemma 19.10) we arrive at Equation (19.16). Inserting $A_\Lambda = -\frac{1}{\hbar}\mathscr{G}^{-1}_{0,\Lambda}$ and using $\zeta^2 = 1$ yields $\frac{\zeta}{2}\,\mathrm{diag}(\zeta\,\partial_\Lambda A_\Lambda, \partial_\Lambda A_\Lambda^{\mathrm{T}}) = -\frac{1}{2\hbar}\,\mathrm{diag}(\partial_\Lambda \mathscr{G}^{-1}_{0,\Lambda}, \zeta\,\partial_\Lambda \mathscr{G}^{-\mathrm{T}}_{0,\Lambda})$ and thus Equation (19.17).

Remark 19.11.1 The quotient of two matrices is well-defined here, although the matrices do not necessarily commute, because the trace is cyclic. The prefactor $\frac{\zeta}{2}\,\mathrm{Tr}$ is the familiar $\frac{1}{2}\,\mathrm{STr}$ ("supertrace") of the literature: For bosons the one-loop-like term comes with a plus-sign, for fermions with a minus-sign.

Remark 19.11.2 For $\zeta = -1$ Equation (19.16) reduces to Theorem 3.24 in [27]: With $G^{-1}_{0,\Lambda}\big|_{\mathrm{MT}} = A_\Lambda$ and the fact that the second derivatives of [27] (one derivative from the left, one from the right) differ from the left-derivatives used here by an overall sign (for even functionals), i.e. $\delta^2\Gamma_\Lambda\big|_{\mathrm{MT}} = -\boldsymbol{\Gamma}^{(2)}_\Lambda$, the right-hand side of Theorem 3.24 in [27] becomes $+\frac{1}{2}\,\mathrm{Tr}(\mathrm{diag}(\partial_\Lambda A_\Lambda, -\partial_\Lambda A_\Lambda^{\mathrm{T}})/\boldsymbol{\Gamma}^{(2)}_\Lambda) + \sum_{k,l}\overline{\phi}_k(\partial_\Lambda A_\Lambda)_{k,l}\phi_l$, which is Equation (19.16) for $\zeta = -1$.

Remark 19.11.3 (Consistency check.) For $S_{\text{int}} = 0$ one obtains from Remark 19.5.2 with $j = A_\Lambda \phi$ and $\overline{j}_k = \sum_i \overline{\phi}_i (A_\Lambda)_{i,k}$

$$\Gamma_{0,\Lambda}[\phi, \overline{\phi}] = -\log Z_{0,\Lambda} + \sum_{k,l} \overline{\phi}_k (A_\Lambda)_{k,l} \phi_l,$$

i.e. the Tree-Level-Approximation is exact. With Lemma 19.9 we have $(\boldsymbol{\Gamma}^{(2)}_{0,\Lambda})^{-1} = \operatorname{diag}(\zeta A_\Lambda^{-1}, A_\Lambda^{-\mathrm{T}})$, such that the trace-term in Equation (19.16) becomes $\frac{\zeta}{2}(\operatorname{Tr}(\partial_\Lambda A_\Lambda A_\Lambda^{-1}) + \operatorname{Tr}(\partial_\Lambda A_\Lambda^{\mathrm{T}} A_\Lambda^{-\mathrm{T}})) = \zeta \operatorname{Tr}(A_\Lambda^{-1} \partial_\Lambda A_\Lambda) = -\partial_\Lambda \log Z_{0,\Lambda}$, as it should.

Remark 19.11.4 In the literature [29] one oftentimes uses the so-called "Wetterich-Legendre-transformation"

$$\Gamma^{\mathrm{We}}_\Lambda[\phi, \overline{\phi}] := \Gamma_\Lambda[\phi, \overline{\phi}] - \sum_{k,l} \overline{\phi}_k \left(R_\Lambda\right)_{k,l} \phi_l, \qquad R_\Lambda = A_\Lambda - A.$$

With $\partial_\Lambda \boldsymbol{R}_\Lambda = \partial_\Lambda A_\Lambda$, $\boldsymbol{R}^{(2)}_\Lambda = \operatorname{diag}(\zeta R_\Lambda, R_\Lambda^{\mathrm{T}})$ (Lemma 19.9) and $\boldsymbol{\Gamma}^{(2)}_\Lambda = \boldsymbol{\Gamma}^{\mathrm{We},(2)}_\Lambda + \boldsymbol{R}^{(2)}_\Lambda$, Equation (19.16) turns into the standard form of the Wetterich-equation

$$\partial_\Lambda \Gamma^{\mathrm{We}}_\Lambda[\phi, \overline{\phi}] = \frac{\zeta}{2} \operatorname{Tr}\left(\partial_\Lambda \boldsymbol{R}^{(2)}_\Lambda \cdot \left(\boldsymbol{\Gamma}^{\mathrm{We},(2)}_\Lambda[\phi, \overline{\phi}] + \boldsymbol{R}^{(2)}_\Lambda\right)^{-1}\right),$$

in which the term $\sum_{k,l} \overline{\phi}_k (\partial_\Lambda A_\Lambda)_{k,l} \phi_l$ has been absorbed.

Notation 19.12 For notational simplicity we introduce the following abbreviations

- $\boldsymbol{G}_\Lambda \quad := \left(\boldsymbol{\Gamma}^{(2)}_\Lambda[0,0]\right)^{-1}$,
- $\boldsymbol{\mathcal{V}}_\Lambda[\phi, \overline{\phi}] := \boldsymbol{\Gamma}^{(2)}_\Lambda[0,0] - \boldsymbol{\Gamma}^{(2)}_\Lambda[\phi, \overline{\phi}]$,
- $\boldsymbol{G}^{-1}_{0,\Lambda} := \boldsymbol{S}^{(2)}_{0,\Lambda} = \begin{pmatrix} \zeta A_\Lambda & 0 \\ 0 & A_\Lambda^{\mathrm{T}} \end{pmatrix}$,
- $\boldsymbol{S}_\Lambda \quad := -\boldsymbol{G}_\Lambda \cdot \partial_\Lambda \boldsymbol{G}^{-1}_{0,\Lambda} \cdot \boldsymbol{G}_\Lambda$.

Lemma 19.13 Assume (in addition to Notation 19.1) that there is no spontaneous symmetry breaking, such that Γ_Λ shares the U(1)-invariance of S (Theorem 18.3, Remark 18.3.2), i.e. it contains only monomials with equally many ϕ's and $\overline{\phi}$'s. Denote by $\gamma_\Lambda(a \mid b)$ the coefficients of the quadratic part $\sum_{a,b} \overline{\phi}_a \gamma_\Lambda(a \mid b) \phi_b$ of Γ_Λ (Notation 16.36) and by $\gamma^{(2)}_\Lambda$ the corresponding $\mathrm{D} \times \mathrm{D}$-matrix. Then

1. $\boldsymbol{\Gamma}^{(2)}_\Lambda[0,0] = \operatorname{diag}(\zeta \gamma^{(2)}_\Lambda, \gamma^{(2),\mathrm{T}}_\Lambda)$ and $\boldsymbol{G}_\Lambda = \operatorname{diag}(\zeta G_\Lambda, G_\Lambda^{\mathrm{T}})$ with $G_\Lambda := (\gamma^{(2)}_\Lambda)^{-1}$,
2. $G_\Lambda(i \mid i') = \left\langle \psi_i \overline{\psi}_{i'} \right\rangle_\Lambda$, i.e. $G_\Lambda = -\hbar \mathscr{G}_\Lambda$ (Equation (16.33)),
3. $\gamma_\Lambda(a \mid b) = (A_\Lambda)_{a,b} + \frac{1}{\hbar}\Sigma_\Lambda(a \mid b)$, i.e. $G^{-1}_\Lambda = G^{-1}_{0,\Lambda} + \frac{1}{\hbar}\Sigma_\Lambda$, with the self-energy Σ_Λ from $\mathscr{G}^{-1}_\Lambda = \mathscr{G}^{-1}_{0,\Lambda} - \Sigma_\Lambda$ (Remark 16.46.1),

4. $\boldsymbol{G}_{0,\Lambda} = \mathrm{diag}(\zeta G_{0,\Lambda}, G_{0,\Lambda}^{\mathrm{T}})$ and $\boldsymbol{S}_\Lambda = \mathrm{diag}(\zeta S_\Lambda, S_\Lambda^{\mathrm{T}})$ with the *single-scale propagator*

$$S_\Lambda := -G_\Lambda \left(\partial_\Lambda G_{0,\Lambda}^{-1}\right) G_\Lambda = -G_\Lambda \left(\partial_\Lambda A_\Lambda\right) G_\Lambda = -\hbar\, \mathscr{S}_\Lambda, \qquad \mathscr{S}_\Lambda := -\mathscr{G}_\Lambda \left(\partial_\Lambda \mathscr{G}_{0,\Lambda}^{-1}\right) \mathscr{G}_\Lambda. \tag{19.18}$$

Proof 19.13 1. At $\phi = \overline{\phi} = 0$ only the quadratic part of Γ_Λ contributes to the second derivatives (all other monomials either contain more than two fields or, like $\phi\phi$ or $\overline{\phi}\overline{\phi}$, are excluded by the U(1)-invariance). Lemma 19.9 with $M = \gamma_\Lambda^{(2)}$ gives the first statement, and the inverse of a block-diagonal matrix is block-diagonal with $(\zeta\gamma_\Lambda^{(2)})^{-1} = \zeta G_\Lambda$.

2. At $\phi = \overline{\phi} = 0$ (i.e. $j = \overline{j} = 0$) the inverse-rule (Lemma 19.10) gives $\mathbf{W}_{22} = G_\Lambda^{\mathrm{T}}$, i.e. $\frac{\partial^2 W_\Lambda}{\partial j_k\, \partial \overline{j}_l}\Big|_0 = G_\Lambda(l \mid k)$. On the other hand, Lemma 19.4 gives at vanishing sources (where $\phi = \overline{\phi} = 0$) $\frac{\partial^2 W_\Lambda}{\partial j_k\, \partial \overline{j}_l}\Big|_0 = \left\langle \psi_l \overline{\psi}_k \right\rangle_\Lambda$.

3. Follows from 2., $G_{0,\Lambda} = -\hbar \mathscr{G}_{0,\Lambda}$ and the Dyson-equation: $\gamma_\Lambda^{(2)} = G_\Lambda^{-1} = -\frac{1}{\hbar}\mathscr{G}_\Lambda^{-1} = -\frac{1}{\hbar}\mathscr{G}_{0,\Lambda}^{-1} + \frac{1}{\hbar}\Sigma_\Lambda = A_\Lambda + \frac{1}{\hbar}\Sigma_\Lambda$. (This is consistent with $\mathrm{Vert}_\Lambda(a \mid b) = -\hbar\, \gamma_\Lambda(a \mid b)$ and $\mathrm{Vert}_\Lambda = \mathscr{G}_\Lambda^{-1}$, cf. Equation (16.63).)

4. Multiplying the block-diagonal matrices gives $\boldsymbol{S}_\Lambda = -\,\mathrm{diag}(\zeta G_\Lambda \cdot \zeta \partial_\Lambda A_\Lambda \cdot \zeta G_\Lambda\,,\, G_\Lambda^{\mathrm{T}} \partial_\Lambda A_\Lambda^{\mathrm{T}} G_\Lambda^{\mathrm{T}}) = \mathrm{diag}(\zeta S_\Lambda, S_\Lambda^{\mathrm{T}})$. Finally, $-G_\Lambda(\partial_\Lambda A_\Lambda)G_\Lambda = -(-\hbar)^2 \mathscr{G}_\Lambda(-\frac{1}{\hbar}\partial_\Lambda \mathscr{G}_{0,\Lambda}^{-1})\mathscr{G}_\Lambda = -\hbar\, \mathscr{S}_\Lambda$.

Remark 19.13.1 The quantity S_Λ (or $\mathscr{S}_\Lambda$) is known as the "single-scale propagator" [29, 36]. In Lemma 19.21 it will become clear why. It is the derivative of the propagator w.r.t. the *explicit* Λ-dependence,

$$S_\Lambda = \partial_\Lambda G_\Lambda\Big|_{\Sigma_\Lambda \text{ fixed}}, \qquad \partial_\Lambda G_\Lambda = S_\Lambda - \frac{1}{\hbar} G_\Lambda \left(\partial_\Lambda \Sigma_\Lambda\right) G_\Lambda,$$

which follows from $G_\Lambda = (G_{0,\Lambda}^{-1} + \frac{1}{\hbar}\Sigma_\Lambda)^{-1}$ and $\partial_\Lambda X^{-1} = -X^{-1}(\partial_\Lambda X)X^{-1}$. Notice that the sign-convention for $\boldsymbol{S}_\Lambda$ differs from Notation 3.25 in [27] (there $\boldsymbol{S}_\Lambda$ was defined without the minus-sign); we follow [36].

Theorem 19.14 With the abbreviations of Notation 19.12 and under the assumptions of Lemma 19.13, the Wetterich-equation can be expanded as

$$\begin{aligned} \partial_\Lambda \Gamma_\Lambda[\phi, \overline{\phi}] \quad = \quad & \zeta\, \mathrm{Tr}\left(\partial_\Lambda A_\Lambda \cdot G_\Lambda\right) \quad + \quad \sum_{k,l} \overline{\phi}_k \left(\partial_\Lambda A_\Lambda\right)_{k,l} \phi_l \\ & - \quad \frac{\zeta}{2}\, \mathrm{Tr}\left(\boldsymbol{S}_\Lambda \cdot \boldsymbol{\mathcal{V}}_\Lambda\right) \\ & - \quad \frac{\zeta}{2}\, \mathrm{Tr}\left(\boldsymbol{S}_\Lambda \cdot \boldsymbol{\mathcal{V}}_\Lambda \cdot \boldsymbol{G}_\Lambda \cdot \boldsymbol{\mathcal{V}}_\Lambda\right) \\ & - \quad \frac{\zeta}{2}\, \mathrm{Tr}\left(\boldsymbol{S}_\Lambda \cdot \boldsymbol{\mathcal{V}}_\Lambda \cdot \boldsymbol{G}_\Lambda \cdot \boldsymbol{\mathcal{V}}_\Lambda \cdot \boldsymbol{G}_\Lambda \cdot \boldsymbol{\mathcal{V}}_\Lambda\right) \\ & - \quad \ldots \end{aligned} \tag{19.19}$$

The field-independent term can also be written as $\zeta\, \mathrm{Tr}(\partial_\Lambda A_\Lambda \cdot G_\Lambda) = \zeta\, \mathrm{Tr}(\partial_\Lambda \mathscr{G}_{0,\Lambda}^{-1} \cdot \mathscr{G}_\Lambda)$.

Proof 19.14 With $\boldsymbol{\Gamma}_\Lambda^{(2)}[\phi, \overline{\phi}] = \boldsymbol{G}_\Lambda^{-1} - \boldsymbol{\mathcal{V}}_\Lambda[\phi, \overline{\phi}]$, $(AB)^{-1} = B^{-1}A^{-1}$ and the (Neumann- or geometric) series we obtain

$$\left(\boldsymbol{\Gamma}^{(2)}_{\Lambda}\right)^{-1} = \left(\boldsymbol{G}^{-1}_{\Lambda} - \boldsymbol{\mathcal{V}}_{\Lambda}\right)^{-1} = \left(1 - \boldsymbol{G}_{\Lambda}\boldsymbol{\mathcal{V}}_{\Lambda}\right)^{-1}\boldsymbol{G}_{\Lambda} = \left(1 + \boldsymbol{G}_{\Lambda}\boldsymbol{\mathcal{V}}_{\Lambda} + \boldsymbol{G}_{\Lambda}\boldsymbol{\mathcal{V}}_{\Lambda}\boldsymbol{G}_{\Lambda}\boldsymbol{\mathcal{V}}_{\Lambda} + \ldots\right)\boldsymbol{G}_{\Lambda}.$$

The series is justified as follows: Since $\boldsymbol{\mathcal{V}}_{\Lambda}[0,0] = 0$, all entries of $\boldsymbol{\mathcal{V}}_{\Lambda}$ have vanishing body. For $\zeta = -1$ they are therefore nilpotent, such that the series terminates after finitely many terms and is exact. For $\zeta = +1$ the series is a formal power-series in the fields, which is all we need for comparing coefficients. Inserting this into the first term of Equation (19.16), $\frac{\zeta}{2}\operatorname{Tr}(\partial_{\Lambda}\boldsymbol{G}^{-1}_{0,\Lambda}\cdot(\boldsymbol{\Gamma}^{(2)}_{\Lambda})^{-1})$, and using the cyclicity of the trace (the entries of all matrices are even and commute) gives for the term of order $n \geq 1$ in $\boldsymbol{\mathcal{V}}_{\Lambda}$

$$\frac{\zeta}{2}\operatorname{Tr}\left(\partial_{\Lambda}\boldsymbol{G}^{-1}_{0,\Lambda}\left(\boldsymbol{G}_{\Lambda}\boldsymbol{\mathcal{V}}_{\Lambda}\right)^{n}\boldsymbol{G}_{\Lambda}\right) = \frac{\zeta}{2}\operatorname{Tr}\left(\boldsymbol{G}_{\Lambda}\partial_{\Lambda}\boldsymbol{G}^{-1}_{0,\Lambda}\boldsymbol{G}_{\Lambda}\boldsymbol{\mathcal{V}}_{\Lambda}\left(\boldsymbol{G}_{\Lambda}\boldsymbol{\mathcal{V}}_{\Lambda}\right)^{n-1}\right) = -\frac{\zeta}{2}\operatorname{Tr}\left(\boldsymbol{S}_{\Lambda}\boldsymbol{\mathcal{V}}_{\Lambda}\left(\boldsymbol{G}_{\Lambda}\boldsymbol{\mathcal{V}}_{\Lambda}\right)^{n-1}\right).$$

The term of order $n = 0$ is evaluated with Lemma 19.13:

$$\frac{\zeta}{2}\operatorname{Tr}\left(\partial_{\Lambda}\boldsymbol{G}^{-1}_{0,\Lambda}\boldsymbol{G}_{\Lambda}\right) = \frac{\zeta}{2}\left(\operatorname{Tr}\left(\zeta\,\partial_{\Lambda}A_{\Lambda}\cdot\zeta\,G_{\Lambda}\right) + \operatorname{Tr}\left(\partial_{\Lambda}A^{\mathrm{T}}_{\Lambda}G^{\mathrm{T}}_{\Lambda}\right)\right) = \zeta\operatorname{Tr}\left(\partial_{\Lambda}A_{\Lambda}\cdot G_{\Lambda}\right).$$

Finally, $\partial_{\Lambda}A_{\Lambda}\cdot G_{\Lambda} = (-\frac{1}{\hbar}\partial_{\Lambda}\mathscr{G}^{-1}_{0,\Lambda})(-\hbar\,\mathscr{G}_{\Lambda})$.

Remark 19.14.1 At this point we notice why the sign-convention of $\boldsymbol{\mathcal{V}}_{\Lambda}$ in Notation 19.12 is reasonable, although defying the convention: In the Wetterich-equation, this gives us an infinite sum *without* alternating sign.

Remark 19.14.2 The field-independent term gives the flow of $\Gamma_{\Lambda}[0,0] = -W_{\Lambda}[0,0] = -\log Z_{\Lambda}$, i.e. (up to the factor $k_B T$) of the natural energy of the system (Remark 16.30.1). Notice that in Theorem 3.26 of [27] this term was written as $-\operatorname{Tr}(G^{-1}_{\Lambda}\cdot\partial_{\Lambda}G^{-1}_{0,\Lambda})$, which is a typo: The correct expression (for $\zeta = -1$) is $-\operatorname{Tr}(G_{\Lambda}\cdot\partial_{\Lambda}G^{-1}_{0,\Lambda})$.

Remark 19.14.3 In the next section we will express the individual terms by Feynman-diagrams.

The above equation represents an infinite system of coupled differential equations for the vertex-functions. We are particularly interested in the vertex-functions corresponding to the two-point- and four-point-correlators. A common approach is the following simplification.

Approximation 19.15 In a *level-2 truncation*[1] one neglects all terms above the quadratic order in the interaction $\boldsymbol{\mathcal{V}}_{\Lambda}$. Thus one arrives at the approximation

$$\begin{aligned}\partial_{\Lambda}\Gamma_{\Lambda}[\phi,\overline{\phi}] \quad &\approx \quad \zeta\operatorname{Tr}\left(\partial_{\Lambda}A_{\Lambda}\cdot G_{\Lambda}\right) \quad + \quad \sum_{k,l}\overline{\phi}_k\left(\partial_{\Lambda}A_{\Lambda}\right)_{k,l}\phi_l \\ &- \quad \frac{\zeta}{2}\operatorname{Tr}\left(\boldsymbol{S}_{\Lambda}\cdot\boldsymbol{\mathcal{V}}_{\Lambda}\right) \quad - \quad \frac{\zeta}{2}\operatorname{Tr}\left(\boldsymbol{S}_{\Lambda}\cdot\boldsymbol{\mathcal{V}}_{\Lambda}\cdot\boldsymbol{G}_{\Lambda}\cdot\boldsymbol{\mathcal{V}}_{\Lambda}\right).\end{aligned} \tag{19.20}$$

[1] More generally, for $n \in \mathbb{N}_{>0}$ one can introduce a level-n truncation.

19.3. An Example for Flow-Equations

Fact 19.16 To apply this formalism to concrete problems (i.e. actions of the shape in Equation (19.1)) we need two things:

1. A concrete shape of the regulator in Equation (19.3).
2. An approximation / ansatz[2] for the effective action Γ_Λ.

Remark 19.16.1 The most general ansatz for the effective action Γ_Λ is its full series-expansion (Notation 16.36). At least for non-trivial systems, it is obvious that this approach inevitably leads to a giant combinatorial puzzle. It is also said in [43], p. 10 (with references to these notes [...] inserted for better understanding):

> *"Unfortunately, the direct solution of the functional flow equation* [Equation (19.20)] *is only possible for a very small number of systems. However, in practice, one is primarily interested in a few number of 1PI vertex functions. It is therefore convenient to expand both sides of* [Equation (19.20)] *in powers of the fields, and calculate the flow only for certain coefficients."*

To reduce the number of vertex-functions to a "small number", one usually exploits the fact that the effective action has the same symmetries as the action itself (Remark 18.3.2). One can then do the following things:

- One can either stare at the action of the concrete problem and conclude by symmetry considerations (Chapter 18), analogous to the calculations in [43], to what extent the shape of the vertices can be restricted,
- or one can start from a Tree-Level- or One-Loop-Approximation (Approximations 16.55 and 16.57) to make an ansatz for the effective action.

The advantage of the latter procedure is that one does not have to bother with the details of symmetry transformations: The non-vanishing vertex-functions of the Tree-Level-Approximation satisfy the required symmetry properties *by construction* (Theorem 18.3). Another common strategy is to classify the appearing terms on the right-hand side of the flow-equations by their magnitude.

Hypothesis 19.17 *The only* vertex-functions that govern the macroscopic behaviour of the system[3] are those, that flow under the influence of terms that diverge in the limit $\Lambda \to 0$ (assuming their existence).

Remark 19.17.1 Building on the analogy to Wilson's RG-procedure one also realizes that diverging terms not only govern the contributions to the effective action (with decreasing Λ), but as one follows the flow, most of the other terms also drop out due to their "scaling dimension". Thus it is also said in [29], p. 78-79

> *"Microscopic lattice models are usually characterized by infinitely many coupling constants with negative scaling dimensions, implying the existence of infinitely many irrelevant scaling variables. (...) As the RG is iterated there is an enormous reduction of the dimensionality of the coupling space and all irrelevant terms drop out. The leading singular behavior of physical observables is controlled by a small number of relevant (and marginally relevant) couplings."*

[2] There are at least two common ansatzes for the effective action; the first one is a so-called "derivative expansion" [29], also known as "gradient expansion" [36], whereas the other common ansatz (which we will focus on here) is a so-called "vertex expansion" [29].

[3] The vertex-functions correspond to correlators, which are known to form the bridge between theory and experiment.

In the remainder of this section we make two concrete choices, derive the resulting flow-equations *with* self-energy-feedback (Theorem 19.25), and show how they reproduce the One-Loop-Approximation (Corollary 19.27, cf. Theorem 3.30 in [27]).

Choice 1: Regulator

Notation 19.18 In Equation (19.3) we choose the multiplicative regulator

$$\mathscr{G}_{0,\Lambda} := \Theta_{\Lambda,\epsilon} \cdot \mathscr{G}_0 \qquad \Longleftrightarrow \qquad G_{0,\Lambda} = \Theta_{\Lambda,\epsilon} \cdot G_0 \qquad \Longleftrightarrow \qquad A_\Lambda = A \cdot \Theta^{-1}_{\Lambda,\epsilon}, \tag{19.21}$$

where $\Theta_{\Lambda,\epsilon}$ denotes the diagonal, regularized Heaviside-matrix

$$\Theta_{\Lambda,\epsilon}(i,i') := \delta_{i,i'}\, \theta_\epsilon\left(f(i) - \Lambda\right), \tag{19.22}$$

with ...

- a "usual" regularized Heaviside-function θ_ϵ with $0 < \theta_\epsilon < 1$, for example $\theta_\epsilon(x) = \frac{1}{\pi}\arctan(x/\epsilon) + \frac{1}{2}$,
- a regularization-parameter $\epsilon > 0$,
- a system specific function $f(i) > 0$ of the (discrete) index i (for example the modulus of a band-energy measured from the chemical potential).

We denote by $\delta_\epsilon := \theta'_\epsilon$ the corresponding regularized Dirac-delta, such that $\partial_\Lambda \theta_\epsilon(f(i) - \Lambda) = -\delta_\epsilon(f(i) - \Lambda)$.

Remark 19.18.1 A sharp cutoff ($\epsilon \to 0$) sometimes leads to technical complications, like products of Heaviside-*and* Dirac-functions (see Remark 19.21.2). It is a prime example of non-commuting limits in physics. However, a regularized step-function is in many cases still much easier to work with than other choices. For notational simplicity it is usual to neglect the ϵ-dependence most of the time and to just bring it up when one needs it [29].

Choice 2: Approximation / Ansatz for the Effective Action

Approximation 19.19 For the effective action we choose the ansatz (vertex expansion, truncated after the four-point vertex)

$$\Gamma_\Lambda[\phi,\overline{\phi}] \overset{\text{Ansatz}}{\approx} \Gamma_\Lambda[0,0] + \Gamma_{2,\Lambda}[\phi,\overline{\phi}] + \Gamma_{\text{int},\Lambda}[\phi,\overline{\phi}], \tag{19.23}$$

where ...

- $\Gamma_\Lambda[0,0]$ is a field-independent (formal) constant (in [27] denoted as $c(\Lambda)$),
- the quadratic part with the self-energy Σ_Λ (Lemma 19.13)

$$\Gamma_{2,\Lambda}[\phi,\overline{\phi}] = \sum_{a,b} \overline{\phi}_a\, \gamma_\Lambda(a \mid b)\, \phi_b, \qquad \gamma_\Lambda(a \mid b) = (A_\Lambda)_{a,b} + \frac{1}{\hbar}\Sigma_\Lambda(a \mid b),$$

- the quartic part with the (anti)symmetric four-point vertex

$$\Gamma_{\text{int},\Lambda}[\phi,\overline{\phi}] = \frac{1}{(2!)^2} \sum_{a_1,a_2,b_1,b_2} \overline{\phi}_{a_1} \overline{\phi}_{a_2}\, \gamma_\Lambda(a_1,a_2 \mid b_1,b_2)\, \phi_{b_2} \phi_{b_1},$$

with $\gamma_\Lambda(a_2, a_1 \mid b_1, b_2) = \gamma_\Lambda(a_1, a_2 \mid b_2, b_1) = \zeta\, \gamma_\Lambda(a_1, a_2 \mid b_1, b_2)$,

- all vertex-functions with more than four legs are neglected,

and we consider (for simplicity) a purely quartic interaction $S_{\text{int}}[\psi, \overline{\psi}] = \frac{1}{(2!)^2} \sum \overline{\psi}_{a_1} \overline{\psi}_{a_2}\, s(a_1, a_2 \mid b_1, b_2)\, \psi_{b_2} \psi_{b_1}$ (Notation 16.36) with the initial conditions

$$\Sigma_{\Lambda_0} = 0, \qquad \gamma_{\Lambda_0}(a_1, a_2 \mid b_1, b_2) = s(a_1, a_2 \mid b_1, b_2), \qquad \text{i.e.} \qquad \Gamma_{\Lambda_0}[\phi, \overline{\phi}] = S_{\Lambda_0}[\phi, \overline{\phi}] + \text{const.} \tag{19.24}$$

Remark 19.19.1 The initial conditions express that for $\Lambda \to \Lambda_0$ all fluctuations are frozen ($G_{0,\Lambda_0} = 0$), such that all loop-contributions (which contain at least one propagator) vanish and the Tree-Level-Approximation becomes exact. For example, integrating Equation (19.30) below to lowest order gives $\frac{1}{\hbar}\Sigma_\Lambda(a \mid b) \approx \zeta \sum_{x,y}(G_{0,\Lambda} - G_{0,\Lambda_0})(y \mid x)\, s(x, a \mid y, b)$. With finitely many (discrete) indices this is unproblematic. In the limit of infinitely many indices (e.g. infinitely many Matsubara-frequencies) the limits $\Lambda \to \Lambda_0$ and $\mathrm{D} \to \infty$ need not commute (the equal-time contractions in the first-order term converge only conditionally), and the first-order contribution may then have to be included in the initial condition.

Remark 19.19.2 In comparison to Choice 2 in [27], we do *not* neglect the self-energy: The full propagator $G_\Lambda = (G_{0,\Lambda}^{-1} + \frac{1}{\hbar}\Sigma_\Lambda)^{-1}$ (and thus S_Λ) is fed back into the flow-equations, and Σ_Λ itself flows according to Equation (19.30). As in [27] one can additionally restrict the four-point vertex to the set $I = \{(a_1, a_2, b_1, b_2) \mid s(a_1, a_2 \mid b_1, b_2) \neq 0\}$, i.e. keep the structure of the interaction from the bare action, but *include* a Λ-dependence of the vertex-functions. A similar strategy was used in [29], p. 229-232 and [36], p. 312.

Corollary 19.20 These two choices satisfy all the requirements demanded by Lemma 19.13 and Equation (19.4) (for $\epsilon \to 0$ and with $\Lambda_0 = \infty$).

Proof 19.20 The ansatz contains only monomials with equally many ϕ's and $\overline{\phi}$'s and thus satisfies the U(1)-invariance by construction (Theorem 18.3). For the regulator we have for $\Lambda = 0$

$$\theta_\epsilon(f(i) - 0) = \frac{1}{\pi} \arctan\left(\frac{f(i)}{\epsilon}\right) + \frac{1}{2} \to 1 \quad \text{for} \quad \epsilon \to 0,$$

since $f(i) > 0$, such that $\mathscr{G}_{0,0} \to \mathscr{G}_0$. Similarly, for $\Lambda \gg f(i)$ (for all of the finitely many indices i) the limiting behaviour is

$$\theta_\epsilon(f(i) - \Lambda) \approx \frac{1}{\pi} \arctan\left(\frac{-\Lambda}{\epsilon}\right) + \frac{1}{2} \to 0 \quad \text{for} \quad \Lambda \to \infty,$$

such that $\mathscr{G}_{0,\Lambda} \to 0$, i.e. $\mathscr{G}_{0,\Lambda}^{-1} \to \infty$.

Lemma 19.21 With Choice 1 the single-scale propagator (Equation (19.18)) reads

$$S_\Lambda = G_\Lambda\, G_0^{-1}\, \Theta_{\Lambda,\epsilon}^{-1} \left(\partial_\Lambda \Theta_{\Lambda,\epsilon}\right) \Theta_{\Lambda,\epsilon}^{-1}\, G_\Lambda, \qquad \left(\partial_\Lambda \Theta_{\Lambda,\epsilon}\right)(i, i') = -\delta_{i,i'}\, \delta_\epsilon\left(f(i) - \Lambda\right). \tag{19.25}$$

In particular …

1. without self-energy ($\Sigma_\Lambda = 0$, i.e. $G_\Lambda = G_{0,\Lambda}$) one has $S_\Lambda = (\partial_\Lambda \Theta_{\Lambda,\epsilon})\, G_0 = \partial_\Lambda G_{0,\Lambda}$, i.e. $S_\Lambda(i \mid i') = -\delta_\epsilon(f(i) - \Lambda)\, G_0(i \mid i')$,
2. if G_0 and Σ_Λ are diagonal (e.g. in a basis of conserved quantum numbers), one has

$$S_\Lambda(i \mid i) = -\frac{\delta_\epsilon(f(i) - \Lambda)\, G_0(i \mid i)}{\Big(1 + \frac{1}{\hbar}\theta_\epsilon(f(i) - \Lambda)\, G_0(i \mid i)\, \Sigma_\Lambda(i \mid i)\Big)^2}, \qquad \mathscr{S}_\Lambda(i \mid i) = -\frac{\delta_\epsilon(f(i) - \Lambda)\, \mathscr{G}_0(i \mid i)}{\big(1 - \theta_\epsilon(f(i) - \Lambda)\, \mathscr{G}_0(i \mid i)\, \Sigma_\Lambda(i \mid i)\big)^2}. \tag{19.26}$$

Proof 19.21 From $G_{0,\Lambda}^{-1} = A_\Lambda = G_0^{-1}\Theta_{\Lambda,\epsilon}^{-1}$ we get $\partial_\Lambda G_{0,\Lambda}^{-1} = -G_0^{-1}\Theta_{\Lambda,\epsilon}^{-1}(\partial_\Lambda \Theta_{\Lambda,\epsilon})\Theta_{\Lambda,\epsilon}^{-1}$, and inserting this into $S_\Lambda = -G_\Lambda(\partial_\Lambda G_{0,\Lambda}^{-1})G_\Lambda$ gives Equation (19.25).

1. With $G_\Lambda = G_{0,\Lambda} = \Theta_{\Lambda,\epsilon} G_0$ we obtain $S_\Lambda = \Theta_{\Lambda,\epsilon} G_0 G_0^{-1}\Theta_{\Lambda,\epsilon}^{-1}(\partial_\Lambda \Theta_{\Lambda,\epsilon})\Theta_{\Lambda,\epsilon}^{-1}\Theta_{\Lambda,\epsilon} G_0 = (\partial_\Lambda \Theta_{\Lambda,\epsilon}) G_0$.

2. For diagonal matrices all factors commute. With the abbreviations $g_0 \equiv G_0(i \mid i)$, $\theta \equiv \theta_\epsilon(f(i) - \Lambda)$ and $\sigma \equiv \Sigma_\Lambda(i \mid i)$ we have

$$G_\Lambda(i \mid i) = \left(\frac{1}{\theta g_0} + \frac{\sigma}{\hbar}\right)^{-1} = \frac{\theta g_0}{1 + \frac{1}{\hbar}\theta g_0 \sigma}, \qquad S_\Lambda(i \mid i) = G_\Lambda(i \mid i)^2\, \frac{\partial_\Lambda \theta}{g_0\, \theta^2} = \frac{(\partial_\Lambda \theta)\, g_0}{\Big(1 + \frac{1}{\hbar}\theta g_0 \sigma\Big)^2},$$

and $\partial_\Lambda \theta = -\delta_\epsilon(f(i) - \Lambda)$. The second identity follows with $G_0 = -\hbar \mathscr{G}_0$ and $S_\Lambda = -\hbar \mathscr{S}_\Lambda$.

Remark 19.21.1 With the appearance of the regularized Dirac-delta δ_ϵ in S_Λ one immediately grasps the name "single-scale propagator": only indices with $f(i) \approx \Lambda$ contribute. Statement 1. is Corollary 3.32 in [27] (up to the sign-convention of S_Λ, see Remark 19.13.1).

Remark 19.21.2 In the sharp-cutoff limit $\epsilon \to 0$ one encounters products of δ_ϵ with functions of θ_ϵ, which are to be interpreted (as distributions in Λ) by [36]

$$\delta_\epsilon(x)\, F\big(\theta_\epsilon(x)\big) \longrightarrow \delta(x) \int_0^1 \mathrm{d}t\, F(t) \qquad (\epsilon \to 0),$$

since $\delta_\epsilon = \theta_\epsilon'$. Applied to Equation (19.26) with $F(t) = g_0/(1 + \frac{1}{\hbar} t g_0 \sigma)^2$ and $\int_0^1 \mathrm{d}t\, (1 + tc)^{-2} = (1 + c)^{-1}$ this gives

$$S_\Lambda(i \mid i) \longrightarrow -\delta\,(f(i) - \Lambda)\, \frac{G_0(i \mid i)}{1 + \frac{1}{\hbar} G_0(i \mid i)\, \Sigma_\Lambda(i \mid i)}.$$

Lemma 19.22 For $\Gamma_{\mathrm{int},\Lambda}$ from Choice 2 one has (suppressing the index Λ)

$$\frac{\partial^2 \Gamma_{\mathrm{int}}}{\partial \overline{\phi}_x\, \partial \phi_y} = \zeta \sum_{a,b} \overline{\phi}_a\, \gamma(x, a \mid y, b)\, \phi_b, \qquad \frac{\partial^2 \Gamma_{\mathrm{int}}}{\partial \phi_x\, \partial \overline{\phi}_y} = \sum_{a,b} \overline{\phi}_a\, \gamma(y, a \mid x, b)\, \phi_b,$$
$$\frac{\partial^2 \Gamma_{\mathrm{int}}}{\partial \overline{\phi}_x\, \partial \overline{\phi}_y} = \frac{\zeta}{2} \sum_{b_1, b_2} \gamma(x, y \mid b_1, b_2)\, \phi_{b_2} \phi_{b_1}, \qquad \frac{\partial^2 \Gamma_{\mathrm{int}}}{\partial \phi_x\, \partial \phi_y} = \frac{1}{2} \sum_{a_1, a_2} \overline{\phi}_{a_1} \overline{\phi}_{a_2}\, \gamma(a_1, a_2 \mid x, y).$$

Proof 19.22 For the first derivatives we use the graded chain-rule (Theorem 16.9) and the (anti)symmetry of γ:

$$\begin{aligned}
\frac{\partial\Gamma_{\text{int}}}{\partial\overline{\phi}_y} &= \frac{1}{4}\sum\Big(\delta_{y,a_1}\overline{\phi}_{a_2} + \zeta\,\overline{\phi}_{a_1}\delta_{y,a_2}\Big)\,\gamma(a_1,a_2\,|\,b_1,b_2)\,\phi_{b_2}\phi_{b_1} \\
&= \frac{1}{4}\sum\overline{\phi}_a\Big(\gamma(y,a\,|\,b_1,b_2) + \zeta\,\gamma(a,y\,|\,b_1,b_2)\Big)\phi_{b_2}\phi_{b_1} = \frac{1}{2}\sum\overline{\phi}_a\,\gamma(y,a\,|\,b_1,b_2)\,\phi_{b_2}\phi_{b_1}, \\
\frac{\partial\Gamma_{\text{int}}}{\partial\phi_y} &= \frac{1}{4}\sum\overline{\phi}_{a_1}\overline{\phi}_{a_2}\,\gamma(a_1,a_2\,|\,b_1,b_2)\,\big(\delta_{y,b_2}\phi_{b_1} + \zeta\,\phi_{b_2}\delta_{y,b_1}\big) = \frac{1}{2}\sum\overline{\phi}_{a_1}\overline{\phi}_{a_2}\,\gamma(a_1,a_2\,|\,b,y)\,\phi_b,
\end{aligned}$$

where in the second line the derivative passed the even pair $\overline{\phi}_{a_1}\overline{\phi}_{a_2}$ without sign. Differentiating once more gives

$$\begin{aligned}
\frac{\partial^2\Gamma_{\text{int}}}{\partial\overline{\phi}_x\,\partial\overline{\phi}_y} &= \frac{1}{2}\sum\gamma(y,x\,|\,b_1,b_2)\,\phi_{b_2}\phi_{b_1} = \frac{\zeta}{2}\sum\gamma(x,y\,|\,b_1,b_2)\,\phi_{b_2}\phi_{b_1}, \\
\frac{\partial^2\Gamma_{\text{int}}}{\partial\phi_x\,\partial\phi_y} &= \frac{1}{2}\sum\overline{\phi}_{a_1}\overline{\phi}_{a_2}\,\gamma(a_1,a_2\,|\,x,y), \\
\frac{\partial^2\Gamma_{\text{int}}}{\partial\phi_x\,\partial\overline{\phi}_y} &= \frac{\zeta}{2}\sum\overline{\phi}_a\,\gamma(y,a\,|\,b_1,b_2)\,\big(\delta_{x,b_2}\phi_{b_1} + \zeta\,\phi_{b_2}\delta_{x,b_1}\big) \\
&= \frac{\zeta}{2}\sum\overline{\phi}_a\Big(\gamma(y,a\,|\,b,x) + \zeta\,\gamma(y,a\,|\,x,b)\Big)\phi_b = \sum\overline{\phi}_a\,\gamma(y,a\,|\,x,b)\,\phi_b,
\end{aligned}$$

where the prefactor ζ in the last line stems from passing $\overline{\phi}_a$. The remaining block follows from Lemma 19.8: $\frac{\partial^2\Gamma_{\text{int}}}{\partial\overline{\phi}_x\,\partial\phi_y} = \zeta\frac{\partial^2\Gamma_{\text{int}}}{\partial\phi_y\,\partial\overline{\phi}_x}$.

Theorem 19.23 With the ansatz of Choice 2 (and any regulator), the level-2 truncation (Approximation 19.15) becomes

$$\begin{aligned}
\partial_\Lambda\Gamma_\Lambda[\phi,\overline{\phi}] \;\approx\; & \zeta\,\mathrm{Tr}\,\big(\partial_\Lambda A_\Lambda\cdot G_\Lambda\big) \;+\; \sum_{k,l}\overline{\phi}_k\,\big(\partial_\Lambda A_\Lambda\big)_{k,l}\,\phi_l \;+\; \mathrm{Tr}\,\Big[S_\Lambda\cdot\frac{\partial^2\Gamma_{\text{int},\Lambda}}{\partial\overline{\phi}\,\partial\phi}\Big] \\
& -\;\zeta\,\mathrm{Tr}\,\Big[S_\Lambda\cdot\frac{\partial^2\Gamma_{\text{int},\Lambda}}{\partial\overline{\phi}\,\partial\phi}\cdot G_\Lambda\cdot\frac{\partial^2\Gamma_{\text{int},\Lambda}}{\partial\overline{\phi}\,\partial\phi}\Big] \;-\; \mathrm{Tr}\,\Big[S_\Lambda\cdot\frac{\partial^2\Gamma_{\text{int},\Lambda}}{\partial\overline{\phi}\,\partial\overline{\phi}}\cdot G_\Lambda^{\mathrm{T}}\cdot\frac{\partial^2\Gamma_{\text{int},\Lambda}}{\partial\phi\,\partial\phi}\Big],
\end{aligned}\tag{19.27}$$

with $G_\Lambda = (G_{0,\Lambda}^{-1} + \frac{1}{\hbar}\Sigma_\Lambda)^{-1}$ and $S_\Lambda = -G_\Lambda(\partial_\Lambda A_\Lambda)G_\Lambda$ (Lemma 19.13).

Proof 19.23 Within the ansatz, $\boldsymbol{\Gamma}_\Lambda^{(2)}[\phi,\overline{\phi}] = \boldsymbol{\Gamma}_{2,\Lambda}^{(2)} + \boldsymbol{\Gamma}_{\text{int},\Lambda}^{(2)}[\phi,\overline{\phi}]$, where $\boldsymbol{\Gamma}_{2,\Lambda}^{(2)} = \boldsymbol{\Gamma}_\Lambda^{(2)}[0,0]$ is field-independent (Lemma 19.9) and $\boldsymbol{\Gamma}_{\text{int},\Lambda}^{(2)}[0,0] = 0$. Hence $\boldsymbol{\mathcal{V}}_\Lambda = -\boldsymbol{\Gamma}_{\text{int},\Lambda}^{(2)}$. We abbreviate the blocks of $\boldsymbol{\Gamma}_{\text{int},\Lambda}^{(2)}$ by $\Gamma_{\overline{\phi}\phi} \equiv \frac{\partial^2\Gamma_{\text{int},\Lambda}}{\partial\overline{\phi}\,\partial\phi}$, $\Gamma_{\overline{\phi}\overline{\phi}}$, $\Gamma_{\phi\phi}$, $\Gamma_{\phi\overline{\phi}}$ and recall $\boldsymbol{S}_\Lambda = \mathrm{diag}(\zeta S_\Lambda, S_\Lambda^{\mathrm{T}})$, $\boldsymbol{G}_\Lambda = \mathrm{diag}(\zeta G_\Lambda, G_\Lambda^{\mathrm{T}})$ (Lemma 19.13). In the following we use the cyclicity of the trace, $\mathrm{Tr}\,X^{\mathrm{T}} = \mathrm{Tr}\,X$, $(XY)^{\mathrm{T}} = Y^{\mathrm{T}}X^{\mathrm{T}}$ (valid since all entries are even and commute), and the relations $\Gamma_{\phi\overline{\phi}} = \zeta\Gamma_{\overline{\phi}\phi}^{\mathrm{T}}$, $\Gamma_{\overline{\phi}\phi}^{\mathrm{T}} = \zeta\Gamma_{\overline{\phi}\overline{\phi}}$, $\Gamma_{\phi\phi}^{\mathrm{T}} = \zeta\Gamma_{\phi\phi}$ (Lemma 19.8).

Linear term. We have

$$-\frac{\zeta}{2}\operatorname{Tr}\left(\boldsymbol{S}_\Lambda\boldsymbol{\mathcal{V}}_\Lambda\right)=\frac{\zeta}{2}\left(\operatorname{Tr}\left(\zeta S_\Lambda\Gamma_{\bar\phi\phi}\right)+\operatorname{Tr}\left(S_\Lambda^{\mathrm{T}}\Gamma_{\phi\bar\phi}\right)\right)=\frac{\zeta}{2}\left(\zeta\operatorname{Tr}\left(S_\Lambda\Gamma_{\bar\phi\phi}\right)+\zeta\operatorname{Tr}\left(\left(\Gamma_{\bar\phi\phi}S_\Lambda\right)^{\mathrm{T}}\right)\right)=\operatorname{Tr}\left(S_\Lambda\Gamma_{\bar\phi\phi}\right).$$

Quadratic term. We first multiply the matrices

$$\boldsymbol{S}_\Lambda\boldsymbol{\Gamma}^{(2)}_{\mathrm{int},\Lambda}=\begin{pmatrix}\zeta S_\Lambda\Gamma_{\bar\phi\phi} & \zeta S_\Lambda\Gamma_{\overline{\phi\phi}}\\ S_\Lambda^{\mathrm{T}}\Gamma_{\phi\phi} & S_\Lambda^{\mathrm{T}}\Gamma_{\phi\bar\phi}\end{pmatrix},\qquad \boldsymbol{G}_\Lambda\boldsymbol{\Gamma}^{(2)}_{\mathrm{int},\Lambda}=\begin{pmatrix}\zeta G_\Lambda\Gamma_{\bar\phi\phi} & \zeta G_\Lambda\Gamma_{\overline{\phi\phi}}\\ G_\Lambda^{\mathrm{T}}\Gamma_{\phi\phi} & G_\Lambda^{\mathrm{T}}\Gamma_{\phi\bar\phi}\end{pmatrix},$$

such that

$$\boldsymbol{S}_\Lambda\boldsymbol{\mathcal{V}}_\Lambda\boldsymbol{G}_\Lambda\boldsymbol{\mathcal{V}}_\Lambda=\boldsymbol{S}_\Lambda\boldsymbol{\Gamma}^{(2)}_{\mathrm{int},\Lambda}\boldsymbol{G}_\Lambda\boldsymbol{\Gamma}^{(2)}_{\mathrm{int},\Lambda}=\begin{pmatrix}\mathcal{A}+\mathcal{B} & \cdots\\ \cdots & \mathcal{C}+\mathcal{D}\end{pmatrix}$$

(the off-diagonal blocks are irrelevant for the trace) with

$$\begin{aligned}\mathcal{A}&=S_\Lambda\Gamma_{\bar\phi\phi}G_\Lambda\Gamma_{\bar\phi\phi},\qquad &\mathcal{B}&=\zeta\,S_\Lambda\Gamma_{\overline{\phi\phi}}G_\Lambda^{\mathrm{T}}\Gamma_{\phi\phi},\\ \mathcal{C}&=\zeta\,S_\Lambda^{\mathrm{T}}\Gamma_{\phi\phi}G_\Lambda\Gamma_{\overline{\phi\phi}},\qquad &\mathcal{D}&=S_\Lambda^{\mathrm{T}}\Gamma_{\phi\bar\phi}G_\Lambda^{\mathrm{T}}\Gamma_{\phi\bar\phi}.\end{aligned}$$

Now

$$\begin{aligned}\operatorname{Tr}\mathcal{D}&=\zeta^2\operatorname{Tr}\left(S_\Lambda^{\mathrm{T}}\Gamma^{\mathrm{T}}_{\bar\phi\phi}G_\Lambda^{\mathrm{T}}\Gamma^{\mathrm{T}}_{\bar\phi\phi}\right)=\operatorname{Tr}\left(\left(\Gamma_{\bar\phi\phi}G_\Lambda\Gamma_{\bar\phi\phi}S_\Lambda\right)^{\mathrm{T}}\right)=\operatorname{Tr}\mathcal{A},\\ \operatorname{Tr}\mathcal{C}&=\zeta\operatorname{Tr}\left(\Gamma^{\mathrm{T}}_{\overline{\phi\phi}}G_\Lambda^{\mathrm{T}}\Gamma^{\mathrm{T}}_{\phi\phi}S_\Lambda\right)=\zeta^3\operatorname{Tr}\left(S_\Lambda\Gamma_{\overline{\phi\phi}}G_\Lambda^{\mathrm{T}}\Gamma_{\phi\phi}\right)=\operatorname{Tr}\mathcal{B},\end{aligned}$$

such that

$$-\frac{\zeta}{2}\operatorname{Tr}\left(\boldsymbol{S}_\Lambda\boldsymbol{\mathcal{V}}_\Lambda\boldsymbol{G}_\Lambda\boldsymbol{\mathcal{V}}_\Lambda\right)=-\zeta\left(\operatorname{Tr}\mathcal{A}+\operatorname{Tr}\mathcal{B}\right)=-\zeta\operatorname{Tr}\left(S_\Lambda\Gamma_{\bar\phi\phi}G_\Lambda\Gamma_{\bar\phi\phi}\right)-\operatorname{Tr}\left(S_\Lambda\Gamma_{\overline{\phi\phi}}G_\Lambda^{\mathrm{T}}\Gamma_{\phi\phi}\right).$$

Remark 19.23.1 For $\zeta=-1$, $\Sigma_\Lambda=0$ (such that $S_\Lambda=\partial_\Lambda G_{0,\Lambda}$, Lemma 19.21) the last two terms read $+\operatorname{Tr}[\partial_\Lambda G_{0,\Lambda}\Gamma_{\bar\phi\phi}G_{0,\Lambda}\Gamma_{\bar\phi\phi}]-\operatorname{Tr}[\partial_\Lambda G_{0,\Lambda}\Gamma_{\overline{\phi\phi}}G^{\mathrm{T}}_{0,\Lambda}\Gamma_{\phi\phi}]$, which has the same form as Equation (3.24) (Theorem 3.33) in [27]; the different sign-conventions of the second derivatives cancel there, since each term contains two of them.

Lemma 19.24 Let $\widetilde{f}(a_1,a_2\,|\,b_1,b_2)$ be arbitrary complex coefficients (without any symmetry properties). Then

$$\sum_{a_1,a_2,b_1,b_2}\overline{\phi}_{a_1}\overline{\phi}_{a_2}\,\widetilde{f}(a_1,a_2\,|\,b_1,b_2)\,\phi_{b_2}\phi_{b_1}=\frac{1}{(2!)^2}\sum_{a_1,a_2,b_1,b_2}\overline{\phi}_{a_1}\overline{\phi}_{a_2}\,f(a_1,a_2\,|\,b_1,b_2)\,\phi_{b_2}\phi_{b_1}\tag{19.28}$$

with the (anti)symmetric coefficients

$$f(a_1,a_2\,|\,b_1,b_2):=\widetilde{f}(a_1,a_2\,|\,b_1,b_2)+\zeta\,\widetilde{f}(a_2,a_1\,|\,b_1,b_2)+\zeta\,\widetilde{f}(a_1,a_2\,|\,b_2,b_1)+\widetilde{f}(a_2,a_1\,|\,b_2,b_1).$$

Since (anti)symmetric coefficients are uniquely determined by the functional (Lemma 16.39), we can compare coefficients in this form. For quadratic terms $\sum_{a,b} \overline{\phi}_a \widetilde{f}(a \mid b) \phi_b$ no symmetrization is needed.

Proof 19.24 Renaming $a_1 \leftrightarrow a_2$ in the summation and using $\overline{\phi}_{a_2}\overline{\phi}_{a_1} = \zeta \overline{\phi}_{a_1}\overline{\phi}_{a_2}$ shows that the left-hand side is equal to $\sum \overline{\phi}_{a_1}\overline{\phi}_{a_2}\, \zeta\, \widetilde{f}(a_2, a_1 \mid b_1, b_2)\, \phi_{b_2}\phi_{b_1}$, and analogously for $b_1 \leftrightarrow b_2$ and for both renamings. Taking the mean value of these four equal expressions gives the claim. The (anti)symmetry of f is checked directly.

Theorem 19.25 With the ansatz of Choice 2 (and any regulator) the level-2 truncation yields the following flow-equations[4] with self-energy-feedback:

1. The field-independent part (natural energy):

$$\partial_\Lambda \Gamma_\Lambda[0,0] = \zeta \operatorname{Tr}\left(\partial_\Lambda A_\Lambda \cdot G_\Lambda\right) = \zeta \operatorname{Tr}\left(\partial_\Lambda \mathscr{G}_{0,\Lambda}^{-1} \cdot \mathscr{G}_\Lambda\right). \tag{19.29}$$

2. The self-energy:

$$\partial_\Lambda \Sigma_\Lambda(a \mid b) = \zeta \hbar \sum_{x,y} S_\Lambda(y \mid x)\, \gamma_\Lambda(x, a \mid y, b). \tag{19.30}$$

3. The four-point vertex ("effective interaction", cf. Remark 16.42.2):

$$\begin{aligned} \partial_\Lambda \gamma_\Lambda(a_1, a_2 \mid b_1, b_2) \quad = \quad & -\frac{1}{2} \sum \gamma_\Lambda(a_1, a_2 \mid u, v)\, \dot{L}_\Lambda(u, v \mid x, y)\, \gamma_\Lambda(x, y \mid b_1, b_2) && \text{(particle-particle)} \\ & -\zeta \sum \gamma_\Lambda(a_1, x \mid b_1, y)\, \dot{L}_\Lambda(y, v \mid u, x)\, \gamma_\Lambda(a_2, u \mid b_2, v) && \text{(particle-hole, direct)} \\ & -\sum \gamma_\Lambda(a_1, x \mid b_2, y)\, \dot{L}_\Lambda(y, v \mid u, x)\, \gamma_\Lambda(a_2, u \mid b_1, v) && \text{(particle-hole, crossed)} \end{aligned} \tag{19.31}$$

with the full propagator $G_\Lambda = (G_{0,\Lambda}^{-1} + \frac{1}{\hbar}\Sigma_\Lambda)^{-1}$, the single-scale propagator S_Λ (Equation (19.18)) and the "loop-kernel"

$$\dot{L}_\Lambda(p, q \mid r, s) := S_\Lambda(p \mid r)\, G_\Lambda(q \mid s) + G_\Lambda(p \mid r)\, S_\Lambda(q \mid s) = \partial_\Lambda \Big(G_\Lambda(p \mid r)\, G_\Lambda(q \mid s) \Big)\Big|_{\Sigma_\Lambda \text{ fixed}}. \tag{19.32}$$

Proof 19.25 We insert the ansatz into Theorem 19.23 and use Lemma 19.22. Both sides of Equation (19.27) then only contain monomials of order 0, 2 and 4 in the fields, whose coefficients we compare with Lemma 19.24.

Order 0. The only field-independent term on the right-hand side is $\zeta \operatorname{Tr}(\partial_\Lambda A_\Lambda G_\Lambda)$. The second form follows from Theorem 19.14.

Order 2. On the left-hand side we have $\sum_{a,b} \overline{\phi}_a\, \partial_\Lambda \gamma_\Lambda(a \mid b)\, \phi_b$ with $\partial_\Lambda \gamma_\Lambda(a \mid b) = (\partial_\Lambda A_\Lambda)_{a,b} + \frac{1}{\hbar}\partial_\Lambda \Sigma_\Lambda(a \mid b)$. On the right-hand side we have $\sum_{a,b} \overline{\phi}_a (\partial_\Lambda A_\Lambda)_{a,b} \phi_b$ and

$$\operatorname{Tr}\left(S_\Lambda \Gamma_{\overline{\phi}\phi}\right) = \sum_{x,y} S_\Lambda(y \mid x)\, \frac{\partial^2 \Gamma_{\text{int},\Lambda}}{\partial \overline{\phi}_x\, \partial \phi_y} = \sum_{a,b} \overline{\phi}_a \left(\zeta \sum_{x,y} S_\Lambda(y \mid x)\, \gamma_\Lambda(x, a \mid y, b) \right) \phi_b.$$

[4] All sums run over the internal indices $x, y, u, v \in \{1, \dots, \mathrm{D}\}$.

The terms with $\partial_\Lambda A_\Lambda$ cancel, which gives Equation (19.30).

Order 4, particle-particle term. With $(G_\Lambda^{\mathrm{T}})(y,u) = G_\Lambda(u \mid y)$ we have

$$-\operatorname{Tr}\left(S_\Lambda \Gamma_{\overline{\phi}\overline{\phi}} G_\Lambda^{\mathrm{T}} \Gamma_{\phi\phi}\right) = -\sum_{x,y,u,v} S_\Lambda(v \mid x)\, \Gamma_{\overline{\phi}\overline{\phi}}(x,y)\, G_\Lambda(u \mid y)\, \Gamma_{\phi\phi}(u,v).$$

Since the even pair $\phi_{b_2}\phi_{b_1}$ commutes with everything, Lemma 19.22 gives

$$\Gamma_{\overline{\phi}\overline{\phi}}(x,y)\, \Gamma_{\phi\phi}(u,v) = \frac{\zeta}{4} \sum_{a_1,a_2,b_1,b_2} \overline{\phi}_{a_1} \overline{\phi}_{a_2}\, \gamma_\Lambda(a_1,a_2 \mid u,v)\, \gamma_\Lambda(x,y \mid b_1,b_2)\, \phi_{b_2}\phi_{b_1}.$$

The resulting coefficient

$$\widetilde{f}^{\mathrm{pp}}(a_1,a_2 \mid b_1,b_2) = -\frac{\zeta}{4} \sum_{x,y,u,v} S_\Lambda(v \mid x)\, G_\Lambda(u \mid y)\, \gamma_\Lambda(a_1,a_2 \mid u,v)\, \gamma_\Lambda(x,y \mid b_1,b_2)$$

is already (anti)symmetric, such that Lemma 19.24 gives the contribution $f^{\mathrm{pp}} = 4\widetilde{f}^{\mathrm{pp}}$. Renaming $x \leftrightarrow y$, $u \leftrightarrow v$ and using the (anti)symmetry of both vertices twice shows $\sum S_\Lambda(v \mid x) G_\Lambda(u \mid y)\gamma\gamma = \sum G_\Lambda(v \mid x) S_\Lambda(u \mid y)\gamma\gamma$, such that

$$\begin{aligned} f^{\mathrm{pp}}(a_1,a_2 \mid b_1,b_2) &= -\frac{\zeta}{2} \sum \gamma_\Lambda(a_1,a_2 \mid u,v)\, \dot{L}_\Lambda(u,v \mid y,x)\, \gamma_\Lambda(x,y \mid b_1,b_2) \\ &= -\frac{1}{2} \sum \gamma_\Lambda(a_1,a_2 \mid u,v)\, \dot{L}_\Lambda(u,v \mid x,y)\, \gamma_\Lambda(x,y \mid b_1,b_2), \end{aligned}$$

where in the last step we used $\gamma_\Lambda(x,y \mid b_1,b_2) = \zeta\gamma_\Lambda(y,x \mid b_1,b_2)$ and renamed $x \leftrightarrow y$.

Order 4, particle-hole terms. We have

$$-\zeta \operatorname{Tr}\left(S_\Lambda \Gamma_{\overline{\phi}\phi} G_\Lambda \Gamma_{\overline{\phi}\phi}\right) = -\zeta \sum_{x,y,u,v} S_\Lambda(v \mid x)\, \Gamma_{\overline{\phi}\phi}(x,y)\, G_\Lambda(y \mid u)\, \Gamma_{\overline{\phi}\phi}(u,v).$$

With $\phi_b\overline{\phi}_c\phi_d = \zeta\overline{\phi}_c\phi_b\phi_d = \overline{\phi}_c\phi_d\phi_b$ we obtain from Lemma 19.22

$$\begin{aligned} \Gamma_{\overline{\phi}\phi}(x,y)\, \Gamma_{\overline{\phi}\phi}(u,v) &= \zeta^2 \sum_{a,b,c,d} \overline{\phi}_a \gamma_\Lambda(x,a \mid y,b) \phi_b\, \overline{\phi}_c \gamma_\Lambda(u,c \mid v,d) \phi_d \\ &= \sum_{a_1,a_2,b_1,b_2} \overline{\phi}_{a_1} \overline{\phi}_{a_2}\, \gamma_\Lambda(x,a_1 \mid y,b_1)\, \gamma_\Lambda(u,a_2 \mid v,b_2)\, \phi_{b_2}\phi_{b_1}. \end{aligned}$$

Thus the unsymmetrized coefficient is

$$\widetilde{f}^{\mathrm{ph}}(a_1,a_2 \mid b_1,b_2) = -\zeta \sum_{x,y,u,v} S_\Lambda(v \mid x)\, G_\Lambda(y \mid u)\, \gamma_\Lambda(x,a_1 \mid y,b_1)\, \gamma_\Lambda(u,a_2 \mid v,b_2).$$

In $\widetilde{f}^{\mathrm{ph}}(a_2,a_1 \mid b_2,b_1)$ we rename $(x,y) \leftrightarrow (u,v)$ and obtain

$$\begin{aligned} \widetilde{f}^{\mathrm{ph}}(a_1,a_2 \mid b_1,b_2) + \widetilde{f}^{\mathrm{ph}}(a_2,a_1 \mid b_2,b_1) = -\zeta \sum \Big(& S_\Lambda(v \mid x) G_\Lambda(y \mid u) + G_\Lambda(v \mid x) S_\Lambda(y \mid u) \Big) \\ & \times \gamma_\Lambda(x,a_1 \mid y,b_1)\, \gamma_\Lambda(u,a_2 \mid v,b_2), \end{aligned}$$

and analogously

$$\zeta\Big(\widetilde{f}^{\mathrm{ph}}(a_2,a_1\,|\,b_1,b_2)+\widetilde{f}^{\mathrm{ph}}(a_1,a_2\,|\,b_2,b_1)\Big)=-\sum\Big(S_\Lambda(v\,|\,x)G_\Lambda(y\,|\,u)+G_\Lambda(v\,|\,x)S_\Lambda(y\,|\,u)\Big)\\ \times\gamma_\Lambda(x,a_1\,|\,y,b_2)\,\gamma_\Lambda(u,a_2\,|\,v,b_1).$$

The bracket is $\dot{L}_\Lambda(y,v\,|\,u,x)$, and $\gamma_\Lambda(x,a_1\,|\,y,b)=\gamma_\Lambda(a_1,x\,|\,b,y)$ (two transpositions). Adding the particle-particle and the particle-hole contributions (Lemma 19.24) gives Equation (19.31). The second form of $\dot{L}_\Lambda$ follows from Remark 19.13.1.

Remark 19.25.1 The flow-equations (19.29) and (19.30) are *exact* (they hold without any truncation, as long as the exact four-point vertex is inserted), since the terms of order 0 and 2 in the fields only receive contributions from the first two lines of Equation (19.19). Equation (19.31) becomes exact, if one adds the contribution of the six-point vertex $\Gamma_{6,\Lambda}=\frac{1}{(3!)^2}\sum\overline{\phi}_{a_1}\overline{\phi}_{a_2}\overline{\phi}_{a_3}\gamma_\Lambda(a_1,a_2,a_3\,|\,b_1,b_2,b_3)\phi_{b_3}\phi_{b_2}\phi_{b_1}$, which enters through the linear term $\mathrm{Tr}(S_\Lambda\cdot\partial^2\Gamma_{6,\Lambda}/\partial\overline{\phi}\,\partial\phi)$ and gives (analogously to Lemma 19.22)

$$\partial_\Lambda\gamma_\Lambda(a_1,a_2\,|\,b_1,b_2)\;\ni\;\zeta\sum_{x,y}S_\Lambda(y\,|\,x)\,\gamma_\Lambda(x,a_1,a_2\,|\,y,b_1,b_2).$$

This follows the same pattern as Equation (19.30): The $(2n+2)$-point vertex enters the flow of the $2n$-point vertex by closing two of its legs with the single-scale propagator. In the level-2 truncation with Choice 2 this term is neglected.

Corollary 19.26 In terms of the vertex-functions $\mathrm{Vert}_\Lambda(a_1,a_2\,|\,b_1,b_2)=(-\hbar)^2\gamma_\Lambda(a_1,a_2\,|\,b_1,b_2)$ (cf. the Definition of Vert in Chapter 16), the Green-function $\mathscr{G}_\Lambda=-\frac{1}{\hbar}G_\Lambda$ and $\mathscr{S}_\Lambda=-\frac{1}{\hbar}S_\Lambda$, the flow-equations read

$$\partial_\Lambda\Sigma_\Lambda(a\,|\,b)=-\zeta\sum_{x,y}\mathscr{S}_\Lambda(y\,|\,x)\;\mathrm{Vert}_\Lambda(x,a\,|\,y,b), \tag{19.33}$$

$$\begin{aligned}\partial_\Lambda\,\mathrm{Vert}_\Lambda(a_1,a_2\,|\,b_1,b_2)\;\;=&\\ &-\frac{1}{2}\sum\mathrm{Vert}_\Lambda(a_1,a_2\,|\,u,v)\,\dot{\mathscr{L}}_\Lambda(u,v\,|\,x,y)\;\mathrm{Vert}_\Lambda(x,y\,|\,b_1,b_2)\\ &-\zeta\sum\mathrm{Vert}_\Lambda(a_1,x\,|\,b_1,y)\,\dot{\mathscr{L}}_\Lambda(y,v\,|\,u,x)\;\mathrm{Vert}_\Lambda(a_2,u\,|\,b_2,v)\\ &-\sum\mathrm{Vert}_\Lambda(a_1,x\,|\,b_2,y)\,\dot{\mathscr{L}}_\Lambda(y,v\,|\,u,x)\;\mathrm{Vert}_\Lambda(a_2,u\,|\,b_1,v),\end{aligned} \tag{19.34}$$

with $\dot{\mathscr{L}}_\Lambda(p,q\,|\,r,s):=\mathscr{S}_\Lambda(p\,|\,r)\mathscr{G}_\Lambda(q\,|\,s)+\mathscr{G}_\Lambda(p\,|\,r)\mathscr{S}_\Lambda(q\,|\,s)$. The six-point contribution of Remark 19.25.1 reads $+\zeta\sum_{x,y}\mathscr{S}_\Lambda(y\,|\,x)\,\mathrm{Vert}_\Lambda(x,a_1,a_2\,|\,y,b_1,b_2)$ with $\mathrm{Vert}^{(6)}_\Lambda=(-\hbar)^3\gamma^{(6)}_\Lambda$.

Proof 19.26 With $G_\Lambda=-\hbar\mathscr{G}_\Lambda$ and $S_\Lambda=-\hbar\mathscr{S}_\Lambda$ one has $\dot{L}_\Lambda=\hbar^2\dot{\mathscr{L}}_\Lambda$. Then Equation (19.30) becomes $\partial_\Lambda\Sigma_\Lambda=\zeta\hbar\sum(-\hbar\mathscr{S}_\Lambda)\hbar^{-2}\,\mathrm{Vert}_\Lambda$, and multiplying Equation (19.31) by $\hbar^2$ gives the prefactor $\hbar^2\cdot\hbar^{-4}\cdot\hbar^2=1$ in every term. For the six-point term: $\hbar^2\cdot\zeta(-\hbar\mathscr{S}_\Lambda)(-\hbar)^{-3}\,\mathrm{Vert}^{(6)}_\Lambda=\zeta\mathscr{S}_\Lambda\,\mathrm{Vert}^{(6)}_\Lambda$.

Remark 19.26.1 Since the self-energy is fed back, the derivative of the full propagator (Remark 19.13.1)

$$\partial_\Lambda G_\Lambda = S_\Lambda - \frac{1}{\hbar} G_\Lambda \left(\partial_\Lambda \Sigma_\Lambda\right) G_\Lambda$$

differs from S_Λ. Replacing S_Λ by $\partial_\Lambda G_\Lambda$ in the loop-kernel, i.e. $\dot{L}_\Lambda(p,q \mid r,s) \to \partial_\Lambda(G_\Lambda(p \mid r) G_\Lambda(q \mid s))$, captures a part of the neglected six-point contribution ("Katanin-substitution", cf. [36]).

Corollary 19.27 (Correspondence to the One-Loop-Approximation.) If on the right-hand sides of Equations (19.30) and (19.31) one neglects the self-energy ($G_\Lambda \to G_{0,\Lambda}$, $S_\Lambda \to \partial_\Lambda G_{0,\Lambda}$) and replaces the vertex by its initial value ($\gamma_\Lambda \to s$), the right-hand sides become total derivatives, and integrating from Λ_0 (with $G_{0,\Lambda_0} = 0$) to Λ gives

$$\frac{1}{\hbar}\Sigma_\Lambda(a \mid b) \approx \zeta \sum_{x,y} G_{0,\Lambda}(y \mid x)\, s(x,a \mid y,b), \tag{19.35}$$

$$\begin{aligned}\gamma_\Lambda(a_1,a_2 \mid b_1,b_2) \approx & s(a_1,a_2 \mid b_1,b_2) - \frac{1}{2}\sum s(a_1,a_2 \mid u,v)\, G_{0,\Lambda}(u \mid x)\, G_{0,\Lambda}(v \mid y)\, s(x,y \mid b_1,b_2) \\ & - \zeta \sum s(a_1,x \mid b_1,y)\, G_{0,\Lambda}(y \mid u)\, G_{0,\Lambda}(v \mid x)\, s(a_2,u \mid b_2,v) \\ & - \sum s(a_1,x \mid b_2,y)\, G_{0,\Lambda}(y \mid u)\, G_{0,\Lambda}(v \mid x)\, s(a_2,u \mid b_1,v).\end{aligned} \tag{19.36}$$

For $\Lambda \to 0$ this is first- (Hartree-Fock) and second-order perturbation theory for the self-energy and the effective interaction, i.e. the One-Loop-Approximation (Approximation 16.58, written there in the conventions of [27]).

Proof 19.27 Without self-energy one has $S_\Lambda = \partial_\Lambda G_{0,\Lambda}$ (Remark 19.13.1) and therefore

$$\dot{L}_\Lambda(p,q \mid r,s) = \partial_\Lambda\Big(G_{0,\Lambda}(p \mid r)\, G_{0,\Lambda}(q \mid s)\Big).$$

Since s is Λ-independent, the right-hand sides are total derivatives. Integration from Λ_0 to Λ, the initial conditions (19.24) and $G_{0,\Lambda_0} = 0$ give the claim, where we used $L(u,v \mid x,y) = G_{0,\Lambda}(u \mid x) G_{0,\Lambda}(v \mid y)$ and $L(y,v \mid u,x) = G_{0,\Lambda}(y \mid u) G_{0,\Lambda}(v \mid x)$.

Remark 19.27.1 Drawing the corresponding Feynman-diagrams, and denoting the single-scale propagator by a slashed line, one immediately recognizes in Equation (19.31) the typical particle-particle diagram (two propagators running in the same direction between the two vertices), the direct particle-hole diagram (a closed loop through both vertices, which produces the statistics-factor ζ) and the crossed particle-hole diagram (obtained from the direct one by exchanging $b_1 \leftrightarrow b_2$, which produces another factor ζ). Every diagram contains exactly one slashed line, which can sit on either of the two internal lines ($\dot{L}_\Lambda$ is the sum of both possibilities). The self-energy flow (19.30) is the tadpole-diagram (Hartree- and Fock-contribution) with a slashed line. Integrating "$\partial_\Lambda G_\Lambda \cdots G_\Lambda \cdots$" to "$G_\Lambda \cdots G_\Lambda \cdots$" produces the factor $\frac{1}{2}$ of the particle-particle diagram in the One-Loop-Approximation, as pointed out in [10].

Remark 19.27.2 It is reasonable to note that we used different sets of identities to arrive at the respective equations: For the One-Loop-Approximation (Approximation 16.58), one performs a trace-log-expansion up to second order in the interaction. For the level-2 truncation leading to Equation (19.31) we used the Neumann-series and truncated the expansion after the second order in the interaction. Different techniques yielding equivalent sets of equations obviously indicate their correctness.

Remark 19.27.3 For debugging purposes: Theorem 19.5, Lemma 19.10, Theorem 19.11, Theorem 19.23 (up to quartic order in the fields), Theorem 19.25 (including the six-point term of Remark 19.25.1), Corollary 19.26 and Corollary 19.27 have been checked numerically: For fermions ($\zeta = -1$) by an exact implementation of the Graßmann-algebra with $D = 3$ and $D = 4$, for bosons ($\zeta = +1$) perturbatively (up to fifth order in the interaction) with $D = 2$; in both cases with random complex matrices $A_\Lambda = A + \Lambda B$ and random (anti)symmetric s, computing Γ_Λ by an explicit Legendre-transformation and ∂_Λ by finite differences. Flipping, e.g., the sign of the crossed particle-hole term makes the check fail.

20. Thermal Quantum Field Theory

20.1. Many-Body Quantum Field Theory - Pure Systems

20.1.1. Coherent States and Resolutions of Identity

In the previous chapter we learned many techniques on how to evaluate (functional) integrals. In this chapter, we will provide the bridge between the many-body-concepts developed earlier, and the (functional) integral formalism. For this we still require some tools.

Definition 20.1 We consider a polynomial algebra $\mathscr{P}_\zeta$ as in Definition 16.1 and a Fock-space $\mathscr{H}_\eta$ that is generated by creation and annihilation-operators, as in Equation (10.4). We then construct[1] a [G]eneralized [H]ilbert-space $\mathscr{GH}_{\eta,\zeta}$ as the set of linear combinations of states of the Hilbert-space $\mathscr{H}_\eta$ with coefficients in the polynomial algebra $\mathscr{P}_\zeta$.

Remark 20.1.1 Notice that this implies, that any vector $|\psi\rangle$ in the generalized Hilbert-space can be expanded as

$$|\psi\rangle = \sum_\alpha \chi_\alpha |\phi_\alpha\rangle \tag{20.1}$$

where the χ_α are elements of the polynomial algebra and the $|\phi_\alpha\rangle$ vectors of the Hilbert-space.

In order to treat expressions containing combinations of polynomial-algebra-generators and creation- and annihilation-operators, it is necessary to specify commutation-relations between the ψ's and c's.

Definition 20.2 In the generalized Hilbert-space, we define commutation-relations as

$$[\psi_i, c_j]_\zeta := 0 \tag{20.2}$$

etc. for the other combinations.

Definition 20.3 We define a *coherent state* $|\psi\rangle \in \mathscr{GH}_{\eta,\zeta}$ as an eigenstate of the statistical annihilation-operator, i.e. fulfilling the equation

$$c_j|\psi\rangle = \psi_j|\psi\rangle \tag{20.3}$$

with $\psi_j \in \mathscr{P}_\zeta$.

[1] Cf. [38] p. 29 for this part, or [33] p. 64 for the enlarged Fock-space for fermionic coherent states.

Theorem 20.4 The state $|\psi\rangle$ defined through

$$|\psi\rangle = \exp\left(\sum_{j=1}^{\mathrm{d}_\eta} c_j^\dagger \psi_j\right)|0\rangle \tag{20.4}$$

is a *coherent state with respect to generators* $\{c_1, c_1^\dagger, \dots, c_{\mathrm{d}_\eta}, c_{\mathrm{d}_\eta}^\dagger\}$ of $\mathscr{H}$ *and* $\{\psi_1, \overline{\psi}_1, \dots, \psi_{\mathrm{d}_\eta}, \overline{\psi}_{\mathrm{d}_\eta}\}$ of $\mathscr{P}_\zeta$, i.e. it is an eigenstate of the statistical annihilation-operators fulfilling

$$c_j|\psi\rangle = \psi_j|\psi\rangle \quad \text{for all } j \in \{1, \dots, \mathrm{d}_\eta\} \tag{20.5}$$

Proof 20.4 See Appendix, Proofs, page 596.

Remark 20.4.1 Notice that we have $\mathrm{D} = \mathrm{d}_\eta$ in the sense of Definition 16.1.

Corollary 20.5 By taking the hermitian conjugate of Equation (20.4) we find that the „bra" $\langle\psi|$ associated with the „ket" $|\psi\rangle$ is a left-eigenstate of the set of creation-operators, i.e. for

$$\langle\psi| = \langle 0|\exp\left(\sum_{j=1}^{\mathrm{d}_\eta} \overline{\psi}_j c_j\right) \tag{20.6}$$

it holds

$$\langle\psi|c_j^\dagger = \langle\psi|\overline{\psi}_j \tag{20.7}$$

Proof 20.5 See Appendix, Proofs, page 596.

Lemma 20.6 One finds the *derivative-identities* for the coherent states as

$$\langle\psi|c_j = \frac{\partial}{\partial\overline{\psi}_j}\langle\psi|, \qquad c_j^\dagger|\psi\rangle = \zeta\frac{\partial}{\partial\psi_j}|\psi\rangle \tag{20.8}$$

Proof 20.6 See Appendix, Proofs, page 596.

Theorem 20.7 One finds for the overlap between two coherent states

$$\langle\psi'|\psi\rangle = \exp\left(\sum_{j=1}^{\mathrm{d}_\eta} \overline{\psi}_j'\psi_j\right) \tag{20.9}$$

Proof 20.7 See, for example, [4], Chapter 4.

Theorem 20.8 Taking $\mathrm{D} = \mathrm{d}_\eta$ in Definition 16.1, we obtain the *completeness-relation*

$$\mathbb{1}_{\mathscr{H}} = \int \mathrm{d}_\zeta(\overline{\psi}, \psi)\, \mathrm{e}^{-\sum_{j=1}^{\mathrm{d}_\eta} \overline{\psi}_j \psi_j} |\psi\rangle\langle\psi| \tag{20.10}$$

with integration-measure as in Definition 16.16

$$\mathrm{d}_\zeta(\overline{\psi}, \psi) \equiv \prod_{j=1}^{\mathrm{d}_\eta} \frac{\mathrm{d}\overline{\psi}_j \mathrm{d}\psi_j}{(2\pi\mathrm{i})^{\theta(\zeta)}} \tag{20.11}$$

Proof 20.8 See Appendix, Proofs, page 596.

Lemma 20.9 For $\eta = 1$, the Hamiltonian in Equation (10.3) is block-diagonal w.r.t. the number of particles.

Proof 20.9 See Appendix, Proofs, page 596.

Remark 20.9.1 Notice that this theorem implies, that $\langle N|H|N'\rangle = 0$ if $|N\rangle$ and $|N'\rangle$ represents occupation number states with different numbers of particles.

Lemma 20.10 Let $|n\rangle$ and $|n'\rangle$ denote two N-particle states in their occupation-number representation. Then it follows that

$$\langle n|\psi\rangle\langle\psi|n'\rangle = \langle\zeta\psi|n'\rangle\langle n|\psi\rangle. \tag{20.12}$$

Proof 20.10 See Appendix, Proofs, page 596.

Lemma 20.11 For an operator X that is given as a polynomial expression in ladder-operators $X \equiv X(c, c^\dagger)$, we write for the normalized overlap between coherent states

$$\frac{\langle\psi|X|\psi'\rangle}{\langle\psi|\psi'\rangle} \quad = \quad X(\overline{\psi}, \psi'), \tag{20.13}$$

i.e. the normalized overlap is *the* polynomial expression in Graßmann-variables, in which one replaced each ladder-operator by its Graßmann-counterpart.

Proof 20.11 See Appendix, Proofs, page 596.

Remark 20.11.1 Notice that for the Hamiltonian-operators in Fact 8.4, one obtains the identities

$$\frac{\langle\psi|H|\psi'\rangle}{\langle\psi|\psi'\rangle} \equiv H(\overline{\psi},\psi') \equiv \begin{cases} \sum_{i,j=1}^{\mathrm{d}} H_{i,j}\overline{\psi}_i\psi_j + \sum_{i,j,k=1}^{\mathrm{d}} \left(H_{i,j;k}\overline{\psi}_i\overline{\psi}_j\psi_k + H_{i;j,k}\overline{\psi}_i\psi_j\psi_k\right) + \dots & \text{for } \eta = 0 \\ \sum_{i,j=1}^{\mathrm{d}} H_{i,j}\overline{\psi}_i\psi_j + \frac{1}{2}\sum_{i,j,k,l=1}^{\mathrm{d}} H_{i,j;kl}\overline{\psi}_i\overline{\psi}_j\psi_l\psi_k + \dots & \text{for } \eta = 1 \end{cases} \tag{20.14}$$

and the interacting part will be considered in the next subsection.

Lemma 20.12 One finds for the trace of an operator $X \equiv X(c, c^\dagger)$ that is block-diagonal in the number of fermionic particle-number (and arbitrary in the bosonic particle-number)

$$\mathrm{Tr}_{\mathscr{F}_\zeta} X(c,c^\dagger) = \int \mathrm{d}_\zeta(\overline{\psi},\psi)\, \mathrm{e}^{-\sum_{j=1}^{\mathrm{d}_\eta}\overline{\psi}_j\psi_j}\, \langle\zeta\psi|X|\psi\rangle\,. \tag{20.15}$$

with

$$\langle\zeta\psi| \equiv \langle 0|\exp\left(\zeta\sum_{j=1}^{\mathrm{d}_\eta}\overline{\psi}_j c_j\right) \tag{20.16}$$

Proof 20.12 See Appendix, Proofs, page 596.

20.1.2. The Functional Field Integral of the Partition Function

Theorem 20.13 One can rewrite the grand canonical partition function Z as a functional field integral

$$Z = \mathrm{Tr}_{\mathscr{H}_\eta}\, \mathrm{e}^{-\beta(H-\eta\mu N)} = \int \mathscr{D}_\zeta(\psi,\overline{\psi})\, \mathrm{e}^{-S_\eta[\psi,\overline{\psi}]}$$

where the action is written in its *continuum-notation*

$$\begin{aligned} S_\eta[\psi,\overline{\psi}] &\equiv \int_0^{\hbar\beta} \mathrm{d}\tau \left[\overline{\psi}\cdot\partial_\tau\psi + \frac{H(\overline{\psi},\psi) - \eta\mu N(\overline{\psi},\psi)}{\hbar}\right] \\ &\equiv \int_0^{\hbar\beta} \mathrm{d}\tau \left[\overline{\psi}\cdot\partial_\tau\psi + \frac{H_0(\overline{\psi},\psi) - \eta\mu N(\overline{\psi},\psi)}{\hbar}\right] \quad + \int_0^{\hbar\beta} \mathrm{d}\tau\, \frac{V(\overline{\psi}(\tau),\psi(\tau))}{\hbar} \end{aligned} \tag{20.17}$$

and the other symbols will be introduced and explained in the course of the text.

Proof 20.13 See Appendix, Proofs, page 596.

Remark 20.13.1 Notice that the continuum-notation is a bit misleading, as we are strictly speaking dealing with finite sums. However, the charm of the continuum-notation has prevailed.

Remark 20.13.2 We notice, that the field integral above is *almost* in the form of the generic field integral that was introduced in Chapter 16. The only difference is that (in our notation) the action has (or seems to have) a continous variable, whereas we based our formalism only on the discrete case. To this end, we need to translate the action into a discrete form by performing an appropriate variable transformation.

Remark 20.13.3 Notice that for the generic Hamilton-operators in Fact 8.4, one obtains the identities

$$S_\eta[\psi,\overline{\psi}] = \begin{cases} \iint \overline{\psi}_\alpha(\tau)\Big[\partial_\tau \delta_{\alpha\alpha'} + H_{\substack{0\\ \alpha\alpha'}}/\hbar\Big]\psi_{\alpha'}(\tau) + \iint \frac{V_{\alpha,\beta;\gamma}}{\hbar}\overline{\psi}_\alpha(\tau)\overline{\psi}_\beta(\tau)\psi_\gamma(\tau) + \frac{V_{\alpha;\beta,\gamma}}{\hbar}\overline{\psi}_\alpha(\tau)\psi_\beta(\tau)\psi_\gamma(\tau) + \dots & \text{for } \eta = 0 \\ \iint \overline{\psi}_\alpha(\tau)\Big[\Big(\partial_\tau - \frac{\mu}{\hbar}\Big)\delta_{\alpha\alpha'} + H_{\substack{0\\ \alpha\alpha'}}/\hbar\Big]\psi_{\alpha'}(\tau) + \frac{1}{2}\iint \frac{V_{\alpha_1\alpha_2\alpha_3\alpha_4}}{\hbar}\overline{\psi}_{\alpha_1}(\tau)\overline{\psi}_{\alpha_2}(\tau)\psi_{\alpha_4}(\tau)\psi_{\alpha_3}(\tau) + \dots & \text{for } \eta = 1 \end{cases} \tag{20.18}$$

Lemma 20.14 The following transformation is unitary up to a (diverging) scaling-factor

$$\begin{aligned} \psi(\tau) &= \frac{1}{\sqrt{\hbar\beta}}\sum_{\omega_n\in\Omega_\zeta}\psi(\mathrm{i}\omega_n)\,\mathrm{e}^{-\mathrm{i}\omega_n\tau}, \qquad \psi(\mathrm{i}\omega_n) = \frac{1}{\sqrt{\hbar\beta}}\int_0^{\hbar\beta}\mathrm{d}\tau\,\psi(\tau)\,\mathrm{e}^{\mathrm{i}\omega_n\tau} \\ \overline{\psi}(\tau) &= \frac{1}{\sqrt{\hbar\beta}}\sum_{\omega_n\in\Omega_\zeta}\overline{\psi}(\mathrm{i}\omega_n)\,\mathrm{e}^{\mathrm{i}\omega_n\tau}, \qquad \overline{\psi}(\mathrm{i}\omega_n) = \frac{1}{\sqrt{\hbar\beta}}\int_0^{\hbar\beta}\mathrm{d}\tau\,\overline{\psi}(\tau)\,\mathrm{e}^{-\mathrm{i}\omega_n\tau} \end{aligned} \tag{20.19}$$

where

$$\mathbb{Z}\ni n\mapsto \omega_n = \frac{2n+1-\theta(\zeta)}{\hbar\beta}\pi = \begin{cases} 2n\pi/\hbar\beta & \text{for bosons} \\ (2n+1)\pi/\hbar\beta & \text{for fermions} \end{cases} \tag{20.20}$$

Proof 20.14 See Appendix, Proofs, page 597.

Remark 20.14.1 Notice that this is a change of coordinates in the sense of Equation (16.67) with Jacobian-matrix

$$\mathrm{Det}\left(\frac{\partial\psi(\tau_i)}{\partial\psi(\mathrm{i}\omega_j)}\right) = \mathrm{Det}\left(\frac{\partial\overline{\psi}(\tau_i)}{\partial\overline{\psi}(\mathrm{i}\omega_j)}\right) = \text{TBLookedUp} \tag{20.21}$$

Remark 20.14.2 This diverging factor is mostly irrelevant. There are though situations, where it becomes important to keep the diverging factor inside the Equations. Examples are when one computes the natural energy for a non-interacting system in Lemma TBReferenced, or when one considers corrections to the partition-function in the superconducting state.

Remark 20.14.3 Notice that we found in the proof of this Lemma the identity

Kronecker-Delta relations for zeta-transformations. (20.22)

Corollary 20.15 Transforming to Matsubara-frequencies gives in the non-interacting case ($V \equiv 0$)

$$S[\psi, \overline{\psi}] = \sum_{\substack{\omega_n \in \Omega_\zeta \\ \alpha, \alpha' \in \mathscr{A}}} \overline{\psi}_\alpha(\mathrm{i}\omega_n) \Big[\left(-\mathrm{i}\omega_n - \frac{\eta\mu}{\hbar} \right) \delta_{\alpha\alpha'} + H_{0\,\alpha\alpha'}/\hbar \Big] \psi_{\alpha'}(\mathrm{i}\omega_n) \tag{20.23}$$

and for the Hamiltonians in Fact 8.4 …

- in the massless case ($\eta = 0$)

$$\begin{aligned} S[\psi, \overline{\psi}] = & \sum_{\substack{\omega_n \in \Omega_\zeta \\ \alpha, \alpha' \in \mathscr{A}}} \overline{\psi}_\alpha(\mathrm{i}\omega_n) \Big[-\mathrm{i}\omega_n \delta_{\alpha\alpha'} + H_{0\,\alpha\alpha'}/\hbar \Big] \psi_{\alpha'}(\mathrm{i}\omega_n) \\ & + \frac{1}{\hbar} \sum_{\substack{\omega_n, \omega_{n'}, \omega_{n''} \in \Omega_\zeta \\ \alpha, \alpha', \alpha'' \in \mathscr{A}}} \left(H_{\alpha,\alpha';\alpha''} \overline{\psi}_\alpha(\omega_n) \overline{\psi}_{\alpha'}(\omega_{n'}) \psi_{\alpha''}(\omega_{n''}) \delta_{\omega_n + \omega_{n'}, \omega_{n''}} + H_{\alpha;\alpha',\alpha''} \overline{\psi}_\alpha(\omega_n) \psi_{\alpha'}(\omega_{n'}) \psi_{\alpha''}(\omega_{n''}) \delta_{\omega_n, \omega_{n'} + \omega_{n''}} \right) \end{aligned} \tag{20.24}$$

- in the massless case ($\eta = 1$)

$$\begin{aligned} S[\psi, \overline{\psi}] = & \sum_{\substack{\omega_n \in \Omega_\zeta \\ \alpha, \alpha' \in \mathscr{A}}} \overline{\psi}_\alpha(\mathrm{i}\omega_n) \Big[\left(-\mathrm{i}\omega_n - \frac{\mu}{\hbar} \right) \delta_{\alpha\alpha'} + H_{0\,\alpha\alpha'}/\hbar \Big] \psi_{\alpha'}(\mathrm{i}\omega_n) \\ & + \frac{1}{2} \frac{1}{\hbar\beta} \sum_{\substack{\alpha_1\alpha_2\alpha_3\alpha_4 \in \mathscr{A} \\ \omega_{n_1}\omega_{n_2}\omega_{n_3}\omega_{n_4} \in \Omega_\zeta}} \frac{V_{\alpha_1\alpha_2\alpha_3\alpha_4} \delta_{n_1+n_2,\, n_3+n_4}}{\hbar} \overline{\psi}_{\alpha_1}(\mathrm{i}\omega_{n_1}) \overline{\psi}_{\alpha_2}(\mathrm{i}\omega_{n_2}) \psi_{\alpha_4}(\mathrm{i}\omega_{n_4}) \psi_{\alpha_3}(\mathrm{i}\omega_{n_3}) \end{aligned} \tag{20.25}$$

with rescaled[2] partition-function.

Proof 20.15 See Appendix, Proofs, page 600.

Lemma 20.16 The natural energy from Equation (10.8) is …

- in the non-interacting case $V \equiv 0$ given as

$$\Omega_0 = \frac{\zeta}{\beta} \sum_{\alpha \in \mathscr{A}} \log\left(1 - \zeta \mathrm{e}^{-\beta\xi_\alpha}\right) \tag{20.26}$$

  whereas $\xi_{\alpha_1}, \xi_{\alpha_2}, \ldots, \xi_{\alpha_{\mathrm{d}_\mathcal{H}}}$ denote the eigenvalues of $H_0 - \eta\mu$.

- in the interacting case $V \neq 0$ given as

$$\Omega = \Omega_0 - \frac{1}{\beta} \sum \text{"all connected graphs"} \tag{20.27}$$

[2] Notice that this does not change the expectation-value, due to the quotient nature of the generating functional in Equation (16.39).

Proof 20.16 See Appendix, Proofs, page 601.

20.1.3. Imaginary-Time Generalized Green-Functions

From the proof of Theorem 20.17 we see that expectation-values of operators can be computed within the functional integral formalism only if they are normal ordered. Therefore one can compute any generalized Green-function but one has to re-express X and X' through their normal-ordered expressions.

20.1.4. Imaginary-Time Pure n-Body Green-Functions

Theorem 20.17 For $\tau_1, \dots, \tau_n, \tau'_1, \dots, \tau'_n \in (0, \hbar\beta)$ one finds for the imaginary-time n-body Green-Functions

$$\begin{aligned}\mathscr{G}(A_1, \dots, A_n \mid A'_n, \dots, A'_1) &= \left(-\frac{1}{\hbar}\right)^n \frac{1}{Z} \int \mathscr{D}_\zeta(\psi, \overline{\psi})\, \mathrm{e}^{-S[\psi,\overline{\psi}]}\, \psi_{\alpha_1}(\tau_1) \cdots \psi_{\alpha_n}(\tau_n)\, \overline{\psi}_{\alpha'_1}(\tau'_1) \cdots \overline{\psi}_{\alpha'_n}(\tau'_n) \\ &\equiv \left(-\frac{1}{\hbar}\right)^n \left\langle\, \psi(A_1) \cdots \psi(A_n)\, \overline{\psi}(A'_1) \cdots \overline{\psi}(A'_n)\, \right\rangle .\end{aligned}$$

Proof 20.17 See Appendix, Proofs, page 601.

Theorem 20.18 For the one-body-Green-function of a non-interacting (fermionic or bosonic) gas one finds[3]

$$\mathscr{G}_{\substack{0 \\ \alpha,\alpha'}}(\tau) = \frac{1}{\hbar\beta} \sum_{\omega_n \in \Omega_\zeta} \mathscr{G}_{\substack{0 \\ \alpha,\alpha'}}(\mathrm{i}\omega_n)\, \mathrm{e}^{-\mathrm{i}\omega_n \tau} \tag{20.29}$$

with

$$\mathscr{G}_{\substack{0 \\ \alpha,\alpha'}}(\mathrm{i}\omega_n) = \frac{1}{\hbar} \left(\left[\mathrm{i}\omega_n - \frac{H_0 - \eta\mu}{\hbar} \right]^{\mathrm{inv}} \right)_{\alpha,\alpha'} \quad \Longleftrightarrow: \quad \mathscr{G}_0(\mathrm{i}\omega_n) \equiv \frac{1}{\mathrm{i}\hbar\omega_n - (H_0 - \eta\mu)} \tag{20.30}$$

Proof 20.18 See Appendix, Proofs, page 601.

[3] Notice that we are dropping the infinitesimal phases for notational convenience. Keeping track of them yields

$$\mathscr{G}_{\substack{0 \\ \alpha,\alpha'}}(\mathrm{i}\omega_n) = \frac{1}{\hbar} \left(\left[\mathrm{i}\omega_n - \frac{H_0 - \eta\mu}{\hbar} \mathrm{e}^{\mathrm{i}\omega_n \delta} \right]^{\mathrm{inv}} \right)_{\alpha,\alpha'} \tag{20.28}$$

20.1.5. Intermezzo: The Continuum-Notation with it's Perks and Problems

We introduced the mathematical framework of quantum field theory in Chapter 16 based on discrete indices. In the derivation of the field-integral however, we noticed that the resulting expressions are more conveniently written in a continuum-notation. This is a re-occuring phenomenon in physics. For example the action in Equation (20.17) or (equivalently) in Equation (20.18) can also be re-expressed with field operators (which are introduced in Appendix, section 29.8) in a continuum-notation over space, such that the entire action becomes an integral over four variables. The only thing one needs is some mild assumptions about the completeness of the basis-set.

Definition 20.19 We equip our partition-function with external sources and introduce the generating functional with continuum-notation

$$\frac{Z[\bar{j},j]}{Z} = \frac{1}{Z}\int \mathscr{D}_\zeta(\psi,\overline{\psi})\,\mathrm{e}^{-S[\psi,\overline{\psi}]+\oint j^\dagger\psi+\psi^\dagger j} = \left\langle \exp\oint j^\dagger\psi+\psi^\dagger j \right\rangle \tag{20.31}$$

whereas the source-terms are given in their continuum-notation as

$$\oint j^\dagger\psi \equiv \int_0^{\hbar\beta}\mathrm{d}\tau\, j^\dagger(\tau)\psi(\tau) \equiv \int_0^{\hbar\beta}\mathrm{d}\tau \sum_{\alpha\in\mathscr{A}} \bar{j}_\alpha(\tau)\psi_\alpha(\tau) \equiv \Delta\tau \sum_{\substack{\alpha\in\mathscr{A}\\ n=1,\dots,N_\tau}} \bar{j}_\alpha(\tau_n)\psi_\alpha(\tau_n) \tag{20.32}$$

Lemma 20.20 One concludes, that one can determine the n-body Green-function as functional derivative

$$\mathscr{G}(A_1,\dots,A_n \mid A'_1,\dots,A'_n) = \left(-\frac{\zeta}{\hbar}\right)^n \frac{\delta^{2n}}{\delta\bar{j}(A_1)\cdots\delta\bar{j}(A_n)\delta j(A'_n)\cdots\delta j(A'_1)}\frac{Z[\bar{j},j]}{Z}\Big|_{\bar{j}=j=0} \tag{20.33}$$

Proof 20.20 See Appendix, Proofs, page 575.

Notation 20.21 Just as in Definition 16.30, we introduce the analogue of the Gibbs free energy / grand canonical potential

$$W[\bar{j},j] = +\log Z[\bar{j},j] \tag{20.34}$$

Notation 20.22 Just as in Definition 16.41 we introduce the [c]onnected Green-functions

$$\mathscr{G}^{\mathrm{c}}(A_1,\dots,A_n \mid A'_1,\dots,A'_n) = \left(-\frac{\zeta}{\hbar}\right)^n \frac{\delta^{2n}}{\delta\bar{j}(A_1)\cdots\delta\bar{j}(A_n)\delta j(A'_n)\cdots\delta j(A'_1)}W[\bar{j},j]\Big|_{\bar{j}=j=0} \tag{20.35}$$

Theorem 20.23 One has the identity

$$\left\langle c^\dagger_{\alpha'}(0)\, c_\alpha(0)\right\rangle = \frac{\delta^2}{\delta\bar{j}(\tau=0-,\alpha)\delta j(\tau'=0,\alpha')}\frac{Z[\bar{j},j]}{Z}\Big|_{\bar{j}=j=0} \tag{20.36}$$

Proof 20.23 Recall first that from the definition of the Green-function

$$\mathscr{G}(A,A') \equiv \mathscr{G}_{\alpha,\alpha'}(\tau,\tau') \equiv -\frac{1}{\hbar}\frac{\mathrm{Tr}_{\mathscr{F}_\zeta}\, \mathrm{e}^{-\beta(H-\mu N)}\Big[\theta(\tau-\tau')\, c_\alpha(\tau)\, c^\dagger_{\alpha'}(\tau') + \zeta\,\theta(\tau'-\tau)\, c^\dagger_{\alpha'}(\tau')\, c_\alpha(\tau)\Big]}{\mathrm{Tr}_{\mathscr{F}_\zeta}\, \mathrm{e}^{-\beta(H-\mu N)}}$$

one finds the identity

$$\left\langle c^\dagger_{\alpha'}(0)\, c_\alpha(0)\right\rangle = -\frac{\hbar}{\zeta}\mathscr{G}_{\alpha,\alpha'}(\tau=0-,\tau'=0) \tag{20.37}$$

This then implies with Lemma 16.40

$$\begin{aligned}\left\langle c^\dagger_{\alpha'}(0)\, c_\alpha(0)\right\rangle &= -\frac{\hbar}{\zeta}\mathscr{G}_{\alpha,\alpha'}(\tau=0-,\tau'=0)\\ &= -\frac{\hbar}{\zeta}\left(-\frac{\zeta}{\hbar}\right)^1\frac{\delta^2}{\delta\bar{j}(\tau=0-,\alpha)\delta j(\tau'=0,\alpha')}\frac{Z[\bar{j},j]}{Z}\Big|_{\bar{j}=j=0}\\ &= \frac{\delta^2}{\delta\bar{j}(\tau=0-,\alpha)\delta j(\tau'=0,\alpha')}\frac{Z[\bar{j},j]}{Z}\Big|_{\bar{j}=j=0}\end{aligned} \tag{20.38}$$

Lemma 20.24 One can rewrite the source-term derivatives as

$$\frac{\delta}{\delta\bar{j}(\tau=0-,\alpha)} = \frac{1}{\sqrt{\hbar\beta}}\sum_{\omega_n\in\Omega_\zeta}\mathrm{e}^{+\mathrm{i}\omega_n 0^+}\frac{\partial}{\partial\bar{j}(\mathrm{i}\omega_n,\alpha)} \tag{20.39}$$

Proof 20.24 Follows by combining Lemma 16.51 with Lemma 20.14.

20.2. Many-Body Quantum Field Theory - Mixed Systems

We present the formalism at the example of **massive-massless-particles-mixtures**. The generalization to other mixtures is straight-forward.

20.2.1. Coherent States and Resolutions of Identity

In one to one correspondence to the respective creation- and annihilation-operators we again introduce Graßmann-numbers $\left\{\psi_1, \overline{\psi}_1, \dots, \psi_{\mathrm{d}_{m>0}}, \overline{\psi}_{\mathrm{d}_{m>0}}\right\}$ and complex-numbers $\left\{\phi_1, \overline{\phi}_1, \dots, \phi_{\mathrm{d}_{m=0}}, \overline{\phi}_{\mathrm{d}_{m=0}}\right\}$ to form polynomial expressions with them and creation- and annihilation-operators.

Theorem 20.25 The bra- and ket-states $\langle\, \chi \,|$ and $|\, \chi \,\rangle$ as

$$\langle\, \chi \,| \equiv \langle\, \mathrm{vac.} \,| \exp\left(+ \sum_{j=1}^{\mathrm{d}_{m=0}} b_j \overline{\phi}_j \quad - \quad \sum_{j=1}^{\mathrm{d}_{m>0}} c_j \overline{\psi}_j \right), \qquad |\, \chi \,\rangle \equiv \exp\left(+ \sum_{j=1}^{\mathrm{d}_{m=0}} \phi_j b_j^\dagger \quad - \quad \sum_{j=1}^{\mathrm{d}_{m>0}} \psi_j c_j^\dagger \right) |\, \mathrm{vac.} \,\rangle,$$

and are left- and right-eigenstates of creation- and annihilation-operators, implying

$$\langle\, \chi \,| b_\beta^\dagger = \langle\, \chi \,| \overline{\phi}_\beta, \quad \langle\, \chi \,| c_\alpha^\dagger = \langle\, \chi \,| \overline{\psi}_\alpha, \qquad b_\beta |\, \chi \,\rangle = \phi_\beta |\, \chi \,\rangle \quad \text{and} \quad c_\alpha |\, \chi \,\rangle = \psi_\alpha |\, \chi \,\rangle, \tag{20.40}$$

for all $\alpha \in \{1, \dots \mathrm{d}_{m>0}\}$, $\beta \in \{1, \dots, \mathrm{d}_{m=0}\}$.

Proof 20.25 TBD.

Theorem 20.26 It follows

- Overlap
- Completeness Relation for the total Hilbert-space.

Proof 20.26 Follows from the generalization of the identities by straight forwarad computations.

20.2.2. The Functional Field Integral of the Partition Function

Theorem 20.27 One can rewrite the mixed partition function Z as a functional field integral

$$Z = \mathrm{Tr}_{\mathscr{H}} \exp - \beta \left(H_{m>0} - \mu N_{m>0} + H_{m=0} \right) = \int \mathscr{D}(\chi, \overline{\chi})\, \mathrm{e}^{-S[\chi, \overline{\chi}]}$$

where

$$S[\chi,\overline{\chi}] \equiv \quad S_0[\chi,\overline{\chi}] \quad + \quad \underset{\text{int}}{S_{m>0}}[\psi,\overline{\psi}] + \underset{\text{int}}{S_{m=0}}[\phi,\overline{\phi}] + S_{\text{int}}[\chi,\overline{\chi}]$$

$$= \int_0^{\hbar\beta} \mathrm{d}\tau \begin{pmatrix} \boldsymbol{\psi} \\ \boldsymbol{\phi} \end{pmatrix}^{\dagger} \cdot \begin{pmatrix} \partial_\tau + \frac{H_{\underset{m>0}{0}} - \mu}{\hbar} & 0 \\ 0 & \partial_\tau + \frac{H_{\underset{m=0}{0}}}{\hbar} \end{pmatrix} \cdot \begin{pmatrix} \boldsymbol{\psi} \\ \boldsymbol{\phi} \end{pmatrix} \quad + \quad \int_0^{\hbar\beta} \mathrm{d}\tau \, \frac{V_{m>0}(\overline{\boldsymbol{\psi}},\boldsymbol{\psi}) + V_{m=0}(\overline{\boldsymbol{\phi}},\boldsymbol{\phi}) + V_{\text{int}}(\overline{\chi},\chi)}{\hbar}$$

Proof 20.27 Follows from the generalization of the identities by straight forwarad computations.

Remark 20.27.1 Going over to Matsubara-frequencies turns this expression into a real mess, as one has to account for the different statistics within the respective summations. It is however common to use Matsubara-frequencies, as it is still the most tractable way to deal with these integrals.

20.2.3. Pure Imaginary-Time Generalized Green-Functions

TBDigitalized for interaction-expectation-values.

20.2.4. Pure Imaginary-Time n-Body Green-Functions

21. Examples of Self-Energies and Polarizations for Interacting Systems

In this whole section, we consider a situation as in Equation (10.3) or its mixed system generalization, where the total system is written as

$$H \quad = \quad H_0 \quad + \quad V \tag{21.1}$$

whereas H_0 is a Hamiltonian of which the Green-functions are accessible, and V is a perturbation of some kind. The electronic self-energy is the main object of interest. It will be always written in a series

$$\Sigma(\mathrm{i}\omega_n) \quad = \quad \sum_{j=1}^{\infty} \Sigma^{(j)}(\mathrm{i}\omega_n) \quad = \quad \Sigma^{(1)}(\mathrm{i}\omega_n) + \Sigma^{(2)}(\mathrm{i}\omega_n) + \Sigma^{(3)}(\mathrm{i}\omega_n) + \mathcal{O}(\, V^4\,) \tag{21.2}$$

in the interaction-vertices.

21.1. Example: A Diagonalized Gas with Single-Particle-Interactions

Theorem 21.1 The self-energy reads

$$\Sigma_{\beta\beta'}(\mathrm{i}\omega_n) = V_{\beta\beta'} = \text{„frequency-independent“} . \tag{21.3}$$

Proof 21.1 See Appendix, Proofs, page 381.

Remark 21.1.1 Notice that with the Dyson-equation (15.12) one can conclude that this is actually the only term that appears in the self-energy, i.e. $\Sigma^{(1)}_{\beta\beta'} \equiv \Sigma_{\beta\beta'}$ and $\Sigma^{(1)}_{\beta\beta'} = \Sigma^{(2)}_{\beta,\beta'} = \ldots = 0$. When dealing with quadratic perturbations, self-energy concepts are basically useless. It's only when one has other, higher order perturbations on top of it, where it becomes reasonable to compute self-energies.

21.2. Example: A Diagonalized Gas with Quartic Interactions

Theorem 21.2 The electronic self-energy of this system reads can be approximated in the series expansion as[1]

$$\Sigma^{(1)}_{\alpha,\alpha'}(\mathrm{i}\omega_n) \equiv \zeta \sum_{\beta \in \mathscr{A}} \left(V_{\alpha\beta\beta\alpha'} - V_{\alpha\beta\alpha'\beta} \right) \mathrm{n}^{\zeta}_{\hbar\beta}(\epsilon_\beta - \mu) = \text{„frequency-independent“} . \tag{21.4}$$

Proof 21.2 See Appendix, Proofs, page 384.

[1] Cf. also [52] p. 167 - 169.

21.3. Example: A Spin-Independent-Interaction between an Electron-Gas and a Phonon-Gas

Theorem 21.3 The electronic self-energy of this system reads can be approximated in the series expansion as

$$\Sigma^{(1)}_{\substack{\mathbf{k},\mathbf{k}'\\ m,m'\\ \mu,\mu'}}(\mathrm{i}\omega_n) = 0, \tag{21.5}$$

$$\Sigma^{(2)}_{\substack{\mathbf{k},\mathbf{k}'\\ m,m'\\ \mu,\mu'}}(\mathrm{i}\omega_n) = \Sigma^{\mathrm{Hartree}}_{\substack{\mathbf{k},\mathbf{k}'\\ m,m'\\ \mu,\mu'}}(\mathrm{i}\omega_n) + \Sigma^{\mathrm{Fock}}_{\substack{\mathbf{k},\mathbf{k}'\\ m,m'\\ \mu,\mu'}}(\mathrm{i}\omega_n), \tag{21.6}$$

with Hartree-contribution

$$\begin{aligned}\Sigma^{\mathrm{Hartree}}_{\substack{\mathbf{k},\mathbf{k}'\\ m,m'\\ \mu,\mu'}}(\mathrm{i}\omega_n) &= \delta_{\mathbf{k},\mathbf{k}'}\delta_{\mu,\mu'} \sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ \sigma\in\{\downarrow,\uparrow\}\\ n\in\{1,2,\dots\}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}}} \frac{g_{mm'\nu}(\mathbf{k},0)g_{nn\nu}(\mathbf{q},0)}{N_p} \mathscr{D}_{\substack{0\\ \mathbf{0},\mathbf{0}\\ \nu,\nu}}(0)\,\mathrm{F}_\beta(\xi_{n\sigma\mathbf{q}}) \\ &= -\delta_{\mathbf{k},\mathbf{k}'}\delta_{\mu,\mu'} \sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ \sigma\in\{\downarrow,\uparrow\}\\ n\in\{1,2,\dots\}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}}} \frac{g_{mm'\nu}(\mathbf{k},0)g_{nn\nu}(\mathbf{q},0)}{N_p} \frac{\mathrm{F}_\beta(\xi_{n\sigma\mathbf{q}})}{\Omega_\nu(\mathbf{q}'=0)}\end{aligned} \tag{21.7}$$

and Fock-contribution

$$\Sigma^{\mathrm{Fock}}_{\substack{\mathbf{k},\mathbf{k}'\\ m,m'\\ \mu,\mu'}}(\mathrm{i}\omega_n) = \delta_{\mathbf{k},\mathbf{k}'}\delta_{\mu,\mu'} \sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ n\in\{1,2,\dots\}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}}} \frac{g^*_{nm\nu}(\mathbf{k},\mathbf{q})g_{nm'\nu'}(\mathbf{k},\mathbf{q})}{N_p} \left[\frac{\mathrm{B}_\beta(\Omega_\nu(\mathbf{q})) + \mathrm{F}_\beta(\xi_{\mathbf{q}+\mathbf{k}n\mu})}{\mathrm{i}\hbar\omega_n - \xi_{\mathbf{q}+\mathbf{k}n\mu} + \Omega_\nu(\mathbf{q})} + \frac{\mathrm{B}_\beta(\Omega_\nu(\mathbf{q})) + 1 - \mathrm{F}_\beta(\xi_{\mathbf{q}+\mathbf{k}n\mu})}{\mathrm{i}\hbar\omega_n - \xi_{\mathbf{q}+\mathbf{k}n\mu} - \Omega_\nu(\mathbf{q})}\right] \tag{21.8}$$

Proof 21.3 See Appendix, Proofs, page 388.

Remark 21.3.1 In the *diagonal band approximation*, one assumes that the self-energy is diagonal in the band indices, i.e.

$$\Sigma_{\substack{\mathbf{k},\mathbf{k}'\\ m,m'\\ \mu,\mu'}}(\mathrm{i}\omega_n) \approx \delta_{m,m'}\delta_{\mu,\mu'}\Sigma_{\mathbf{k}m\sigma}(\mathrm{i}\omega_n) \qquad \text{with} \qquad \Sigma_{\mathbf{k}m\sigma}(\mathrm{i}\omega_n) \approx \Sigma^{\mathrm{Hartree}}_{\mathbf{k}m\sigma}(\mathrm{i}\omega_n) + \Sigma^{\mathrm{Fock}}_{\mathbf{k}m\sigma}(\mathrm{i}\omega_n), \tag{21.9}$$

and with Hartree-contribution

$$\Sigma^{\mathrm{Hartree}}_{m\sigma\mathbf{k}}(\bullet) = -\sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ \sigma'\in\{\downarrow,\uparrow\}\\ n\in\{1,2,\dots\}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}}} \frac{g_{mm\nu}(\mathbf{k},0)g_{nn\nu}(\mathbf{q},0)}{N_p} \frac{\mathrm{F}_\beta(\epsilon_{n\sigma'\mathbf{q}} - \mu)}{\Omega_\nu(\mathbf{q}'=0)} \quad \in \quad \mathbb{R} \tag{21.10}$$

and Fock-contribution

$$\Sigma^{\text{Fock}}_{m\sigma\mathbf{k}}(\mathrm{i}\omega_n) = \sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ n\in\{1,2,\dots\}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}}} \frac{|g_{nm\nu}(\mathbf{k},\mathbf{q})|^2}{N_p}\left[\frac{\mathrm{B}_\beta(\Omega_\nu(\mathbf{q}))+\mathrm{F}_\beta(\xi_{\mathbf{q}+\mathbf{k}n\sigma})}{\mathrm{i}\omega_n-\xi_{\mathbf{q}+\mathbf{k}n\sigma}+\Omega_\nu(\mathbf{q})}+\frac{\mathrm{B}_\beta(\Omega_\nu(\mathbf{q}))+1-\mathrm{F}_\beta(\xi_{\mathbf{q}+\mathbf{k}n\sigma})}{\mathrm{i}\omega_n-\xi_{\mathbf{q}+\mathbf{k}n\sigma}-\Omega_\nu(\mathbf{q})}\right] \tag{21.11}$$

which is usually motivated by looking at the complex numbers appearing in Equations (21.7), (21.8) and using Remark 8.37.1.

Remark 21.3.2 Another common approximation is the *Migdal approximation*, which neglects the Hartree-term, which is good, when the change of the chemical potential as a function of temperature is small enough.

The Polarization

Theorem 21.4 The polarization of the system is given as

$$\Pi = 2\mathrm{i}\int \frac{\mathrm{d}2}{(2\pi)^4}|g(1,2)|^2 G_0(1)G_0(2) \tag{21.12}$$

or, in coordinates

$$\underset{\nu,\nu'}{\Pi_{\mathbf{q},\mathbf{q}'}}(\mathrm{i}\omega_n) = 2\delta_{\mathbf{q},\mathbf{q}'}\delta_{\nu,\nu'}\int \frac{\mathrm{d}\mathbf{q}}{\Omega_{\mathrm{BZ}}}|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2\frac{\mathrm{F}_\beta(\epsilon_{m\mathbf{k}})-\mathrm{F}_\beta(\epsilon_{m\mathbf{k}+\mathbf{q}})}{\epsilon_{m\mathbf{k}+\mathbf{q}}-\epsilon_{m\mathbf{k}}-\mathrm{i}\omega_n} \tag{21.13}$$

Proof 21.4 See Appendix, Proofs, page 397.

22. Quasi-Equilibrium-Formalism (Kubo-Formalism)

22.1. Kubo-Formula for arbitrary Perturbations

This argument is evidently quite general, and a large class of experiments in which a system is subjected to a weak, controllable external probe is characterized by simple correlation functions of operators at different times (...) - Negele Orland page 51.

Notation 22.1 We consider a time-dependent Hamiltonian $H(t)$ as

$$H(t) = H_0 + V(t) = H_0 + H'(t)\theta(t - t_0) \tag{22.1}$$

and some observable of interest A, given in second quantization as

$$A \equiv A(c, c^\dagger). \tag{22.2}$$

Remark 22.1.1 Recall that the expectation value of an operator A is (in the absence of spontaneous symmetry breaking) given by

$$\langle A(t)\rangle = \mathrm{Tr}_{\mathscr{H}}\left(\rho(t)A\right). \tag{22.3}$$

Theorem 22.2 The *Kubo-formula* gives an expression for the change of the expectation value of an operator A due to a perturbation $V(t)$ as

$$\langle A(t)\rangle = \langle A\rangle_0(t) + \int_{t_0}^{\infty} \mathrm{d}t' G^{\mathrm{ret}}_{\substack{0\\A,H'(t')}}(t,t') + \mathcal{O}(V^2) \tag{22.4}$$

with

$$G^{\mathrm{ret}}_{\substack{0\\A,H'(t')}}(t,t') = -\frac{\mathrm{i}}{\hbar}\theta(t-t')\langle[A(t),H'(t')]\rangle_0 = -\frac{\mathrm{i}}{\hbar}\theta(t-t')\,\mathrm{Tr}_{\mathscr{H}}\Big[\rho_0[A(t),H'(t')]\Big]. \tag{22.5}$$

and we use the notation $\rho_0 \equiv \rho(t_0)$.

Remark 22.2.1 Cf. also Schwabl 2 page 88. [48, Sect. 4.3, p. 88] „dynamic susceptibility“.

Proof 22.2 First we note that with the Lehmann-representation we obtain

$$\rho \equiv \rho(t_0) = \frac{1}{Z}\mathrm{e}^{-\beta(H-\mu N)} = \frac{1}{Z}\sum_n |n\rangle\langle n|\mathrm{e}^{-\beta\xi_n} \tag{22.6}$$

whereas $|n\rangle \equiv |n(t_0)\rangle$. Now, applying the time-evolution of the von Neumann equation onto the density-matrix ρ we obtain

$$\rho(t) = \frac{1}{Z}\sum_n |n(t)\rangle\langle n(t)|\mathrm{e}^{-\beta\xi_n} \tag{22.7}$$

Now we rewrite the ket-vectors $|n(t)\rangle$ in the interaction picture as

$$|n(t)\rangle = \mathrm{e}^{-\mathrm{i}H_0(t-t_0)/\hbar}\hat{U}(t,t_0)|n(t_0)\rangle \tag{22.8}$$

with

$$\hat{U}(t,0) = \mathrm{e}^{\mathrm{i}H_0(t-t_0)/\hbar}U(t,0) \tag{22.9}$$

Before we continue, note the general expression for the time-evolution-operator from Theorem 2.13. Therefore, using now the identity

$$\partial_t U(t,0) = H(t)U(t,0). \tag{22.10}$$

This yields therefore

$$\begin{aligned}
\partial_t\hat{U}(t,0) &= \mathrm{i}\mathrm{e}^{\mathrm{i}H_0(t-t_0)/\hbar}\left(H_0 - H(t)\right)U(t,0)\\
&= -\frac{\mathrm{i}}{\hbar}\mathrm{e}^{\mathrm{i}H_0(t-t_0)/\hbar}V(t)U(t,0)\\
&= -\frac{\mathrm{i}}{\hbar}\mathrm{e}^{\mathrm{i}H_0(t-t_0)/\hbar}V(t)\mathrm{e}^{-\mathrm{i}H_0(t-t_0)/\hbar}\hat{U}(t,0)\\
&= -\frac{\mathrm{i}}{\hbar}V_{H_0}(t)\hat{U}(t,0)
\end{aligned} \tag{22.11}$$

and with this we obtain

$$\begin{aligned}
\hat{U}(t,0) - \hat{U}(0,0) &= -\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathrm{d}t' V_{H_0}(t')\hat{U}(t',0)\\
\Leftrightarrow \hat{U}(t,0) &= 1 - \frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathrm{d}t' V_{H_0}(t')\hat{U}(t',0)\\
\Leftrightarrow \hat{U}(t,0) &= 1 - \frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathrm{d}t' V_{H_0}(t') + \mathcal{O}(V^2)
\end{aligned} \tag{22.12}$$

this gives us then

$$|n(t)\rangle = \mathrm{e}^{-\mathrm{i}H_0(t-t_0)/\hbar}\left(1 - \frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathrm{d}t' V_{H_0}(t') + \mathcal{O}(V^2)\right)|n(t_0)\rangle \tag{22.13}$$

This gives us, inserting it into the definition of the expectation value,

$$\begin{aligned}\langle A(t)\rangle &= \mathrm{Tr}_{\mathscr{H}}\left(\rho(t)A\right)\\ &= \frac{1}{Z}\sum_n \mathrm{e}^{-\beta\xi_n}\,\mathrm{Tr}_{\mathscr{H}}\left(|n(t)\rangle\langle n(t)|A\right)\\ &= \dots\end{aligned} \tag{22.14}$$

now we compute the trace in the last line as

$$\begin{aligned}&\mathrm{Tr}_{\mathscr{H}}\left(|n(t)\rangle\langle n(t)|A\right)\\ &= \mathrm{Tr}_{\mathscr{H}}\left(\mathrm{e}^{-\mathrm{i}H_0(t-t_0)/\hbar}\left(1-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathrm{d}t'\mathrm{d}t'V_{H_0}(t')\right)|n(t_0)\rangle\langle n(t_0)|\left(1+\frac{\mathrm{i}}{\hbar}\int_0^t\mathrm{d}t''V_{H_0}(t'')\right)\mathrm{e}^{+\mathrm{i}H_0(t-t_0)/\hbar}\right)+\mathcal{O}(V^3)\\ &= \mathrm{Tr}_{\mathscr{H}}\left(\mathrm{e}^{-\mathrm{i}H_0(t-t_0)/\hbar}|n(t_0)\rangle\langle n(t_0)|\mathrm{e}^{+\mathrm{i}H_0(t-t_0)/\hbar}A\right)\\ &- \frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathrm{d}t'\,\mathrm{Tr}_{\mathscr{H}}\left(\mathrm{e}^{-\mathrm{i}H_0(t-t_0)/\hbar}V_{H_0}(t')|n(t_0)\rangle\langle n(t_0)|\mathrm{e}^{+\mathrm{i}H_0(t-t_0)/\hbar}A-\mathrm{e}^{-\mathrm{i}H_0(t-t_0)/\hbar}|n(t_0)\rangle\langle n(t_0)|V_{H_0}(t')\mathrm{e}^{+\mathrm{i}H_0(t-t_0)/\hbar}A\right)\\ &= \mathrm{Tr}_{\mathscr{H}}\left(\mathrm{e}^{-\mathrm{i}H_0(t-t_0)/\hbar}|n(t_0)\rangle\langle n(t_0)|\mathrm{e}^{+\mathrm{i}H_0(t-t_0)/\hbar}A\right)\\ &- \frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathrm{d}t'\langle n(t_0)|A_{H_0}(t)V_{H_0}(t')-V_{H_0}(t')A_{H_0}(t)|n(t_0)\rangle\end{aligned} \tag{22.15}$$

inserting this above yields

$$\begin{aligned}\dots &= \langle A\rangle_0(t-t_0)\\ &- \frac{\mathrm{i}}{\hbar}\frac{1}{Z}\sum_n\mathrm{e}^{-\beta\xi_n}\int_{t_0}^{t}\mathrm{d}t'\langle n(t_0)|A_{H_0}(t)V_{H_0}(t')-V_{H_0}(t')A_{H_0}(t)|n(t_0)\rangle+\mathcal{O}(V^2)\\ &= \langle A\rangle_0(t-t_0)-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathrm{d}t'\langle[A_{H_0}(t),V_{H_0}(t')]\rangle_0+\mathcal{O}(V^2)\\ &= \langle A\rangle_0(t-t_0)-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathrm{d}t'\theta(t'-t_0)\langle[A_{H_0}(t),H'_{H_0}(t')]\rangle_0+\mathcal{O}(V^2)\\ &= \dots\end{aligned} \tag{22.16}$$

now we use

$$\theta(t'-t_0)=\begin{cases}1 & t'>t_0\\ 0 & t'<t_0\end{cases} \tag{22.17}$$

which is, within the integral, always fulfilled, and this gives

$$\begin{aligned}\dots &= \langle A\rangle_0(t-t_0)-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathrm{d}t'\langle[A_{H_0}(t),H'_{H_0}(t')]\rangle_0+\mathcal{O}(V^2)\\ &= \dots\end{aligned} \tag{22.18}$$

now we will extend the integral further, by introducing the theta-function as

$$\theta(t-t') = \begin{cases} 1 & t > t' \\ 0 & t < t' \end{cases} \tag{22.19}$$

to rewrite the expression above as

$$\begin{aligned} \ldots &= \langle A \rangle_0 (t-t_0) - \frac{\mathrm{i}}{\hbar} \int_{t_0}^{\infty} \mathrm{d}t' \theta(t-t') \langle [A_{H_0}(t), H'_{H_0}(t')] \rangle_0 + \mathcal{O}(V^2) \\ &= \langle A \rangle_0 (t-t_0) - \int_{t_0}^{\infty} \mathrm{d}t' G^{\mathrm{ret}}{}_{A,H'(t')}^{0}(t,t') + \mathcal{O}(V^2) \end{aligned} \tag{22.20}$$

Part IV.

Applications to Real Materials

Comment on the Applications

In this entire part, we will seek to model real, crystalline materials. To this end we remark, that that we will essentially be focusing on three (four) systems (depending on how one counts). We consider ...

Non-Interacting Electrons

We consider the system from Remark 8.28.1. (which represents a special case of the system in Definition 8.27). We therefore consider the Hamiltonian

$$H_{\text{el}} = \sum_{\substack{\mathbf{k}\in \text{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\dots,\infty\}}} \epsilon_{m\mathbf{k}\sigma} c^\dagger_{m\mathbf{k}\sigma} c_{m\mathbf{k}\sigma} \tag{22.21}$$

Non-Interacting Phonons

We consider the system from Remark 8.28.4 (which represents a special case of the system in Definition 8.27). We therefore consider the Hamiltonian

$$H_{\text{ph}} = \sum_{\substack{\mathbf{q}\in \text{Q} \\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}}} \Omega_\nu(\mathbf{q}) b^\dagger_{\mathbf{q}\nu} b_{\mathbf{q}\nu} \tag{22.22}$$

Non-Interacting Electrons and Phonons (Total Crystal)

We consider the system from Definitions 8.35. We therefore consider the Hamiltonian

$$H = H_{\text{el}} + H_{\text{ph}} = \sum_{\substack{\mathbf{k}\in \text{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\dots,\infty\}}} \epsilon_{m\mathbf{k}\sigma} c^\dagger_{m\mathbf{k}\sigma} c_{m\mathbf{k}\sigma} + \sum_{\substack{\mathbf{q}\in \text{Q} \\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} \Omega_{\mathbf{q},\nu} b^\dagger_{\mathbf{q}\nu} b_{\mathbf{q}\nu} \tag{22.23}$$

Interacting Electrons and Phonons (Total Crystal)

We consider the system from Definitions 8.36. We therefore consider the Hamiltonian

$$H = \sum_{\substack{\mathbf{k}\in \text{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\dots,\infty\}}} \epsilon_{m\mathbf{k}\sigma} c^\dagger_{m\mathbf{k}\sigma} c_{m\mathbf{k}\sigma} + \sum_{\substack{\mathbf{q}\in \text{Q} \\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} \hbar\omega_{\mathbf{q},\nu} b^\dagger_{\mathbf{q}\nu} b_{\mathbf{q}\nu} + \sum_{\substack{\mathbf{k},\mathbf{q}\in \text{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ \nu\in\{1,\dots,rd_{\mathbf{x}}\} \\ m,n\in\{1,\dots,\infty\}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\sqrt{N_p}} c^\dagger_{\mathbf{k}+\mathbf{q}m\sigma} c_{\mathbf{k}n\sigma} \left(b_{\mathbf{q}\nu} + b^\dagger_{-\mathbf{q}\nu} \right) \tag{22.24}$$

23. Thermal Quantum Field Theories of Real Materials

23.1. Non-Interacting Systems

23.1.1. Non-Interacting Electrons

Fact 23.1 Recall that the retarded Green-function for the electrons is given by analytical continuation of the Matsubara-Green-function according to Theorem 14.20 which is determined as

$$\mathscr{G}^{}_{\substack{m,m'\\ \sigma,\sigma'}}(\mathrm{i}\omega_n,\mathbf{k}) = \frac{\delta_{\sigma,\sigma'}}{\hbar}\left(\frac{1}{\mathrm{i}\omega_n - \left(H_{0,\sigma}(\mathbf{k})-\mu\right)/\hbar}\right)_{m,m'} = \frac{\delta_{\sigma,\sigma'}}{\mathrm{i}\hbar\omega_n - \left(\epsilon_{m\sigma}(\mathbf{k})-\mu\right)} \tag{23.1}$$

with non-interacting band-dispersion-matrix $H_{0,\sigma}(\mathbf{k}) \equiv \mathrm{diag}(\epsilon_{1,\sigma}(\mathbf{k}),\ldots,\epsilon_{n_{\mathrm{bnds}},\sigma}(\mathbf{k}))$, whereas n_{bnds} represents the number of bands that are under consideration[1].

Fact 23.2 Going over to the field-integral-description of the problem gives the action

$$S[\psi,\overline{\psi}] \equiv S_{\mathrm{el}}[\psi,\overline{\psi}] \tag{23.2}$$

with

- $S_{\mathrm{el}}[\psi,\overline{\psi}] = \sum\!\!\!\!\!\!\int\limits_{\substack{\mathbf{k}\in\mathrm{Q}\\ \sigma\in\{\downarrow,\uparrow\}\\ \tau\in(0,\hbar\beta)\\ m\in\{1,2,\ldots,\infty\}}} \overline{\psi}_{m\sigma}(\tau,\mathbf{k})\left(\partial_\tau + \frac{\epsilon_{m\sigma}(\mathbf{k})-\mu}{\hbar}\right)\psi_{m\sigma}(\tau,\mathbf{k})$

Notation 23.3 We implement external sources into the partition-function as

$$Z \mapsto Z[j_{\mathrm{el}},\overline{j}_{\mathrm{el}}] \equiv \int \mathscr{D}(\overline{\psi},\psi)\,\exp\Big[-S_{\mathrm{el}}[\psi,\overline{\psi}] + \overline{j}_{\mathrm{el}}\psi + \overline{\psi}j_{\mathrm{el}}\Big] \tag{23.3}$$

with abbreviations

- $\overline{j}_{\mathrm{el}}\psi \equiv \sum\!\!\!\!\!\!\int\limits_{\substack{\mathbf{k}\in\mathrm{Q}\\ \sigma\in\{\downarrow,\uparrow\}\\ \tau\in(0,\hbar\beta)\\ m\in\{1,2,\ldots,\infty\}}} \overline{j}_{m\sigma}(\tau,\mathbf{k})\psi_{m\sigma}(\tau,\mathbf{k})$
- $\overline{\psi}j_{\mathrm{el}} \equiv \sum\!\!\!\!\!\!\int\limits_{\substack{\mathbf{k}\in\mathrm{Q}\\ \sigma\in\{\downarrow,\uparrow\}\\ \tau\in(0,\hbar\beta)\\ m\in\{1,2,\ldots,\infty\}}} \overline{\psi}_{m\sigma}(\tau,\mathbf{k})j_{m\sigma}(\tau,\mathbf{k})$

[1] Usually this is the number of bands were are reproduced in the Wannierization-procedure.

Lemma 23.4 Going over to Matsubara-frequencies and introducing the four-momenta $k \equiv (\mathrm{i}\omega_n, \mathbf{k}) \in \mathrm{i}\Omega_{-1} \times \mathrm{Q}$, we obtain

$$S_{[j,\bar{j}]}[\psi, \overline{\psi}] = S_{\mathrm{el}}[\psi, \overline{\psi}] - \left(\bar{j}_{\mathrm{el}} \psi + \overline{\psi} j_{\mathrm{el}} \right)$$

with

- $S_{\mathrm{el}}[\psi, \overline{\psi}] = \sum_{\substack{\sigma \in \{\downarrow,\uparrow\} \\ k \in \mathrm{i}\Omega_{-1} \times \mathrm{Q} \\ m \in \{1,2,\ldots,\infty\}}} \overline{\psi}_{m\sigma}(k) \left(-\mathrm{i}\omega_k + \frac{\epsilon_{m\sigma}(\mathbf{k}) - \mu}{\hbar} \right) \psi_{m\sigma}(k) \equiv \sum_{\substack{\sigma \in \{\downarrow,\uparrow\} \\ k \in \mathrm{i}\Omega_{-1} \times \mathrm{Q} \\ m \in \{1,2,\ldots,\infty\}}} \overline{\psi}_{m\sigma}(k) \left(-\frac{1}{\hbar} \mathcal{G}^{-\mathrm{el}}_{0\ m,\sigma}(k) \right) \psi_{m\sigma}(k)$

with negative four-momentum $-q \equiv (-\mathrm{i}\omega_m, -\mathbf{q})$.

Proof 23.4 Follows from Corollary 20.15.

23.1.2. Non-Interacting Phonons

Fact 23.5 Going over to the field-integral-description of the problem gives the action

$$S[\phi, \overline{\phi}] = S_{\mathrm{ph}}[\phi, \overline{\phi}] \tag{23.4}$$

with

- $S_{\mathrm{ph}}[\phi, \overline{\phi}] = \sum\!\!\!\!\!\!\int_{\substack{\mathbf{q} \in \mathrm{Q} \\ \tau \in (0,\hbar\beta) \\ \nu \in \{1,2,\ldots,rd_{\mathbf{x}}\}}} \overline{\phi}_\nu(\tau, \mathbf{q}) \left(\partial_\tau + \omega_\nu(\mathbf{q}) \right) \phi_\nu(\tau, \mathbf{q})$

Notation 23.6 We implement external sources into the partition-function as

$$Z \mapsto Z[j_{\mathrm{ph}}, \bar{j}_{\mathrm{ph}}] \equiv \int \mathscr{D}(\overline{\phi}, \phi)\ \exp\left[-S_{\mathrm{ph}}[\phi, \overline{\phi}] + \sum_{\bullet \in \{\mathrm{el},\mathrm{ph}\}} \bar{j}_{\mathrm{ph}} \phi_\bullet + \overline{\phi} j_{\mathrm{ph}} \right] \tag{23.5}$$

with abbreviations

- $\bar{j}_{\mathrm{ph}} \phi \equiv \sum\!\!\!\!\!\!\int_{\substack{\mathbf{q} \in \mathrm{Q} \\ \tau \in (0,\hbar\beta) \\ \nu \in \{1,2,\ldots,rd_{\mathbf{x}}\}}} \bar{j}_\nu(\tau, \mathbf{q}) \phi_\nu(\tau, \mathbf{q})$
- $\overline{\phi} j_{\mathrm{ph}} \equiv \sum\!\!\!\!\!\!\int_{\substack{\mathbf{q} \in \mathrm{Q} \\ \tau \in (0,\hbar\beta) \\ \nu \in \{1,2,\ldots,rd_{\mathbf{x}}\}}} \overline{\phi}_\nu(\tau, \mathbf{q}) j_\nu(\tau, \mathbf{q})$

Lemma 23.7 Going over to Matsubara-frequencies and introducing the four-momenta $q \equiv (\mathrm{i}\omega_m, \mathbf{q}) \in \mathrm{i}\Omega_{+1} \times \mathrm{Q}$ and $k \equiv (\mathrm{i}\omega_n, \mathbf{k}) \in \mathrm{i}\Omega_{-1} \times \mathrm{Q}$, we obtain

$$S_{[j,\bar{j}]}[\phi,\overline{\phi}] = S_{\mathrm{ph}}[\phi,\overline{\phi}] - \left(\bar{j}_{\mathrm{ph}}\phi_{\mathrm{ph}} + \overline{\phi}_{\mathrm{ph}} j_{\mathrm{ph}}\right)$$

with

- $S_{\mathrm{ph}}[\phi,\overline{\phi}] = \sum_{\substack{q\in \mathrm{i}\Omega_{+1}\times \mathrm{Q} \\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} \overline{\phi}_\nu(q)\left(-\mathrm{i}\omega_q + \omega_\nu(\mathbf{q})\right)\phi_\nu(q) \equiv \sum_{\substack{q\in \mathrm{i}\Omega_{+1}\times \mathrm{Q} \\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} \overline{\phi}_\nu(q)\left(-\frac{1}{\hbar}\mathscr{G}^{-\mathrm{ph}}_{0,\nu}(q)\right)\phi_\nu(q)$

with negative four-momentum $-q \equiv (-\mathrm{i}\omega_m, -\mathbf{q})$.

Proof 23.7 Follows from Corollary 20.15.

Notice that in the case of phonons, one can also simplify the action by changing the field-variables. This is elaborated in Section 29.6.

23.1.3. Non-Interacting Electrons and Phonons (Total Crystal)

We consider the system from Definition 8.35.

Fact 23.8 Going over to the field-integral-description of the problem gives the action

$$S[\chi,\overline{\chi}] = S_{\mathrm{el}}[\psi,\overline{\psi}] + S_{\mathrm{ph}}[\phi,\overline{\phi}] \tag{23.6}$$

with

- $S_{\mathrm{el}}[\psi,\overline{\psi}] = \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}\in \mathrm{Q} \\ \sigma\in\{\downarrow,\uparrow\} \\ \tau\in(0,\hbar\beta) \\ m\in\{1,2,\ldots,\infty\}}} \overline{\psi}_{m\sigma}(\tau,\mathbf{k})\left(\partial_\tau + \frac{\epsilon_{m\sigma}(\mathbf{k})-\mu}{\hbar}\right)\psi_{m\sigma}(\tau,\mathbf{k})$
- $S_{\mathrm{ph}}[\phi,\overline{\phi}] = \sum\!\!\!\!\!\!\int_{\substack{\mathbf{q}\in \mathrm{Q} \\ \tau\in(0,\hbar\beta) \\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} \overline{\phi}_\nu(\tau,\mathbf{q})\left(\partial_\tau + \omega_\nu(\mathbf{q})\right)\phi_\nu(\tau,\mathbf{q})$

Notation 23.9 We implement external sources into the partition-function as

$$Z \mapsto Z[j_{\mathrm{el}},\bar{j}_{\mathrm{el}},j_{\mathrm{ph}},\bar{j}_{\mathrm{ph}}] \equiv \int \mathscr{D}(\overline{\chi},\chi)\,\exp\left[-\left(S_{\mathrm{el}}[\psi,\overline{\psi}] + S_{\mathrm{ph}}[\phi,\overline{\phi}]\right) + \sum_{\bullet\in\{\mathrm{el},\mathrm{ph}\}} \bar{j}_\bullet.\chi_\bullet. + \overline{\chi}_\bullet.j_\bullet.\right] \tag{23.7}$$

with abbreviations

- $\bar{j}_{\mathrm{el}}\chi_{\mathrm{el}} \equiv \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}\in \mathrm{Q} \\ \sigma\in\{\downarrow,\uparrow\} \\ \tau\in(0,\hbar\beta) \\ m\in\{1,2,\ldots,\infty\}}} \bar{j}_{m\sigma}(\tau,\mathbf{k})\psi_{m\sigma}(\tau,\mathbf{k})$
- $\bar{j}_{\mathrm{ph}}\chi_{\mathrm{ph}} \equiv \sum\!\!\!\!\!\!\int_{\substack{\mathbf{q}\in \mathrm{Q} \\ \tau\in(0,\hbar\beta) \\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} \bar{j}_\nu(\tau,\mathbf{q})\phi_\nu(\tau,\mathbf{q})$

- etc...

Lemma 23.10 Going over to Matsubara-frequencies and introducing the four-momenta $q \equiv (\mathrm{i}\omega_m, \mathbf{q}) \in \mathrm{i}\Omega_{+1} \times \mathrm{Q}$ and $k \equiv (\mathrm{i}\omega_n, \mathbf{k}) \in \mathrm{i}\Omega_{-1} \times \mathrm{Q}$, we obtain

$$S_{[j,\bar{j}]}[\chi, \overline{\chi}] = S_{\mathrm{el}}[\psi, \overline{\psi}] + S_{\mathrm{ph}}[\phi, \overline{\phi}] - \sum_{\bullet \in \{\mathrm{el},\mathrm{ph}\}} \left(\bar{j}_\bullet \chi_\bullet + \overline{\chi}_\bullet j_\bullet \right)$$

with

- $$S_{\mathrm{el}}[\psi, \overline{\psi}] = \sum_{\substack{\sigma \in \{\downarrow,\uparrow\} \\ k \in \mathrm{i}\Omega_{-1} \times \mathrm{Q} \\ m \in \{1,2,\ldots,\infty\}}} \overline{\psi}_{m\sigma}(k) \left(-\mathrm{i}\omega_k + \frac{\epsilon_{m\sigma}(\mathbf{k}) - \mu}{\hbar} \right) \psi_{m\sigma}(k) \equiv \sum_{\substack{\sigma \in \{\downarrow,\uparrow\} \\ k \in \mathrm{i}\Omega_{-1} \times \mathrm{Q} \\ m \in \{1,2,\ldots,\infty\}}} \overline{\psi}_{m\sigma}(k) \left(-\frac{1}{\hbar} \mathcal{G}^{-\mathrm{el}}_{0\ m,\sigma}(k) \right) \psi_{m\sigma}(k)$$
- $$S_{\mathrm{ph}}[\phi, \overline{\phi}] = \sum_{\substack{q \in \mathrm{i}\Omega_{+1} \times \mathrm{Q} \\ \nu \in \{1,2,\ldots,rd_{\mathbf{x}}\}}} \overline{\phi}_\nu(q) \left(-\mathrm{i}\omega_q + \omega_\nu(\mathbf{q}) \right) \phi_\nu(q) \equiv \sum_{\substack{q \in \mathrm{i}\Omega_{+1} \times \mathrm{Q} \\ \nu \in \{1,2,\ldots,rd_{\mathbf{x}}\}}} \overline{\phi}_\nu(q) \left(-\frac{1}{\hbar} \mathcal{G}^{-\mathrm{ph}}_{0,\nu}(q) \right) \phi_\nu(q)$$

with negative four-momentum $-q \equiv (-\mathrm{i}\omega_m, -\mathbf{q})$.

Proof 23.10 See Appendix, Proofs, page 491.

23.2. Interacting Electrons and Phonons (Total Crystal)

23.2.1. Introduction

Fact 23.11 Recall that the retarded Green-function for the electrons is given by analytical continuation of the Matsubara-Green-function according to Theorem 14.20 which is determined by solving the Dyson-equation (15.13) as

$$\mathcal{G}_{\substack{m,m' \\ \sigma,\sigma'}}(\mathrm{i}\omega_n, \mathbf{k}) = \frac{\delta_{\sigma,\sigma'}}{\hbar} \left(\frac{1}{\mathrm{i}\omega_n - \left(H_{0,\sigma}(\mathbf{k}) + \Sigma_\sigma(\mathbf{k}, \mathrm{i}\omega_n) - \mu \right) / \hbar} \right)_{m,m'} \tag{23.8}$$

with non-interacting band-dispersion-matrix $H_{0,\sigma}(\mathbf{k}) \equiv \mathrm{diag}(\epsilon_{1,\sigma}(\mathbf{k}), \ldots, \epsilon_{n_{\mathrm{bnds}},\sigma}(\mathbf{k}))$, whereas n_{bnds} represents the number of bands that are under consideration[2].

Remark 23.11.1 Notice further that we have determined the self-energy in this system up to second / third order perturbation theory in Theorem 21.3.

Remark 23.11.2 Usually, we enumerate the indices in such a way, that the matrix-representation of the Green-function becomes

[2] Usually this is the number of bands were are reproduced in the Wannierization-procedure.

$$\mathscr{G}(\mathrm{i}\omega_n, \mathbf{k}) = \begin{pmatrix} \mathscr{G}_{\uparrow,\uparrow}(\mathrm{i}\omega_n, \mathbf{k}) & \mathbf{0} \\ \mathbf{0} & \mathscr{G}_{\downarrow,\downarrow}(\mathrm{i}\omega_n, \mathbf{k}) \end{pmatrix}.$$

with individual blocks for spin-up and spin-down electrons. More explicitly, this means

$$\mathscr{G}(\mathrm{i}\omega_n, \mathbf{k}) = \begin{pmatrix} \mathscr{G}^{1,1}_{\uparrow,\uparrow} & \mathscr{G}^{1,2}_{\uparrow,\uparrow} & \cdots & \mathscr{G}^{1,n_{\mathrm{bnds}}}_{\uparrow,\uparrow} & 0 & 0 & \cdots & 0 \\ \mathscr{G}^{2,1}_{\uparrow,\uparrow} & \mathscr{G}^{2,2}_{\uparrow,\uparrow} & \cdots & \mathscr{G}^{2,n_{\mathrm{bnds}}}_{\uparrow,\uparrow} & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathscr{G}^{n_{\mathrm{bnds}},1}_{\uparrow,\uparrow} & \mathscr{G}^{n_{\mathrm{bnds}},2}_{\uparrow,\uparrow} & \cdots & \mathscr{G}^{n_{\mathrm{bnds}},n_{\mathrm{bnds}}}_{\uparrow,\uparrow} & 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 & \mathscr{G}^{1,1}_{\downarrow,\downarrow} & \mathscr{G}^{1,2}_{\downarrow,\downarrow} & \cdots & \mathscr{G}^{1,n_{\mathrm{bnds}}}_{\downarrow,\downarrow} \\ 0 & 0 & \cdots & 0 & \mathscr{G}^{2,1}_{\downarrow,\downarrow} & \mathscr{G}^{2,2}_{\downarrow,\downarrow} & \cdots & \mathscr{G}^{2,n_{\mathrm{bnds}}}_{\downarrow,\downarrow} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & \mathscr{G}^{n_{\mathrm{bnds}},1}_{\downarrow,\downarrow} & \mathscr{G}^{n_{\mathrm{bnds}},2}_{\downarrow,\downarrow} & \cdots & \mathscr{G}^{n_{\mathrm{bnds}},n_{\mathrm{bnds}}}_{\downarrow,\downarrow} \end{pmatrix} (\mathrm{i}\omega_n, \mathbf{k}).$$

Notation 23.12 We simplify the notation further, by recalling that the self-energy is, within the diagonal-band-approximation (cf. Remark 21.3.1), diagonal in spin and wave-vector indices, such that we can write

$$G^{\mathrm{ret}}_{\substack{m,m' \\ \sigma,\sigma' \\ \mathbf{k},\mathbf{k}'}}(E + \mathrm{i}\delta) \equiv \delta_{\mathbf{k},\mathbf{k}'}\delta_{\sigma,\sigma'} G^{\mathrm{ret}}_{\substack{m,m' \\ \sigma,\sigma'}}(E + \mathrm{i}\delta, \mathbf{k}) \tag{23.9}$$

whereas we keep the double spin-indices explicit for reasons that will become clear in the chapter about superconductivity.

Fact 23.13 Going over to the field-integral-description of the problem gives the action

$$S[\chi, \overline{\chi}] = S_{\mathrm{el}}[\psi, \overline{\psi}] + S_{\mathrm{ph}}[\phi, \overline{\phi}] + S_{\text{el-ph-int}}[\chi, \overline{\chi}] \tag{23.10}$$

with

- $S_{\mathrm{el}}[\psi, \overline{\psi}] = \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}\in\mathrm{Q} \\ \sigma\in\{\downarrow,\uparrow\} \\ \tau\in(0,\hbar\beta) \\ m\in\{1,2,\ldots,\infty\}}} \overline{\psi}_{m\sigma}(\tau, \mathbf{k}) \left(\partial_\tau + \frac{\epsilon_{m\sigma}(\mathbf{k}) - \mu}{\hbar}\right) \psi_{m\sigma}(\tau, \mathbf{k})$
- $S_{\mathrm{ph}}[\phi, \overline{\phi}] = \sum\!\!\!\!\!\!\int_{\substack{\mathbf{q}\in\mathrm{Q} \\ \tau\in(0,\hbar\beta) \\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} \overline{\phi}_\nu(\tau, \mathbf{q}) \left(\partial_\tau + \omega_\nu(\mathbf{q})\right) \phi_\nu(\tau, \mathbf{q})$
- $S_{\text{el-ph-int}}[\chi, \overline{\chi}] = \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k},\mathbf{q}\in\mathrm{Q} \\ \tau\in(0,\hbar\beta) \\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\} \\ m,n\in\{1,2,\ldots,\infty\} \\ \sigma\in\{\downarrow,\uparrow\}}} \frac{g_{mn\nu}(\mathbf{k}, \mathbf{q})}{\hbar\sqrt{N_p}} \left(\phi_\nu(\tau, \mathbf{q}) + \overline{\phi}_\nu(\tau, -\mathbf{q})\right) \overline{\psi}_{m\sigma}(\tau, \mathbf{k} + \mathbf{q}) \psi_{n\sigma}(\tau, \mathbf{k})$

Notation 23.14 We implement external sources into the partition-function as

$$Z \mapsto Z[j_{\text{el}}, \bar{j}_{\text{el}}, j_{\text{ph}}, \bar{j}_{\text{ph}}] \equiv \int \mathscr{D}(\overline{\chi}, \chi) \, \exp\left[- \left(S_{\text{el}}[\psi, \overline{\psi}] + S_{\text{ph}}[\phi, \overline{\phi}] + S_{\text{el-ph-int}}[\chi, \overline{\chi}] \right) + \sum_{\bullet \in \{\text{el,ph}\}} \bar{j}_\bullet . \chi_\bullet + \overline{\chi}_\bullet . j_\bullet \right] \tag{23.11}$$

with abbreviations

- $\bar{j}_{\text{el}} \chi_{\text{el}} \equiv \sum\!\!\!\!\!\!\int\limits_{\substack{\mathbf{k} \in \mathrm{Q} \\ \sigma \in \{\downarrow,\uparrow\} \\ \tau \in (0,\hbar\beta) \\ m \in \{1,2,\ldots,\infty\}}} \bar{j}_{m\sigma}(\tau, \mathbf{k}) \psi_{m\sigma}(\tau, \mathbf{k})$
- $\bar{j}_{\text{ph}} \chi_{\text{ph}} \equiv \sum\!\!\!\!\!\!\int\limits_{\substack{\mathbf{q} \in \mathrm{Q} \\ \tau \in (0,\hbar\beta) \\ \nu \in \{1,2,\ldots,rd_{\mathbf{x}}\}}} \bar{j}_{\nu}(\tau, \mathbf{q}) \phi_{\nu}(\tau, \mathbf{q})$
- etc...

Lemma 23.15 Going over to Matsubara-frequencies and introducing the four-momenta $q \equiv (\mathrm{i}\omega_m, \mathbf{q}) \in \mathrm{i}\Omega_{+1} \times \mathrm{Q}$ and $k \equiv (\mathrm{i}\omega_n, \mathbf{k}) \in \mathrm{i}\Omega_{-1} \times \mathrm{Q}$, we obtain

$$S_{[j,\bar{j}]}[\chi, \overline{\chi}] = S_{\text{el}}[\psi, \overline{\psi}] + S_{\text{ph}}[\phi, \overline{\phi}] + S_{\text{el-ph-int}}[\chi, \overline{\chi}] - \sum_{\bullet \in \{\text{el,ph}\}} \left(\bar{j}_\bullet . \chi_\bullet + \overline{\chi}_\bullet . j_\bullet \right)$$

with

- $S_{\text{el}}[\psi, \overline{\psi}] = \sum_{\substack{\sigma \in \{\downarrow,\uparrow\} \\ k \in \mathrm{i}\Omega_{-1} \times \mathrm{Q} \\ m \in \{1,2,\ldots,\infty\}}} \overline{\psi}_{m\sigma}(k) \left(-\mathrm{i}\omega_k + \frac{\epsilon_{m\sigma}(\mathbf{k}) - \mu}{\hbar} \right) \psi_{m\sigma}(k) \equiv \sum_{\substack{\sigma \in \{\downarrow,\uparrow\} \\ k \in \mathrm{i}\Omega_{-1} \times \mathrm{Q} \\ m \in \{1,2,\ldots,\infty\}}} \overline{\psi}_{m\sigma}(k) \left(-\frac{1}{\hbar} \mathscr{G}_{0\ m,\sigma}^{-\text{el}}(k) \right) \psi_{m\sigma}(k)$
- $S_{\text{ph}}[\phi, \overline{\phi}] = \sum_{\substack{q \in \mathrm{i}\Omega_{+1} \times \mathrm{Q} \\ \nu \in \{1,2,\ldots,rd_{\mathbf{x}}\}}} \overline{\phi}_{\nu}(q) \left(-\mathrm{i}\omega_q + \omega_{\nu}(\mathbf{q}) \right) \phi_{\nu}(q) \equiv \sum_{\substack{q \in \mathrm{i}\Omega_{+1} \times \mathrm{Q} \\ \nu \in \{1,2,\ldots,rd_{\mathbf{x}}\}}} \overline{\phi}_{\nu}(q) \left(-\frac{1}{\hbar} \mathscr{G}_{0,\nu}^{-\text{ph}}(q) \right) \phi_{\nu}(q)$
- $S_{\text{el-ph-int}}[\chi, \overline{\chi}] = \frac{1}{\sqrt{\hbar\beta}} \sum_{\substack{k \in \mathrm{i}\Omega_{-1} \times \mathrm{Q} \\ q \in \mathrm{i}\Omega_{+1} \times \mathrm{Q} \\ \nu \in \{1,2,\ldots,rd_{\mathbf{x}}\} \\ m,n \in \{1,2,\ldots,\infty\} \\ \sigma \in \{\downarrow,\uparrow\}}} \frac{g_{mn\nu}(\mathbf{k}, \mathbf{q})}{\hbar\sqrt{N_p}} \left(\phi_{\nu}(q) + \overline{\phi}_{\nu}(-q) \right) \overline{\psi}_{m\sigma}(q + k) \psi_{n\sigma}(k)$

with negative four-momentum $-q \equiv (-\mathrm{i}\omega_m, -\mathbf{q})$.

Proof 23.15 See Appendix, Proofs, page 491.

Lemma 23.16 We can rewrite the interaction-term as

$$\begin{aligned} S_{\substack{\text{el-ph-int}\\[j_{\text{ph}},\bar{j}_{\text{ph}}]}}[\chi,\overline{\chi}] &= \left(S_{\text{el-ph-int}} + S_{\substack{\text{ph-sources}\\[j_{\text{ph}},\bar{j}_{\text{ph}}]}} \right)[\chi,\overline{\chi}] \\ &= \sum_{\substack{q\in \mathrm{i}\Omega_{+1}\times\mathbb{Q}\\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} \phi_\nu(q)\left(\rho_\nu(q)-\bar{j}_\nu(q)\right) + \overline{\phi}_\nu(q)\left(\rho_\nu(-q)-j_\nu(q)\right) \end{aligned}$$

with density-like-interaction

$$\rho_\nu(q) = \frac{1}{\sqrt{\hbar\beta N_p}} \sum_{\substack{\sigma\in\{\downarrow,\uparrow\}\\ k\in\mathrm{i}\Omega_{-1}\times\mathbb{Q}\\ n,m\in\{1,\dots,\infty\}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\hbar}\overline{\psi}_{m\sigma}(k+q)\psi_{n\sigma}(k) \tag{23.12}$$

Proof 23.16 See Appendix, Proofs, page 603.

Corollary 23.17 One finds

$$\overline{\rho_\nu(-q)} = \rho_\nu(q) \tag{23.13}$$

Proof 23.17 We compute straightforwardly

$$\begin{aligned} \overline{\rho_\nu(-q)} &= \frac{1}{\sqrt{\hbar\beta N_p}} \sum_{\substack{\sigma\in\{\downarrow,\uparrow\}\\ k\in\mathrm{i}\Omega_{-1}\times\mathbb{Q}\\ n,m\in\{1,2,\dots,\infty\}}} g_{mn\nu}(\mathbf{k},-\mathbf{q})^*\left(\overline{\psi}_{m\sigma}(k-q)\psi_{n\sigma}(k)\right)^\dagger \\ &\overset{\text{conj. rule}}{=} \frac{1}{\sqrt{\hbar\beta N_p}} \sum_{\substack{\sigma\in\{\downarrow,\uparrow\}\\ k\in\mathrm{i}\Omega_{-1}\times\mathbb{Q}\\ n,m\in\{1,2,\dots,\infty\}}} g_{mn\nu}(\mathbf{k},-\mathbf{q})^*\overline{\psi}_{n\sigma}(k)\psi_{m\sigma}(k-q) \\ &\overset{\substack{m\mapsto\tilde{n}\\ n\mapsto\tilde{m}}}{=} \frac{1}{\sqrt{\hbar\beta N_p}} \sum_{\substack{\sigma\in\{\downarrow,\uparrow\}\\ k\in\mathrm{i}\Omega_{-1}\times\mathbb{Q}\\ \tilde{n},\tilde{m}\in\{1,2,\dots,\infty\}}} g_{\tilde{n}\tilde{m}\nu}(\mathbf{k},-\mathbf{q})^*\overline{\psi}_{\tilde{m}\sigma}(k)\psi_{\tilde{n}\sigma}(k-q) \\ &\overset{\text{Lemma 8.37}}{=} \frac{1}{\sqrt{\hbar\beta N_p}} \sum_{\substack{\sigma\in\{\downarrow,\uparrow\}\\ k\in\mathrm{i}\Omega_{-1}\times\mathbb{Q}\\ \tilde{n},\tilde{m}\in\{1,2,\dots,\infty\}}} g_{\tilde{m}\tilde{n}\nu}(\mathbf{k}-\mathbf{q},+\mathbf{q})\overline{\psi}_{\tilde{m}\sigma}(k)\psi_{\tilde{n}\sigma}(k-q) \\ &\overset{k\mapsto k+q}{=} \frac{1}{\sqrt{\hbar\beta N_p}} \sum_{\substack{\sigma\in\{\downarrow,\uparrow\}\\ k\in\mathrm{i}\Omega_{-1}\times\mathbb{Q}\\ \tilde{n},\tilde{m}\in\{1,2,\dots,\infty\}}} g_{\tilde{m}\tilde{n}\nu}(\mathbf{k},\mathbf{q})\overline{\psi}_{\tilde{m}\sigma}(k+q)\psi_{\tilde{n}\sigma}(k) \\ &= \rho_\nu(q) \end{aligned} \tag{23.14}$$

23.2.2. Integrating out the Phonons

Lemma 23.18 Changing variables in a standard way allows us to integrate out the phonons, such that we obtain the effective fermionic action

$$\begin{aligned} S_{[j,\bar{j}]}[\psi,\overline{\psi}] &= S_{\text{el}}[\psi,\overline{\psi}] + S_{\substack{\text{el-el-int}\\[j_{\text{ph}},\bar{j}_{\text{ph}}]}}[\psi,\overline{\psi}] - \left(\bar{j}_{\text{el}}\psi + \overline{\psi} j_{\text{el}}\right) \\ &= \sum_{\substack{\sigma\in\{\downarrow,\uparrow\}\\ k\in \mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ m\in\{1,2,\ldots,\infty\}}} \overline{\psi}_{m\sigma}(k)\left(-\frac{1}{\hbar}\mathscr{G}^{-\text{el}}_{0\,m,\sigma}(k)\right)\psi_{m\sigma}(k) + S_{\substack{\text{el-el-int}\\[j_{\text{ph}},\bar{j}_{\text{ph}}]}}[\psi,\overline{\psi}] - \left(\bar{j}_{\text{el}}\psi + \overline{\psi} j_{\text{el}}\right) \end{aligned} \tag{23.15}$$

giving four terms, whereas the term that is quartic in the fermionic fields can be simplified to

$$\begin{aligned} S_{\substack{\text{el-el-int}\\[j_{\text{ph}},\bar{j}_{\text{ph}}]}}[\psi,\overline{\psi}] = &- \sum_{\substack{q\in \mathrm{i}\Omega_{+1}\times\mathrm{Q}\\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\}}} \frac{\omega_\nu(\mathbf{q})}{\omega_m^2+\omega_\nu^2(\mathbf{q})}\rho_\nu(q)\rho_\nu(-q) \\ &- \hbar \sum_{\substack{q\in \mathrm{i}\Omega_{+1}\times\mathrm{Q}\\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\}}} \rho_\nu(q)\mathscr{G}_{0,\nu}(q)j_\nu(q) - \hbar \sum_{\substack{q\in \mathrm{i}\Omega_{+1}\times\mathrm{Q}\\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\}}} \bar{j}_\nu(q)\mathscr{G}_{0,\nu}(q)\rho_\nu(-q) \\ &+ \hbar \sum_{\substack{q\in \mathrm{i}\Omega_{+1}\times\mathrm{Q}\\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\}}} \bar{j}_\nu(q)\mathscr{G}_{0,\nu}(q)j_\nu(q) \end{aligned} \tag{23.16}$$

Proof 23.18 See Appendix, Proofs, page 512.

Remark 23.18.1 Notice that this could be computed much simpler with Remark 16.28.1.

Lemma 23.19 Introducing the multi-index

$$\alpha \equiv (m_\alpha, \sigma_\alpha, \mathrm{i}\omega_\alpha, \mathbf{k}_\alpha) \in \{1,2,\ldots\}\times\{\downarrow,\uparrow\}\times \mathrm{i}\Omega_{-1}\times\mathrm{Q} \equiv \Xi, \tag{23.17}$$

one can rewrite the interaction-term-contribution that is quartic in the Graßmann-variables as generalised bilinear-form

$$S_{\text{el-el-int}}[\psi,\overline{\psi}] = \sum_{\alpha_1,\ldots,\alpha_4\in\Xi} \overline{\psi}_{\alpha_1}\overline{\psi}_{\alpha_2} V_{\alpha_1,\alpha_2;\alpha_3,\alpha_4}\psi_{\alpha_4}\psi_{\alpha_3}$$

with

$$
\begin{aligned}
&V_{\alpha_1,\alpha_2;\alpha_3,\alpha_4} \\
&= \frac{1}{\hbar\beta N_p} \sum_{\nu\in\{1,\dots,rd_{\mathbf{x}}\}} \frac{\omega_\nu(\mathbf{k}_{\alpha_1}-\mathbf{k}_{\alpha_4})}{\omega^2_{\alpha_1-\alpha_4}+\omega^2_\nu(\mathbf{k}_{\alpha_1}-\mathbf{k}_{\alpha_4})} \frac{g_{m_{\alpha_1}m_{\alpha_4}\nu}(\mathbf{k}_{\alpha_4},\mathbf{k}_{\alpha_1}-\mathbf{k}_{\alpha_4}) g^*_{m_{\alpha_3}m_{\alpha_2}\nu}(\mathbf{k}_{\alpha_2},\mathbf{k}_{\alpha_1}-\mathbf{k}_{\alpha_4})}{\hbar^2} \delta_{k_{\alpha_3}+k_{\alpha_4},k_{\alpha_2}+k_{\alpha_1}} \delta_{\sigma_{\alpha_1},\sigma_{\alpha_4}} \delta_{\sigma_{\alpha_2},\sigma_{\alpha_3}} \\
&= \frac{1}{\hbar\beta N_p} \sum_{\nu\in\{1,\dots,rd_{\mathbf{x}}\}} \frac{\omega_\nu(\mathbf{k}_{\alpha_1}-\mathbf{k}_{\alpha_4})}{\omega^2_{\alpha_1-\alpha_4}+\omega^2_\nu(\mathbf{k}_{\alpha_1}-\mathbf{k}_{\alpha_4})} \frac{g_{m_{\alpha_1}m_{\alpha_4}\nu}(\mathbf{k}_{\alpha_4},\mathbf{k}_{\alpha_1}-\mathbf{k}_{\alpha_4}) g_{m_{\alpha_2}m_{\alpha_3}\nu}(\mathbf{k}_{\alpha_2}+\mathbf{k}_{\alpha_1}-\mathbf{k}_{\alpha_4},-\mathbf{k}_{\alpha_1}+\mathbf{k}_{\alpha_4})}{\hbar^2} \delta_{k_{\alpha_3}+k_{\alpha_4},k_{\alpha_2}+k_{\alpha_1}} \delta_{\sigma_{\alpha_1},\sigma_{\alpha_4}} \delta_{\sigma_{\alpha_2},\sigma_{\alpha_3}}
\end{aligned}
\tag{23.18}
$$

Proof 23.19 See Appendix, Proofs, page 606.

Corollary 23.20 This[3] action is invariant under conjugation.

Proof 23.20 See Appendix, Proofs, page 513.

23.2.3. Expectation-Values as Source-Derivatives

Notation 23.21 We assume that we have a partition-function with ($Z[j_{\text{el}},\bar{j}_{\text{el}},j_{\text{ph}},\bar{j}_{\text{ph}}]$) and without ($Z$) electronic and phononic source-terms consider the ratio as generating functional

$$
\frac{Z[j_{\text{el}},\bar{j}_{\text{el}},j_{\text{ph}},\bar{j}_{\text{ph}}]}{Z} \equiv \frac{Z[j,\bar{j}]}{Z} \tag{23.19}
$$

whereas the external sources enter the partition function as in Notation 16.27. After obtaining a final expression for the partition function, we compute various quantities by taking functional derivatives.

Remark 23.21.1 Notice that the partition function can be simplified, by integrating out the phonons. Then one obtains Equation (23.15), which we rewrite here symbolically as

$$
\begin{aligned}
Z[j,\bar{j}] &\equiv \int \mathscr{D}(\overline{\chi},\chi)\, \exp\Big[-\Big(S_{\text{el}}[\psi,\overline{\psi}] + S_{\text{ph}}[\phi,\overline{\phi}] + S_{\text{el-ph-int}}[\chi,\overline{\chi}]\Big) \quad + \sum_{\bullet\in\{\text{el,ph}\}} \bar{j}_\bullet.\chi_\bullet + \overline{\chi}_\bullet.j_\bullet \Big] \\
&= \int \mathscr{D}(\overline{\psi},\psi)\, \exp -S_{[j,\bar{j}]}[\psi,\overline{\psi}] \\
&= \int \mathscr{D}(\overline{\psi},\psi)\, \exp -\left(S_{\text{el}}[\psi,\overline{\psi}] + S_{\substack{\text{el-el-int}\\ [j_{\text{ph}},\bar{j}_{\text{ph}}]}}[\psi,\overline{\psi}] - \left(\bar{j}_{\text{el}}\psi + \overline{\psi} j_{\text{el}}\right)\right) \\
&= \int \mathscr{D}(\overline{\psi},\psi)\, \exp\left(\bar{j}_{\text{el}}\psi + \overline{\psi} j_{\text{el}}\right) \exp -\left(S_{\text{el}} + S_{\substack{\text{el-el-int}\\ [j_{\text{ph}},\bar{j}_{\text{ph}}]}}\right)[\psi,\overline{\psi}]
\end{aligned}
\tag{23.20}
$$

[3] This is actually a much more general theorem that should hold IN GENERAL. This should be implemented somewhere in the text...

Corollary 23.22 Under the assumption, that the Matsubara-Green-function is diagonal w.r.t. the Matsubara-frequencies, we can re-express the following quantities as functional derivatives of the partition function:

Electronic Observables:

- The expectation-value of an occupation-number-operator w.r.t. the electronic state $(n, \sigma, \mathbf{k})$

$$\langle n_{n\sigma}(\mathbf{k})\rangle = \frac{1}{\hbar\beta}\sum_{\omega_m \in \Omega_{-1}} \mathrm{e}^{+\mathrm{i}\omega_m 0^+} \frac{\partial^2}{\partial \bar{j}_{n,\sigma}(\mathrm{i}\omega_m, \mathbf{k}) \partial j_{n,\sigma}(\mathrm{i}\omega_m, \mathbf{k})} \frac{Z[j_{\mathrm{el}}, \bar{j}_{\mathrm{el}}, j_{\mathrm{ph}}, \bar{j}_{\mathrm{ph}}]}{Z}\Big|_{\bar{j}=j=0}, \tag{23.21}$$

- the total particle number

$$\langle N\rangle = \frac{1}{\hbar\beta} \sum_{\substack{\sigma \in \{\downarrow,\uparrow\} \\ k \in \mathrm{i}\Omega_{-1}\times\mathrm{Q} \\ n \in \{1,2,\ldots,\infty\}}} \mathrm{e}^{+\mathrm{i}\omega_k 0^+} \frac{\partial^2}{\partial \bar{j}_{n,\sigma}(k) \partial j_{n,\sigma}(k)} \frac{Z[j_{\mathrm{el}}, \bar{j}_{\mathrm{el}}, j_{\mathrm{ph}}, \bar{j}_{\mathrm{ph}}]}{Z}\Big|_{\bar{j}=j=0}, \tag{23.22}$$

- the electronic contribution to the total energy we have

$$\langle H_{\mathrm{el}}\rangle = \frac{1}{\hbar\beta} \sum_{\substack{\sigma \in \{\downarrow,\uparrow\} \\ k \in \mathrm{i}\Omega_{-1}\times\mathrm{Q} \\ n \in \{1,2,\ldots,\infty\}}} \mathrm{e}^{+\mathrm{i}\omega_k 0^+} \epsilon_{n\sigma}(\mathbf{k}) \frac{\partial^2}{\partial \bar{j}_{n,\sigma}(k) \partial j_{n,\sigma}(k)} \frac{Z[j_{\mathrm{el}}, \bar{j}_{\mathrm{el}}, j_{\mathrm{ph}}, \bar{j}_{\mathrm{ph}}]}{Z}\Big|_{\bar{j}=j=0}, \tag{23.23}$$

Phononic Observables:

- the phononic occupation-number-operator

$$\langle n_\nu(\mathbf{q})\rangle = \frac{1}{\hbar\beta}\sum_{\omega_m \in \Omega_{+1}} \mathrm{e}^{+\mathrm{i}\omega_m 0^+} \frac{\partial^2}{\partial \bar{j}_\nu(\mathrm{i}\omega_m, \mathbf{q}) \partial j_\nu(\mathrm{i}\omega_m, \mathbf{q})} \frac{Z[j_{\mathrm{el}}, \bar{j}_{\mathrm{el}}, j_{\mathrm{ph}}, \bar{j}_{\mathrm{ph}}]}{Z}\Big|_{\bar{j}=j=0},$$

- the phononic contribution to the total energy we have

$$\left\langle H_{\mathrm{ph}}\right\rangle = \frac{1}{\hbar\beta} \sum_{\substack{q \in \mathrm{i}\Omega_{+1}\times\mathrm{Q} \\ \nu \in \{1,2,\ldots,rd_{\mathbf{x}}\}}} \mathrm{e}^{+\mathrm{i}\omega_q 0^+} \Omega_\nu(\mathbf{q}) \frac{\partial^2}{\partial \bar{j}_\nu(q) \partial j_\nu(q)} \frac{Z[j_{\mathrm{el}}, \bar{j}_{\mathrm{el}}, j_{\mathrm{ph}}, \bar{j}_{\mathrm{ph}}]}{Z}\Big|_{\bar{j}=j=0}. \tag{23.24}$$

Interaction Observables:

- the electron-phonon-interaction energy is given by

$$\left\langle c^\dagger_{\mathbf{k}+\mathbf{q}m\sigma} c_{\mathbf{k}n\sigma} \left(b_{\mathbf{q}\nu} + b^\dagger_{-\mathbf{q}\nu}\right)\right\rangle = \frac{1}{\sqrt{\hbar\beta}^3} \sum_{\substack{\omega_m \in \Omega_{+1} \\ \omega_n, \omega_{n'} \in \Omega_{-1}}} \mathrm{e}^{\mathrm{i}\omega_n 0^+} \frac{\partial^2}{\partial \bar{j}_{n\sigma\mathbf{k}}(\mathrm{i}\omega_n) \partial j_{m\sigma\mathbf{k}+\mathbf{q}}(\mathrm{i}\omega_{n'})} \left(\frac{\partial}{\partial \bar{j}_\nu(\mathrm{i}\omega_m, \mathbf{q})} + \frac{\partial}{\partial j_\nu(-\mathrm{i}\omega_m, -\mathbf{q})}\right) \frac{Z[j_{\mathrm{el}}, \bar{j}_{\mathrm{el}}, j_{\mathrm{ph}}, \bar{j}_{\mathrm{ph}}]}{Z}\Big|_{\bar{j}=j=0}. \tag{23.25}$$

Proof 23.22 See Appendix, Proofs, page 610.

Remark 23.22.1 Equations (23.21), (23.21) and (23.23) are merely listed for completeness. The Green-function-techniques developed in the earlier chapters allow us a much more elegant computation of the internal energy, as will become clear in Theorem 25.16.

24. Density of States, Thermodynamic Potential & Conjugated Variables

Motivation and Overview

After this part of the notes you will understand how to calculate for arbitrary materials and for arbitrary temperatures the Band-Structure and [D]ensity [O]f [S]tates (DOS) ...

- ...for a typical non-interacting model, resulting in a plot as in Figure 24.1.
- ...for a typical interacting model, resulting in a plot as in the literature [31].

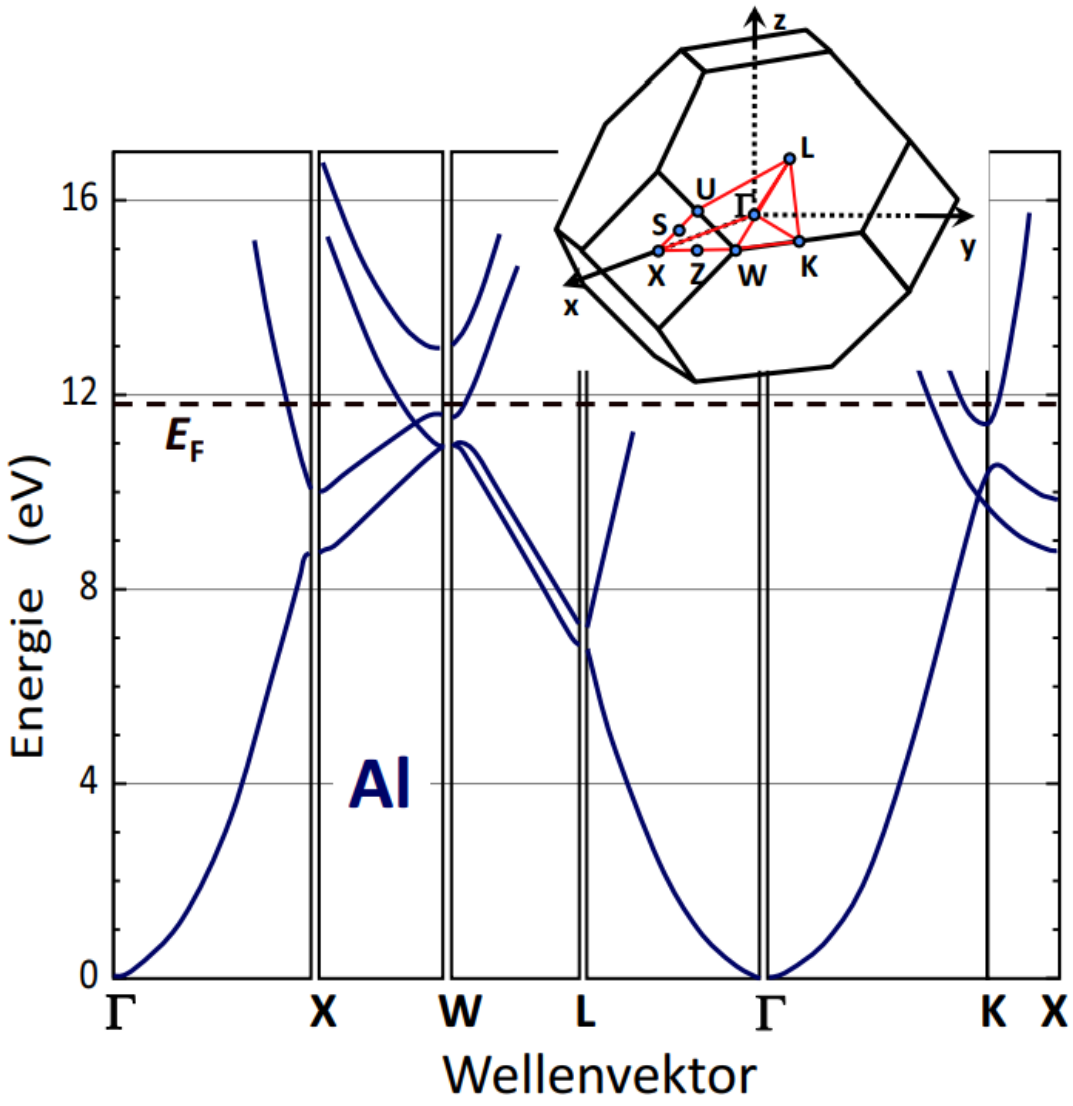


Figure 24.1.: The Band-Structure of Aluminium along the high-symmetry **k**-points. Taken from [22].

24.1. Non-Interacting Gas-Models

24.1.1. Non-Interacting Electrons

Electronic Density of States

Fact 24.1 Recall[1] that using Equation (14.12) we obtain the electronic density of states $\rho_0(E)$ for the system as

$$\rho_0(E) = \sum_{\substack{\mathbf{k}\in\mathrm{Q}\\ \sigma\in\{\uparrow,\downarrow\}\\ m\in\{1,\dots,\infty\}}} \delta(E-(\epsilon_{m\mathbf{k}\sigma}-\mu)) \tag{24.1}$$

Proof 24.1 Follows immediately from the Sokhotski-Plemelj-Theorem in Equation (14.3).

Remark 24.1.1 Notice that this density of states is formally just a sum of Dirac-delta-peaks. However, when physicists *depict* (i.e. plot) the density of states, they recall that this model is just an approximation to a more realistic model which includes interactions. Since interactions usually imply the presence of smearing, one usually "artificially" introduces smearing in the non-interacting density of states by replacing the delta-peaks with Lorentzians or Gaussians.

Remark 24.1.2 We remark that regularizing the delta-functions with Gaussians converges "much faster" (in the number of k-points) than regularizing the delta-functions with Lorentzians.

Notation 24.2 Notice that this quantity is (after introducing cutoffs for the number of bands) normalized to

$$\int \mathrm{d}E\rho_0(E) = N_x N_y N_z \cdot N_{\mathrm{band}} \cdot 2 \tag{24.2}$$

Notice that the factor of 2 originates from spin-degeneracy. The density of states, as computed in [Q]uantum [E]spresso (QE) within the [L]ocal [D]ensity [A]pproximation (LDA), $\rho_{\mathrm{QE}}(E)$ is normalized to the number of bands, i.e.

$$\frac{1}{N_x N_y N_z}\rho_0(E-\mu) = \frac{1}{N_x N_y N_z}\sum_{\substack{\mathbf{k}\in\mathrm{Q}\\ \sigma\in\{\downarrow,\uparrow\}\\ n\in\{1,2,\dots\}}} \delta(E-\epsilon_{n\mathbf{k}}) \mapsto \frac{1}{N_x N_y N_z}\sum_{\substack{\mathbf{k}\in\mathrm{Q}\\ \sigma\in\{\downarrow,\uparrow\}\\ n\in\{1,2,\dots,N_{\mathrm{band}}\}}} \delta(E-\epsilon_{n\mathbf{k}}) \equiv \rho_{\mathrm{QE,\,LDA}}(E) \tag{24.3}$$

such that it is normalized to

$$\int \mathrm{d}E\rho_{\mathrm{QE,\,LDA}}(E) = 2N_{\mathrm{band}} \tag{24.4}$$

[1] Cf. Lemma 14.15.

Electronic Thermodynamic Potential - Landau Potential

Lemma 24.3 The grand canonical potential $\Omega_{0,\mathrm{el}}(\mu, T, V)$ for the electronic system is given as

$$\Omega_{0,\mathrm{el}}(\mu, T, V) = \frac{-1}{\beta} \sum_{\substack{\mathbf{k}\in \mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\dots,\infty\}}} \mathrm{Log}\left(1 + \mathrm{e}^{-\beta(\epsilon_{m\mathbf{k}\sigma}-\mu)}\right) = \frac{-1}{\beta}\int \mathrm{d}E\, \mathrm{Log}\left(1+\mathrm{e}^{-\beta E}\right)\rho_0(E) \tag{24.5}$$

Proof 24.3 See Appendix, Proofs, page 611.

Electronic Thermodynamic Conjugated Variable - Chemical Potential

Fact 24.4 The chemical potential has to be computed by constraining the number of particles according to Lemma 14.14 as

$$\langle N\rangle_0 = \sum_{\substack{\mathbf{k}\in \mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\dots,\infty\}}} \mathrm{F}_\beta(\epsilon_{m\mathbf{k}\sigma}-\mu) = \int_{-\infty}^{+\infty} \mathrm{d}E\, \mathrm{F}_\beta(E)\,\rho_0(E) \quad\Longleftrightarrow\quad \frac{\langle N\rangle_0}{N_x N_y N_z} = \int_{-\infty}^{+\infty} \mathrm{d}E\, \mathrm{F}_\beta(E-\mu)\,\rho_{\mathrm{QE,\,LDA}}(E) \tag{24.6}$$

Remark 24.4.1 Notice that we implicitly assumed that the number of bands is large enough to accommodate all electrons in the system.

Fact 24.5 We first notice that dictating the particle number (for example by requiring [C]harge [N]eutrality of the crystal) through Equation (24.6) can be rewritten as

$$\begin{aligned} F_0(\mu,T) \equiv & \quad \langle N\rangle_0(\mu,T) && - N_{\mathrm{CN}} \\ = & \left[\int_{-\infty}^{+\infty} \mathrm{d}E\, \mathrm{F}_\beta(E)\,\rho_0(E)\right] && - N_{\mathrm{CN}} \\ = & \left[\int_{-\infty}^{+\infty} \mathrm{d}E\, \mathrm{F}_\beta(E-\mu)\,\rho_{\mathrm{QE,\,LDA}}(E)\right] N_x N_y N_z && - N_{\mathrm{CN}} = 0. \end{aligned} \tag{24.7}$$

Remark 24.5.1 Notice that this is an implicit function, meaning that we can use the Theorem for implicit functions to compute, e.g. the derivative of the chemical potential as a function of temperature. Notice further that we dropped the volume-dependence for notational convenience.

Remark 24.5.2 Notice that the chemical potential that is defined through this Equation is unique due to Theorem 9.37.

Remark 24.5.3 Notice further that the partial derivatives of the function F_0 are given as the partial derivatives of the expected particle number $\langle N \rangle_0$, i.e.

$$\left(\partial_T F_0\right)(\mu, T) = \partial_T \langle N \rangle_0(\mu, T), \qquad \left(\partial_\mu F_0\right)(\mu, T) = \partial_\mu \langle N \rangle_0(\mu, T). \tag{24.8}$$

Lemma 24.6 The temperature-derivative of the function F_0 can be computed with Lemma 9.63 and Equation (24.3) as

$$\begin{aligned}
\left(\partial_T F_0\right)(\mu, T) = \partial_T \langle N \rangle_0(\mu, T) = & \quad \frac{\beta}{4T} \sum_{\substack{\mathbf{k} \in \mathrm{Q} \\ \sigma \in \{\uparrow,\downarrow\} \\ m \in \{1,\ldots,\infty\}}} \operatorname{sech}^2\left(\frac{\beta \xi_{m\mathbf{k}\sigma}}{2}\right) \quad \xi_{n\mathbf{k}\sigma} \\
= N_x N_y N_z & \quad \frac{\beta}{4T} \int_{-\infty}^{+\infty} \mathrm{d}E \quad \operatorname{sech}^2\left(\beta \frac{E-\mu}{2}\right) \quad (E-\mu) \quad \rho_{\mathrm{QE,\,LDA}}(E) \\
= & \quad \frac{\beta}{4T} \int_{-\infty}^{+\infty} \mathrm{d}E \quad \operatorname{sech}^2\left(\frac{\beta E}{2}\right) \quad E \quad \rho_0(E) \\
= & \quad \frac{\beta}{T} \int_{-\infty}^{+\infty} \mathrm{d}E \quad \mathrm{F}_\beta(E)\left(1 - \mathrm{F}_\beta(E)\right) \quad E \quad \rho_0(E)
\end{aligned} \tag{24.9}$$

Proof 24.6 The individual identities are proven by referring to Lemma 9.66 and Notation 24.2.

Lemma 24.7 The chemical-potential-derivative of the function F can be computed as ...

$$\begin{aligned}
\left(\partial_\mu F_0\right)(\mu, T) = \partial_\mu \langle N \rangle_0(\mu, T) = & \quad \frac{\beta}{4} \sum_{\substack{\mathbf{k} \in \mathrm{Q} \\ \sigma \in \{\uparrow,\downarrow\} \\ m \in \{1,\ldots,\infty\}}} \operatorname{sech}^2\left(\frac{\xi_{m\mathbf{k}\sigma}}{2k_B T}\right) \\
= N_x N_y N_z & \quad \frac{\beta}{4} \int_{-\infty}^{+\infty} \mathrm{d}E \quad \operatorname{sech}^2\left(\beta \frac{E-\mu}{2}\right) \rho_{\mathrm{QE}}(E) \\
= & \quad \frac{\beta}{4} \int_{-\infty}^{+\infty} \mathrm{d}E \quad \operatorname{sech}^2\left(\frac{\beta E}{2}\right) \rho_0(E)
\end{aligned} \tag{24.10}$$

Proof 24.7 We compute the derivative of the Fermi-function w.r.t. the chemical potential with Equation (24.6) by noticing

$$\mathrm{F}_\beta(\epsilon_{n\mathbf{k}\sigma} - \mu) \equiv \mathrm{n}^{-1}(\beta(\epsilon_{n\mathbf{k}\sigma} - \mu)) \tag{24.11}$$

which implies with Lemma 9.63 and the chain-rule and $\xi_{n\mathbf{k}\sigma} \equiv \epsilon_{n\mathbf{k}\sigma} - \mu$ that

$$\partial_\mu \, \mathrm{n}^{-1}(\beta(\epsilon_{n\mathbf{k}\sigma} - \mu)) = -\frac{1}{4} \operatorname{sech}^2\left(\beta \xi_{n\mathbf{k}\sigma}/2\right) \cdot (-\beta) = \frac{\beta}{4} \operatorname{sech}^2\left(\beta \xi_{n\mathbf{k}\sigma}/2\right) \tag{24.12}$$

proving that the first Equation-sign. The second and the third equation-sign follow from Equation (24.3).

Corollary 24.8 Assuming now we have access[2] to the values $\mu(T)$ that fulfill Equation (24.7), we can compute the temperature derivative of the chemical potential as

$$\left(\frac{\partial\mu}{\partial T}\right)(T) = -\left(\frac{\partial_T F_0}{\partial_\mu F_0}\right)(\mu(T),T) = -\left(\frac{\partial_T\langle N\rangle_0}{\partial_\mu\langle N\rangle_0}\right)(\mu(T),T)\,. \tag{24.13}$$

Proof 24.8 Follows from the Theorem of implicit functions with Equation (24.7).

Remark 24.8.1 Notice that this equation can be rewritten in the physics-notation as

$$\frac{\partial\mu}{\partial T} = -\frac{\partial N}{\partial T}\frac{\partial\mu}{\partial N} \quad\Longleftrightarrow\quad \frac{\partial\mu}{\partial T}\frac{\partial T}{\partial N}\frac{\partial N}{\partial\mu} = -1 \tag{24.14}$$

Corollary 24.9 Notice that this implies for Equation (24.13) in the non-interacting case the formula

$$\left(\frac{\partial\mu}{\partial T}\right)(T) = -\frac{1}{T}\frac{\int_{-\infty}^{+\infty}\mathrm{d}E\,\mathrm{sech}^2\left(\beta\frac{E-\mu(T)}{2}\right)\rho_{\mathrm{QE}}(E)\big[E-\mu(T)\big]}{\int_{-\infty}^{+\infty}\mathrm{d}E\,\mathrm{sech}^2\left(\beta\frac{E-\mu(T)}{2}\right)\rho_{\mathrm{QE}}(E)} \tag{24.15}$$

Proof 24.9 Follows immediately by combining Equation (24.13) with Lemmas 24.7 and 24.7.

Electronic Thermodynamic Conjugated Variable - Pressure

Fact 24.10 Notice that one can compute the pressure $P \equiv P(\mu,T,V)$ with Equations (10.9) and (24.5) as

$$-\frac{\Omega_0(\mu,T,V+\Delta V)-\Omega_0(\mu,T,V)}{\Delta V} \tag{24.16}$$

with $V \equiv N_p V_{\mathrm{UC}}$, $N_p \equiv N_x N_y N_z$ and unit-cell volume

$$V_{\mathrm{UC}} = \int_{\mathrm{span}_{[0,1]}\{\mathbf{a}_1,\mathbf{a}_2,\mathbf{a}_3\}} 1\mathrm{d}^3x = \det(\mathbf{a}_1,\mathbf{a}_2,\mathbf{a}_3) \tag{24.17}$$

[2] Notice that this is the case, as we compute the chemical potential numerically.

Electronic Thermodynamic Conjugated Variable - Entropy

We combine Equations (10.9) and (24.5) and compute the temperature-derivative

$$\begin{aligned} \partial_T \log\left(1+\mathrm{e}^{-\beta E}\right) &= \frac{1}{1+\mathrm{e}^{-\beta E}} \cdot \mathrm{e}^{-\beta E} \cdot \left(\frac{E}{k_{\mathrm{B}} T^2}\right) \\ &\overset{\text{Eq. (9.65)}}{=} \mathrm{F}_\beta(E) \cdot \left(\frac{E}{k_{\mathrm{B}} T^2}\right) \end{aligned} \tag{24.18}$$

which gives us

$$S = -\partial_T \Omega = \boxed{\text{TBD}} \tag{24.19}$$

24.1.2. Non-Interacting Phonons

Phononic Density of States

Definition 24.11 We introduce the *non-interacting phononic density of states* ρ_{ph} as

$$\rho_{\mathrm{ph}}(E) = \frac{1}{N_x N_y N_z} \sum_{\substack{\mathbf{q}\in\mathrm{Q} \\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} \delta(E-\Omega_\nu(\mathbf{q})) = \frac{1}{N_x N_y N_z} \frac{-1}{\pi} \sum_{\substack{\mathbf{q}\in\mathrm{Q} \\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} \lim_{\eta\to 0^+} \mathrm{Im}\, \frac{1}{E+\mathrm{i}\eta-\Omega_\nu(\mathbf{q})} \tag{24.20}$$

Phononic Thermodynamic Potential - Helmholtz Free Energy

Lemma 24.12 The grand canonical potential $\Omega_{0,\mathrm{el}}(\mu,T,V)$ for the electronic system is given as

$$\Omega_{0,\mathrm{ph}}(T,V) = \frac{-1}{\beta} \sum_{\substack{\mathbf{q}\in\mathrm{Q} \\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\}}} \mathrm{Log}\left(1-\mathrm{e}^{-\beta\Omega_{\nu\mathbf{q}}}\right) = \frac{-1}{\beta} \int \mathrm{d}E\, \mathrm{Log}\left(1-\mathrm{e}^{-\beta E}\right) \rho_{0,\mathrm{ph}}(E) \tag{24.21}$$

Proof 24.12 Analogous to the electronic case; Cf. Appendix, Proofs, page 611.

TBD

Phononic Thermodynamic Conjugated Variable - Chemical Potential

This is something that we will not elaborate in the PhD-thesis... However... It's not zero!

Phononic Thermodynamic Conjugated Variable - Pressure

This can be computed in complete analogy to Fact 24.10.

Phononic Thermodynamic Conjugated Variable - Entropy

We combine Equations (10.9) and (24.21) and compute the temperature-derivative

$$\begin{aligned} \partial_T \log\left(1-\mathrm{e}^{-\beta E}\right) &= \frac{1}{1-\mathrm{e}^{-\beta E}} \cdot \left(-\mathrm{e}^{-\beta E}\right) \cdot \left(\frac{E}{k_{\mathrm{B}} T^2}\right) \\ &\overset{\text{Eq. (9.65)}}{=} -\mathrm{B}_\beta(E) \cdot \left(\frac{E}{k_{\mathrm{B}} T^2}\right) \end{aligned} \tag{24.22}$$

which gives us

$$S = -\partial_T \Omega = \text{TBD} \tag{24.23}$$

24.1.3. Non-Interacting Electrons and Phonons (Total Crystal)

Total Crystal Thermodynamic Potential

Fact 24.13 The grand canonical potential $\Omega_0(\mu, T, V)$ is given as

$$\Omega_0(\mu, T, V) = \Omega_{0,\mathrm{el}}(\mu, T, V) + \Omega_{0,\mathrm{ph}}(T, V) \tag{24.24}$$

$$= \frac{-1}{\beta} \sum_{\substack{\mathbf{k}\in \mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\}}} \mathrm{Log}\left(1+\mathrm{e}^{-\beta(\epsilon_{m\sigma}(\mathbf{k})-\mu)}\right) + \frac{1}{\beta} \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\}}} \mathrm{Log}\left(1-\mathrm{e}^{-\beta\Omega_\nu(\mathbf{q})}\right) \tag{24.25}$$

Proof 24.13 Follows from combining

24.2. Interacting Electrons and Phonons (Total Crystal)

24.2.1. Interacting Electrons

Fact 24.14 We compute the chemical potential, by constraining the number of particles according to Lemma 14.14 as

$$\langle N\rangle = \sum_{\substack{\mathbf{k}\in \mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\}}} \langle n_{m\mathbf{k}\sigma}\rangle = \frac{-1}{\pi} \lim_{\delta\to 0} \oint \sum_{\substack{\mathbf{k}\in \mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\} \\ E\in(-\infty,+\infty)}} \mathrm{F}_\beta(E)\, \mathrm{Im}\, G^{\mathrm{ret}}_{\substack{m,m \\ \sigma,\sigma \\ \mathbf{k},\mathbf{k}}}(E+\mathrm{i}\delta) \tag{24.26}$$

Remark 24.14.1 The electronic self-energy depends on the specific system / interaction under consideration, but the formula is always "proper to use".

24.2.2. Interacting Phonons

We only remark that the computation of the occupation-number of phonons is not as straight-forward as in the electronic case. One can write on the one hand

$$\langle N_{\text{ph}} \rangle = \sum_{\substack{\mathbf{q} \in \text{Q} \\ \nu \in \{1,\dots,rd_{\mathbf{x}}\}}} \langle n_{\nu\mathbf{q}} \rangle = \dots ? \tag{24.27}$$

24.2.3. Total Crystal

Theorem 24.15 For the grand canonical potential of the interacting system we have in the lowest order of perturbation theory

TBDigitalized from Pinboard, Topic 17 (24.28)

Proof 24.15 See Appendix, Proofs, page 680.

Remark 24.15.1 Notice further, that one can compute the pressure $P \equiv P(\mu, T, V)$ as

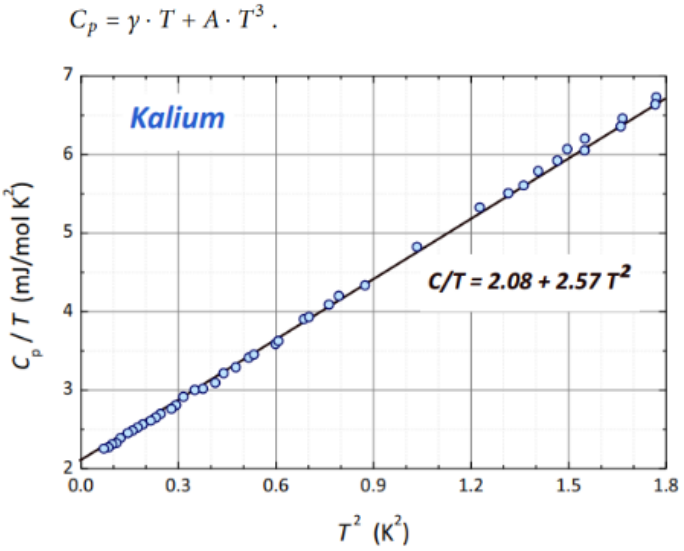
$$-\frac{\Omega(\mu, T, V + \Delta V) - \Omega(\mu, T, V)}{\Delta V} \tag{24.29}$$

with $V \equiv N_p V_{\text{UC}}$, $N_p \equiv N_x N_y N_z$ and unit-cell volume

$$V_{\text{UC}} = \int_{\text{span}_{[0,1]}\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}} 1 \mathrm{d}^3 x = \det(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3) \tag{24.30}$$

25. Internal Energy & Specific Heat (Normal State)

In this part of the notes we will discuss how to calculate the specific heat for arbitrary materials in a typical non-interacting model at low temperatures as in Figures 25.1 and 25.2. We will then extend the discussion to interacting models as well.



Metall	γ_{exp} (10^{-3} J/mol K)	γ_{theor} (10^{-3} J/mol K)	$\gamma_{exp}/\gamma_{theor}$
Li	1.63	0.749	2.18
Na	1.38	1.094	1.26
K	2.08	1.668	1.25
Rb	2.41	1.911	1.26
Cs	3.20	2.238	1.43
Fe	4.98	0.498	10
Co	4.98	0.483	10.3
Ni	7.02	0.458	15.3
Cu	0.695	0.505	1.38
Ag	0.646	0.645	1.00
Au	0.729	0.642	1.14
Sn	1.78	1.41	1.26
Pb	2.98	1.509	1.97

Figure 25.1.: Specific heat of various materials at low temperatures, taken from [22].

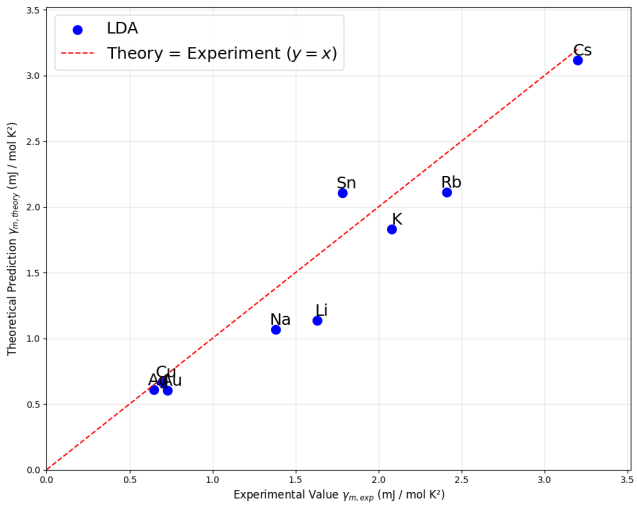


Figure 25.2.: Specific heat of various materials contrasting LDA and Experimental Results. Produced with quantum espresso v7.2 and norm conserving pseudopotentials from sssp.

25.1. Non-Interacting Gas-Models

25.1.1. Non-Interacting Electrons

Theorem 25.1 The expectation-value of the electronic internal energy can be computed as

$$\langle H_{\mathrm{el}} \rangle_0 = \sum_{\substack{\mathbf{k}\in\mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\}}} \epsilon_{m\mathbf{k}\sigma} \left\langle c^{\dagger}_{m\mathbf{k}\sigma} c_{m\mathbf{k}\sigma} \right\rangle_0 = \sum_{\substack{\mathbf{k}\in\mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\}}} \epsilon_{m\mathbf{k}\sigma}\, \mathrm{F}_{\beta}(\epsilon_{m\mathbf{k}\sigma} - \mu) \tag{25.1}$$

Corollary 25.2 Notice, that in the non-interacting case, this formula simplifies to

$$\langle H_{\mathrm{el}} \rangle_0 = \int \mathrm{d}E\; E\; \mathrm{F}_{\beta}(E)\rho_0(E) \quad \Longleftrightarrow \quad \frac{\langle H_{\mathrm{el}} \rangle_0}{N_x N_y N_z} = \int \mathrm{d}E\, (E-\mu)\; \mathrm{F}_{\beta}(E-\mu)\rho_{\mathrm{QE}}(E) \tag{25.2}$$

Proof 25.2 Follows with the Sokhotski-Plemelj theorem from Equation (25.10).

Lemma 25.3 In the absence of interactions one obtains the simple formula

$$\partial_T \frac{\langle H_{\mathrm{el}} \rangle_0}{N_x N_y N_z} = \int \mathrm{d}E \quad \frac{E}{4} \quad \mathrm{sech}^2\left(\frac{E-\mu(T)}{2k_B T}\right) \quad \left[\frac{E-\mu(T)}{k_B T^2}\right] \quad \rho_{\mathrm{QE}}(E) \tag{25.3}$$

Proof 25.3 See Appendix, Proofs, page 611.

Lemma 25.4 In the absence of interactions one obtains the simple formula

$$\begin{aligned} \partial_{\mu} \frac{\langle H_{\mathrm{el}} \rangle_0}{N_x N_y N_z} &= \frac{1}{N_x N_y N_z} \quad \frac{\beta}{4} \quad \sum_{\substack{\mathbf{k}\in\mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\}}} \epsilon_{m\mathbf{k}\sigma} \quad \mathrm{sech}^2\left(\frac{\epsilon_{m\mathbf{k}\sigma}-\mu}{2k_B T}\right) \\ &= \frac{\beta}{4} \quad \int \mathrm{d}E \quad E \quad \mathrm{sech}^2\left(\frac{E-\mu}{2k_B T}\right) \quad \rho_{\mathrm{QE}}(E) \end{aligned} \tag{25.4}$$

Proof 25.4 See Appendix, Proofs, page 613.

25.1.2. Non-Interacting Phonons

Fact 25.5 The expectation-value of the phononic internal energy can be computed as

$$\langle H_{\mathrm{ph}} \rangle_0 = \sum_{\substack{\mathbf{q} \in \mathrm{Q} \\ \nu \in \{1,2,\ldots,rd_{\mathbf{x}}\}}} \Omega_\nu(\mathbf{q})\, \mathrm{B}_\beta(\Omega_\nu(\mathbf{q})) \tag{25.5}$$

Lemma 25.6 The temperature-derivatives of the non-interacting phononic contribution to the internal energy can be computed as

$$\begin{aligned} \partial_T \langle H_{\mathrm{ph}} \rangle_0 &= \frac{\beta}{4T} \sum_{\substack{\mathbf{q} \in \mathrm{Q} \\ \nu \in \{1,2,\ldots,rd_{\mathbf{x}}\}}} \left[\Omega_\nu(\mathbf{q}) \operatorname{csch}(\beta \Omega_\nu(\mathbf{q})/2) \right]^2 \\ &= \frac{\beta}{4T} \int \mathrm{d}E \left[E \operatorname{csch}(\beta E/2) \right]^2 \rho_{\mathrm{ph}}(E) \\ &= \frac{\beta}{4T} \lim_{\eta \to 0^+} \int \mathrm{d}E \left[E \operatorname{csch}(\beta E/2) \right]^2 \left(-\frac{1}{\pi} \right) \sum_{\substack{\mathbf{q} \in \mathrm{Q} \\ \nu \in \{1,2,\ldots,rd_{\mathbf{x}}\}}} \operatorname{Im} \frac{1}{E + \mathrm{i}\eta - \Omega_\nu(\mathbf{q})} \end{aligned} \tag{25.6}$$

Proof 25.6 Follows by using Definition 24.11.

25.1.3. Non-Interacting Electrons and Phonons (Total Crystal)

Fact 25.7 The expectation-value of the total internal energy can be computed as

$$\begin{aligned} \langle H \rangle_0 = &\quad \langle H_{\mathrm{el}} \rangle_0 &&+ \quad \langle H_{\mathrm{ph}} \rangle_0 \\ = &\sum_{\substack{\mathbf{k} \in \mathrm{Q} \\ \sigma \in \{\uparrow,\downarrow\} \\ m \in \{1,\ldots,\infty\}}} \epsilon_{m\mathbf{k}\sigma}\, \mathrm{F}_\beta(\epsilon_{m\mathbf{k}\sigma} - \mu) &&+ \sum_{\substack{\mathbf{q} \in \mathrm{Q} \\ \nu \in \{1,\ldots,rd_{\mathbf{x}}\}}} \Omega_\nu(\mathbf{q})\, \mathrm{B}_\beta(\Omega_\nu(\mathbf{q})) \end{aligned} \tag{25.7}$$

Remark 25.7.1 Notice that these identities can be further simplified by using the density of states for the electronic and / or the phononic system.

Fact 25.8 The basic formula from is according to Equation (9.60)

$$\begin{aligned} c_{N,V}(T) = \frac{C_{N,V}(T)}{n} &= \frac{1}{n} \partial_T \langle H \rangle_{0,N,T,V} \\ &= \frac{1}{n} \Big[\left(\partial_T \langle H \rangle_0 \right)(\mu, T, V) + \left(\partial_\mu \langle H \rangle_0 \right)(\mu, T, V) \cdot \left(\partial_T \mu \right)(N(\mu), V, T) \Big] \end{aligned} \tag{25.8}$$

The Hamiltonian is made up of two contributions

$$H_{\text{tot}} = H_{\text{el}} + H_{\text{ph}} \tag{25.9}$$

Therefore, also for the specific heat, we have contributions from the electronic part and from the phononic part. We further need to account for the temperature derivative of the chemical potential. We consider all three quantities separately and then merge the results.

25.2. Interacting Electrons and Phonons (Total Crystal)

25.2.1. Interacting Electrons

Theorem 25.9 One finds the identity

$$\langle H_{\text{el}} \rangle = \sum_{\substack{\mathbf{k}\in\mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\dots,\infty\}}} \epsilon_{m\mathbf{k}\sigma} \langle n_{m\mathbf{k}\sigma} \rangle = \frac{-1}{\pi} \lim_{\delta\to 0} \oint\!\!\!\!\!\!\sum_{\substack{\mathbf{k}\in\mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\dots,\infty\} \\ E\in(-\infty,+\infty)}} \epsilon_{m\mathbf{k}\sigma}\, \mathrm{F}_\beta(E)\, \mathrm{Im}\, G^{\text{ret}}_{\substack{m,m \\ \sigma,\sigma}}(E+\mathrm{i}\delta,\mathbf{k}) \tag{25.10}$$

Proof 25.9 See Appendix, Proofs, page 613.

The Electronic Contribution

Theorem 25.10 One finds for the interacting system two equivalent identities

$$\frac{\partial^2}{\partial \bar{j}_{n,\sigma}(k)\partial j_{n,\sigma}(k)} \frac{Z[j_{\text{el}},\bar{j}_{\text{el}},j_{\text{ph}},\bar{j}_{\text{ph}}]}{Z}\Big|_{\bar{j}=j=0} = +\hbar \mathscr{G}_{\substack{n,n \\ \sigma,\sigma}}(k,k) \tag{25.11}$$

$$\begin{aligned}\frac{\partial^2}{\partial \bar{j}_{n,\sigma}(k)\partial j_{n,\sigma}(k)} \frac{Z[j_{\text{el}},\bar{j}_{\text{el}},j_{\text{ph}},\bar{j}_{\text{ph}}]}{Z}\Big|_{\bar{j}=j=0} &= +\hbar \mathscr{G}_{\substack{n,n \\ \sigma,\sigma}}{}_0(k,k) \\ &\quad - \frac{\hbar}{\beta N_p} \sum_{\substack{k\in \mathrm{i}\Omega_{-1}\times\mathrm{Q} \\ n'\in\{1,\dots,\infty\} \\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} |g_{nn'\nu}(\mathbf{k},\mathbf{k}'-\mathbf{k})|^2 \mathscr{G}^2_{0,n,\sigma}(k)\mathscr{G}_{0,n',\sigma}(k')\mathscr{D}_{0,\nu}(k'-k) \\ &\quad + \mathcal{O}(g^4)\end{aligned} \tag{25.12}$$

Proof 25.10 See Appendix, Proofs, page 613.

Remark 25.10.1 We only mention the second identity for completeness; In practice, it is difficult to converge this expression. The second identity can be simplified further by evaluating the occuring Matsuara-sums (cf. B-sides). The first identity is the one that is used in practice, since it can be simplified with the fluctuation-dissipation-theorem.

25.2.2. Interacting Phonons

The Phononic Contribution

We first focus on the term in Equation (23.24).

Theorem 25.11 One finds for the interacting system the identity

$$\begin{aligned}\frac{\partial^2}{\partial\bar{j}_\nu(q)\partial j_\nu(q)}\frac{Z[j_{\mathrm{el}},\bar{j}_{\mathrm{el}},j_{\mathrm{ph}},\bar{j}_{\mathrm{ph}}]}{Z}\Big|_{\bar{j}=j=0} \approx & -\hbar\mathscr{G}_{0,\nu}(q)\\ & + \frac{\hbar}{\beta N_p}\mathscr{G}^2_{0,\nu}(q)\delta_{q,0}\sum_{\substack{k,k'\in \mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ n,n'\in\{1,\ldots,\infty\}\\ \sigma,\sigma'\in\{\downarrow,\uparrow\}}} g_{nn\nu}(\mathbf{k},0)g_{n'n'\nu}(\mathbf{k}',0)\mathscr{G}_{0,n,\sigma}(k)\mathscr{G}_{0,n',\sigma'}(k')\\ & - \frac{\hbar}{\beta N_p}\mathscr{G}^2_{0,\nu}(q)\sum_{\substack{k\in \mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ n,n'\in\{1,\ldots,\infty\}\\ \sigma\in\{\downarrow,\uparrow\}}} |g_{n'n\nu}(\mathbf{k},\mathbf{q})|^2\mathscr{G}_{0,n,\sigma}(k)\mathscr{G}_{0,n',\sigma}(k+q) \quad + \quad \mathcal{O}(g^4)\end{aligned} \tag{25.13}$$

whereas the terms of order $\mathcal{O}(g^4)$ are those that are being neglected when one approximates the Bethe-Salpeter-equation.

Proof 25.11 See Appendix, Proofs, page 614.

Lemma 25.12 For the phononic occupation numbers of the interacting system we have the identity

$$\begin{aligned}\langle H_{\mathrm{ph}}\rangle \approx & -\frac{1}{\beta}\sum_{\substack{q\in \mathrm{i}\Omega_{+1}\times\mathrm{Q}\\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} \mathrm{e}^{+\mathrm{i}\omega_q 0^+}\Omega_\nu(\mathbf{q})\mathscr{G}_{0,\nu}(q)\\ & + \frac{1}{\beta^2 N_p}\sum_{\substack{\sigma,\sigma'\in\{\downarrow,\uparrow\}\\ k,k'\in \mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ n,n'\in\{1,\ldots,\infty\}\\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} \Omega_\nu(\mathbf{q}=\mathbf{0})g_{nn\nu}(\mathbf{k},0)g_{n'n'\nu}(\mathbf{k}',0)\mathscr{G}^2_{0,\nu}(q=0)\mathscr{G}_{0,n,\sigma}(k)\mathscr{G}_{0,n',\sigma'}(k')\\ & - \frac{1}{\beta^2 N_p}\sum_{\substack{k\in \mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ q\in \mathrm{i}\Omega_{+1}\times\mathrm{Q}\\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}\\ n,n'\in\{1,\ldots,\infty\}\\ \sigma\in\{\downarrow,\uparrow\}}} \Omega_\nu(\mathbf{q})|g_{n'n\nu}(\mathbf{k},\mathbf{q})|^2\mathscr{G}^2_{0,\nu}(q)\mathscr{G}_{0,n,\sigma}(k)\mathscr{G}_{0,n',\sigma}(k+q) \quad + \quad \mathcal{O}(g^4)\end{aligned} \tag{25.14}$$

whereas the terms of order $\mathcal{O}(g^4)$ are those that are being neglected when one approximates the Bethe-Salpeter-equation.

Proof 25.12 See Appendix, Proofs, page 616.

Remark 25.12.1 Notice that the individual terms have the unit of an energy and are hence consistent.

Corollary 25.13 Evaluating the Matsubara-sums simplifies the individual terms as

$$\begin{aligned}\langle H_{\mathrm{ph}}\rangle \approx & \sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ \nu\in\{1,2,\ldots,rd_{\mathrm{x}}\}}} \Omega_\nu(\mathbf{q})\,\mathrm{B}_\beta(\Omega_\nu(\mathbf{q})) \quad + \quad \sum_{\nu\in\{1,2,\ldots,rd_{\mathrm{x}}\}} A_\nu B_\nu^2 \\ & - \sum_{\substack{\mathbf{k},\mathbf{q}\in\mathrm{Q}\\ \sigma\in\{\downarrow,\uparrow\}\\ \nu\in\{1,2,\ldots,rd_{\mathrm{x}}\}\\ n,n'\in\{1,\ldots,\infty\}}} \frac{\Omega_\nu(\mathbf{q})}{N_p}|g_{n'n\nu}(\mathbf{k},\mathbf{q})|^2\left(\mathrm{F}_\beta(\xi_{n,\sigma,\mathbf{k}})-\mathrm{F}_\beta(\xi_{n',\sigma,\mathbf{k}+\mathbf{q}})\right)\left[\frac{\mathrm{B}_\beta(\Omega_\nu(\mathbf{q}))-\mathrm{B}_\beta(\xi_{n',\sigma,\mathbf{k}+\mathbf{q}}-\xi_{n,\sigma,\mathbf{k}})}{\left(\Omega_\nu(\mathbf{q})+\xi_{n,\sigma,\mathbf{k}}-\xi_{n',\sigma,\mathbf{k}+\mathbf{q}}\right)^2}+\frac{1}{4}\frac{\beta\,\mathrm{csch}(\beta\Omega_\nu(\mathbf{q})/2)^2}{\Omega_\nu(\mathbf{q})+\xi_{n,\sigma,\mathbf{k}}-\xi_{n',\sigma,\mathbf{k}+\mathbf{q}}}\right] \\ & + \mathcal{O}(g^4)\end{aligned}$$

with real coefficients A_ν and B_ν defined as

$$A_\nu = \Omega_\nu(\mathbf{q}=\mathbf{0})\mathscr{G}_{0,\nu}^2(q=0) = \Omega_\nu^{-1}(\mathbf{q}=\mathbf{0}), \qquad B_\nu = \frac{1}{\sqrt{N_p}} \sum_{\substack{\mathbf{k}\in\mathrm{Q}\\ \sigma\in\{\downarrow,\uparrow\}\\ n\in\{1,\ldots,\infty\}}} g_{nn\nu}(\mathbf{k},0)\,\mathrm{F}_\beta(\xi_{n\mathbf{k}\sigma}) \tag{25.15}$$

whereas the terms of order $\mathcal{O}(g^4)$ are those that are being neglected when one approximates the Bethe-Salpeter-equation.

Proof 25.13 See Appendix, Proofs, page 616.

25.2.3. Total Crystal

The Interaction Contribution

Lemma 25.14 One obtains for the electron-phonon-interaction energy the identity

$$\begin{aligned}\langle H_{\mathrm{int}}\rangle &= \sum_{\substack{\mathbf{k},\mathbf{q}\in\mathrm{Q}\\ \sigma\in\{\uparrow,\downarrow\}\\ \nu\in\{1,\ldots,rd_{\mathrm{x}}\}\\ m,n\in\{1,\ldots,\infty\}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\sqrt{N_p}}\left\langle c^\dagger_{\mathbf{k}+\mathbf{q}m\sigma}c_{\mathbf{k}n\sigma}\left(b_{\mathbf{q}\nu}+b^\dagger_{-\mathbf{q}\nu}\right)\right\rangle \\ &= \sum_{\substack{k\in\mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ q\in\mathrm{i}\Omega_{+1}\times\mathrm{Q}\\ \sigma\in\{\downarrow,\uparrow\}\\ \nu\in\{1,2,\ldots,rd_{\mathrm{x}}\}\\ n,m\in\{1,\ldots,\infty\}\\ \omega_{n'}\in\Omega_{-1}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})\hbar}{\sqrt{N_p}\sqrt{\hbar\beta}^3}\left\langle\overline{\psi}_{m\sigma}(\mathrm{i}\omega_{n'},\mathbf{k}+\mathbf{q})\psi_{n\sigma}(\mathrm{i}\omega_n,\mathbf{k})\Big[\rho_\nu(q)\mathscr{G}_{0,\nu}(q)+\mathscr{G}_{0,\nu}(-q)\rho_\nu(q)\Big]\right\rangle\end{aligned} \tag{25.16}$$

Proof 25.14 See Appendix, Proofs, page 619.

Corollary 25.15 Simplifying the above expression with an approximation of the Bethe-Salpeter-equation, and evaluating the Matsubara-sums gives the two contributions

$$\langle H_{\text{int}} \rangle = \text{I} + \text{II} \tag{25.17}$$

Proof 25.15 See Appendix, Proofs, page 620.

Collecting all Contributions

Fact 25.16 For the electronic and phononic occupation numbers of the interacting system we have the identity

$$\langle H_{\text{el}} \rangle = \sum_{\substack{\mathbf{k}\in \text{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\}}} \epsilon_{m\mathbf{k}\sigma} \langle n_{m\mathbf{k}\sigma} \rangle = \frac{-1}{\pi} \lim_{\delta\to 0} \oint \sum_{\substack{\mathbf{k}\in \text{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\} \\ E\in(-\infty,+\infty)}} \epsilon_{m\mathbf{k}\sigma} \, \text{F}_\beta(E) \, \text{Im} \, G^{\text{ret}}_{\substack{m,m \\ \sigma,\sigma}}(E + \text{i}\delta, \mathbf{k}) \tag{25.18}$$

$$\begin{aligned}
\langle H_{\text{ph}} \rangle &= \sum_{\substack{\mathbf{q}\in \text{Q} \\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} \Omega_\nu(\mathbf{q}) \langle n_\nu(\mathbf{q}) \rangle \\
&\approx \sum_{\substack{\mathbf{q}\in \text{Q} \\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} \Omega_\nu(\mathbf{q}) \, \text{B}_\beta(\Omega_\nu(\mathbf{q})) \quad + \quad \sum_{\nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}} A_\nu B_\nu^2 \\
&- \sum_{\substack{\mathbf{k},\mathbf{q}\in \text{Q} \\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\} \\ n,n'\in\{1,\ldots,\infty\} \\ \sigma\in\{\downarrow,\uparrow\}}} \frac{\Omega_\nu(\mathbf{q})}{N_p} |g_{n'n\nu}(\mathbf{k},\mathbf{q})|^2 \left(\text{F}_\beta(\xi_{n,\sigma,\mathbf{k}}) - \text{F}_\beta(\xi_{n',\sigma,\mathbf{k}+\mathbf{q}})\right) \left[\frac{\text{B}_\beta(\Omega_\nu(\mathbf{q})) - \text{B}_\beta(\xi_{n',\sigma,\mathbf{k}+\mathbf{q}} - \xi_{n,\sigma,\mathbf{k}})}{\left(\Omega_\nu(\mathbf{q}) + \xi_{n,\sigma,\mathbf{k}} - \xi_{n',\sigma,\mathbf{k}+\mathbf{q}}\right)^2} + \frac{1}{4} \frac{\beta \, \text{csch}(\beta\Omega_\nu(\mathbf{q})/2)^2}{\Omega_\nu(\mathbf{q}) + \xi_{n,\sigma,\mathbf{k}} - \xi_{n',\sigma,\mathbf{k}+\mathbf{q}}} \right] \\
&+ \mathcal{O}(g^4)
\end{aligned} \tag{25.19}$$

$$\langle H_{\text{int}} \rangle = \text{TBDigitalized from PP3.} \tag{25.20}$$

Proof 25.16 See Appendix, Proofs, page 621.

The Molar Heat Capacity of the Interacting System

We combine Equations (9.59) and (9.52)

$$c_{N,T,V} = \frac{C_{N,V}(T)}{n} = \frac{1}{n} \partial_T \langle H \rangle_{N,T,V} \, . \tag{25.21}$$

Using now Equation (9.60) yields

$$\begin{aligned}
C_{N,V}(T) &= \partial_T \langle H \rangle (N,T,V) \\
&= \left(\partial_T \langle H \rangle\right)(\mu(T,V),T,V) + \left(\partial_\mu \langle H \rangle\right)(\mu(T,V),T,V) \cdot \left(\partial_T \mu\right)(N,V,T)
\end{aligned} \tag{25.22}$$

whereas the Hamiltonian is made up of three contributions

$$H = H_{\text{el}} + H_{\text{ph}} + H_{\text{int}}. \tag{25.23}$$

Therefore, also for the molar heat capacity, we have contributions from the electronic part, from the phononic part, and from the interaction part. We further need to account for the temperature derivative of the chemical potential. We consider all four quantities separately and then merge the results.

25.2.3.1. Temperature-Derivative of the Chemical Potential

Fact 25.17 We first notice that dictating the particle number (for example by requiring [C]harge [N]eutrality of the crystal) through Equation (24.26) can be rewritten as

$$F(\mu, T) \equiv \langle N \rangle(\mu, T) - N_{\text{CN}} = 0. \tag{25.24}$$

Remark 25.17.1 Notice that the chemical potential that is defined through this Equation is unique due to Theorem 9.37.

Corollary 25.18 Assuming now we have access[1] to the values $\mu(T)$ that fulfill Equation (25.24), we can compute the temperature derivative of the chemical potential as

$$\left(\frac{\partial \mu}{\partial T}\right)(T) = -\left(\frac{\partial_T F}{\partial_\mu F}\right)(\mu(T), T)\,. \tag{25.25}$$

Proof 25.18 Follows from the Theorem of implicit functions.

Lemma 25.19 The temperature-derivative of the function F can be computed as

$$\begin{aligned}\left(\partial_T F\right)(\mu, T) = \frac{-1}{\pi}\frac{\beta}{T}\lim_{\delta\to 0}\sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}\in \mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\} \\ E\in(-\infty,+\infty)}} \mathrm{F}_\beta(E)\,\mathrm{Im}\Bigg[\left(1-\mathrm{F}_\beta(E)\right) E \quad & \frac{1}{E+\mathrm{i}\delta-(\xi_{m\mathbf{k}\sigma}+\Sigma^{\text{ret}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta))} \\ + \quad & \frac{k_B T^2 \partial_T \Sigma_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta)}{\left(E+\mathrm{i}\delta-(\xi_{m\mathbf{k}\sigma}+\Sigma^{\text{ret}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta))\right)^2}\Bigg]\end{aligned} \tag{25.26}$$

with partial derivative of the retarded self-energy

$$k_B T^2 \partial_T \Sigma^{\text{ret}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta) \quad = \quad k_B T^2 \partial_T \Sigma^{\text{ret, H}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta) \quad + \quad k_B T^2 \partial_T \Sigma^{\text{ret, F}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta) \tag{25.27}$$

and invididual contributions

[1] Notice that this is the case, as we compute the chemical potential numerically.

$$k_B T^2 \partial_T \Sigma^{\text{ret, H}}_{m\sigma\mathbf{k}}(\bullet) = - \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ \sigma'\in\{\downarrow,\uparrow\} \\ n\in\{1,2,\dots\} \\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}}} \frac{g_{mm\nu}(\mathbf{k},0) g_{nn\nu}(\mathbf{q},0)}{4N_p} \frac{\xi_{n\sigma'\mathbf{q}}}{\Omega_\nu(\mathbf{q}'\equiv 0)} \operatorname{sech}^2\left(\frac{\xi_{n\sigma'\mathbf{q}}}{2k_{\mathrm{B}}T}\right) \tag{25.28}$$

and

$$\begin{aligned} k_B T^2 \partial_T \Sigma^{\text{ret, F}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta) = \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ n\in\{1,2,\dots,\infty\} \\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}}} \frac{|g_{nm\nu}(\mathbf{k},\mathbf{q})|^2}{4N_p} \Bigg[& \frac{\Omega_\nu(\mathbf{q}) \operatorname{csch}^2(\beta\Omega_\nu(\mathbf{q})/2) + \xi_{n,\sigma,\mathbf{k}+\mathbf{q}} \operatorname{sech}^2(\beta\xi_{n,\sigma,\mathbf{k}+\mathbf{q}}/2)}{E+\mathrm{i}\delta-\xi_{n,\sigma,\mathbf{k}+\mathbf{q}}+\Omega_\nu(\mathbf{q})} \\ & + \frac{\Omega_\nu(\mathbf{q}) \operatorname{csch}^2(\beta\Omega_\nu(\mathbf{q})/2) - \xi_{n,\sigma,\mathbf{k}+\mathbf{q}} \operatorname{sech}^2(\beta\xi_{n,\sigma,\mathbf{k}+\mathbf{q}}/2)}{E+\mathrm{i}\delta-\xi_{n,\sigma,\mathbf{k}+\mathbf{q}}-\Omega_\nu(\mathbf{q})} \Bigg] \end{aligned} \tag{25.29}$$

Proof 25.19 See Appendix, Proofs, page 622.

Lemma 25.20 The chemical-potential-derivative of the function F can be computed as

$$\begin{aligned} \left(\partial_\mu F\right)(\mu,T) = \frac{-1}{\pi}\frac{\beta}{4} \lim_{\delta\to 0} \oint \sum_{\substack{\mathbf{k}\in \mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\dots,\infty\} \\ E\in(-\infty,+\infty)}} \mathrm{Im}\Bigg[& \operatorname{sech}^2\left(\frac{\beta E}{2}\right) \frac{1}{E+\mathrm{i}\delta-(\xi_{m\mathbf{k}\sigma}+\Sigma^{\text{ret}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta))} \\ & + \mathrm{F}_\beta(E)\cdot \frac{\sigma_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta)}{\left(E+\mathrm{i}\delta-(\xi_{m\mathbf{k}\sigma}+\Sigma^{\text{ret}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta))\right)^2} \Bigg] \end{aligned} \tag{25.30}$$

with auxiliary function

$$\sigma_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta) = \sigma^{\text{Hartree}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta) + \sigma^{\text{Fock}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta), \tag{25.31}$$

with the Hartree-contribution

$$\sigma^{\text{Hartree}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta) = - \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ \sigma'\in\{\downarrow,\uparrow\} \\ n\in\{1,2,\dots\} \\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}}} \frac{g_{mm\nu}(\mathbf{k},0) g_{nn\nu}(\mathbf{q},0)}{N_p} \frac{1}{\Omega_\nu(\mathbf{q}'=0)} \operatorname{sech}^2\left(\beta\xi_{n\sigma'\mathbf{q}}/2\right) \tag{25.32}$$

and the Fock-contribution

$$\sigma^{\text{Fock}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta) = \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ n\in\{1,2,\dots\} \\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}}} \frac{|g_{nm\nu}(\mathbf{k},\mathbf{q})|^2}{N_p} \operatorname{sech}^2(\beta\xi_{\mathbf{q}+\mathbf{k}n\sigma}/2) \left[\frac{1}{E+\mathrm{i}\delta-\xi_{\mathbf{q}+\mathbf{k}n\sigma}+\Omega_\nu(\mathbf{q})} - \frac{1}{E+\mathrm{i}\delta-\xi_{\mathbf{q}+\mathbf{k}n\sigma}-\Omega_\nu(\mathbf{q})}\right] \tag{25.33}$$

Proof 25.20 See Appendix, Proofs, page 623.

25.2.3.2. Temperature-Derivative of the Electronic Energy

Lemma 25.21 The temperature-derivatives of the electronic contribution to the internal energy can be computed as

$$\partial_T \langle H_{\mathrm{el}} \rangle = \frac{-1}{\pi} \frac{1}{k_B T^2} \lim_{\delta \to 0} \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k} \in \mathrm{Q} \\ \sigma \in \{\uparrow,\downarrow\} \\ m \in \{1,\ldots,\infty\} \\ E \in (-\infty,+\infty)}} \epsilon_{m\mathbf{k}\sigma} \, \mathrm{F}_\beta(E) \, \mathrm{Im} \Bigg[\left(1 - \mathrm{F}_\beta(E)\right) E \frac{1}{E + \mathrm{i}\delta - (\xi_{m\mathbf{k}\sigma} + \Sigma^{\mathrm{ret}}_{m\sigma\mathbf{k}}(E + \mathrm{i}\delta))} + \frac{k_B T^2 \partial_T \Sigma^{\mathrm{ret}}_{m\sigma\mathbf{k}}(E + \mathrm{i}\delta)}{\left(E + \mathrm{i}\delta - (\xi_{m\mathbf{k}\sigma} + \Sigma^{\mathrm{ret}}_{m\sigma\mathbf{k}}(E + \mathrm{i}\delta, \mathbf{k}))\right)^2} \Bigg] \tag{25.34}$$

with partial derivative of the retarded self-energy as in Equation (25.29)

Proof 25.21 See Appendix, Proofs, page 625.

Remark 25.21.1 Notice that this is the very same Equation as (25.26), except for the factor of $\epsilon_{m\mathbf{k}\sigma}$ in the integrand-summand.

Lemma 25.22 The chemical-potential-derivative of the electronic contribution to the internal energy can be computed as

$$\partial_\mu \langle H_{\mathrm{el}} \rangle = \frac{-1}{\pi} \frac{\beta}{4} \lim_{\delta \to 0} \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k} \in \mathrm{Q} \\ \sigma \in \{\uparrow,\downarrow\} \\ m \in \{1,\ldots,\infty\} \\ E \in (-\infty,+\infty)}} \epsilon_{m\mathbf{k}\sigma} \, \mathrm{Im} \Bigg[\mathrm{sech}^2\left(\frac{\beta E}{2}\right) \frac{1}{E + \mathrm{i}\delta - (\xi_{m\mathbf{k}\sigma} + \Sigma^{\mathrm{ret}}_{m\sigma\mathbf{k}}(E + \mathrm{i}\delta))} + \mathrm{F}_\beta(E) \cdot \frac{\sigma_{m\sigma\mathbf{k}}(E + \mathrm{i}\delta)}{\left(E + \mathrm{i}\delta - (\xi_{m\mathbf{k}\sigma} + \Sigma^{\mathrm{ret}}_{m\sigma\mathbf{k}}(E + \mathrm{i}\delta))\right)^2} \Bigg] \tag{25.35}$$

with auxiliary function

$$\sigma_{m\sigma\mathbf{k}}(E + \mathrm{i}\delta) = \sigma^{\mathrm{Hartree}}_{m\sigma\mathbf{k}}(E + \mathrm{i}\delta) + \sigma^{\mathrm{Fock}}_{m\sigma\mathbf{k}}(E + \mathrm{i}\delta), \tag{25.36}$$

as above.

Proof 25.22 Completely analogous to the proof of Lemma 25.20.

25.2.3.3. Temperature-Derivative of the Phononic Energy

Lemma 25.23 The temperature-derivatives of the non-interacting phononic contribution to the internal energy can be computed as

$$\partial_T \langle H_{\text{ph}} \rangle_0 = \frac{1}{4k_B T^2} \sum_{\substack{\mathbf{q}\in \text{Q} \\ \nu \in \{1,2,\ldots,rd_{\mathbf{x}}\}}} \left[\Omega_\nu(\mathbf{q}) \operatorname{csch}(\beta\Omega_\nu(\mathbf{q})/2)\right]^2 \tag{25.37}$$

and for the interacting phononic correction contribution

$$\begin{aligned}
&\partial_T \delta\langle H_{\text{ph}} \rangle \\
&\approx 2 \sum_{\nu \in \{1,2,\ldots,rd_{\mathbf{x}}\}} A_\nu B_\nu \partial_T B_\nu \\
&+ \frac{-1}{N_p} \sum_{\substack{\mathbf{k},\mathbf{q}\in \text{Q} \\ n,n' \in \{1,\ldots,\infty\} \\ \sigma \in \{\downarrow,\uparrow\} \\ \nu \in \{1,2,\ldots,rd_{\mathbf{x}}\}}} \frac{\Omega_\nu(\mathbf{q}) |g_{n'n\nu}(\mathbf{k},\mathbf{q})|^2}{4k_B T^2} \left(\text{F}_\beta(\xi_{n,\sigma,\mathbf{k}}) - \text{F}_\beta(\xi_{n',\sigma,\mathbf{k}+\mathbf{q}})\right) \frac{\operatorname{csch}^2(\beta\Omega_\nu(\mathbf{q})/2)}{\Omega_\nu(\mathbf{q}) + \xi_{n,\sigma,\mathbf{k}} - \xi_{n',\sigma,\mathbf{k}+\mathbf{q}}} \left(\beta\Omega_\nu(\mathbf{q}) \coth\left(\beta\Omega_\nu(\mathbf{q})/2\right) - 1\right) \\
&+ \frac{-1}{N_p} \sum_{\substack{\mathbf{k},\mathbf{q}\in \text{Q} \\ n,n' \in \{1,\ldots,\infty\} \\ \sigma \in \{\downarrow,\uparrow\} \\ \nu \in \{1,2,\ldots,rd_{\mathbf{x}}\}}} \frac{\Omega_\nu(\mathbf{q}) |g_{n'n\nu}(\mathbf{k},\mathbf{q})|^2}{4k_B T^2} \left(\text{F}_\beta(\xi_{n,\sigma,\mathbf{k}}) - \text{F}_\beta(\xi_{n',\sigma,\mathbf{k}+\mathbf{q}})\right) \left[\frac{\Omega_\nu(\mathbf{q}) \operatorname{csch}^2\left(\beta\Omega_\nu(\mathbf{q})/2\right) - (\xi_{n',\sigma,\mathbf{k}+\mathbf{q}} - \xi_{n,\sigma,\mathbf{k}}) \operatorname{csch}^2\left(\frac{\xi_{n',\sigma,\mathbf{k}+\mathbf{q}} - \xi_{n,\sigma,\mathbf{k}}}{2k_B T}\right)}{\left(\Omega_\nu(\mathbf{q}) + \xi_{n,\sigma,\mathbf{k}} - \xi_{n',\sigma,\mathbf{k}+\mathbf{q}}\right)^2}\right] \\
&+ \frac{-1}{N_p} \sum_{\substack{\mathbf{k},\mathbf{q}\in \text{Q} \\ n,n' \in \{1,\ldots,\infty\} \\ \sigma \in \{\downarrow,\uparrow\} \\ \nu \in \{1,2,\ldots,rd_{\mathbf{x}}\}}} \frac{\Omega_\nu(\mathbf{q}) |g_{n'n\nu}(\mathbf{k},\mathbf{q})|^2}{4k_B T^2} \left(\xi_{n,\sigma,\mathbf{k}} \operatorname{sech}^2\left(\beta\xi_{n,\sigma,\mathbf{k}}/2\right) - \xi_{n',\sigma,\mathbf{k}+\mathbf{q}} \operatorname{sech}^2\left(\beta\xi_{n',\sigma,\mathbf{k}+\mathbf{q}}/2\right)\right) \left[\frac{\text{B}_\beta(\Omega_\nu(\mathbf{q})) - \text{B}_\beta(\xi_{n',\sigma,\mathbf{k}+\mathbf{q}} - \xi_{n,\sigma,\mathbf{k}})}{\left(\Omega_\nu(\mathbf{q}) + \xi_{n,\sigma,\mathbf{k}} - \xi_{n',\sigma,\mathbf{k}+\mathbf{q}}\right)^2} + \frac{1}{4} \frac{\beta \operatorname{csch}(\beta\Omega_\nu(\mathbf{q})/2)^2}{\Omega_\nu(\mathbf{q}) + \xi_{n,\sigma,\mathbf{k}} - \xi_{n',\sigma,\mathbf{k}+\mathbf{q}}}\right]
\end{aligned} \tag{25.38}$$

with partial derivative

$$\partial_T B_\nu = \frac{1}{\sqrt{N_p}} \frac{\xi_{n,\sigma,\mathbf{k}}}{4k_B T^2} \sum_{\substack{\mathbf{k}\in \text{Q} \\ n \in \{1,2,\ldots,\infty\} \\ \sigma \in \{\downarrow,\uparrow\}}} g_{nn\nu}(\mathbf{k},0) \operatorname{sech}^2\left(\beta\xi_{n,\sigma,\mathbf{k}}/2\right) \tag{25.39}$$

Proof 25.23 See Appendix, Proofs, page 626.

Lemma 25.24 For the chemical potential-derivative of the phononic correction-term we obtain

$$\begin{aligned}
&\partial_\mu \delta\langle H_{\text{ph}} \rangle \\
&\approx 2 \sum_{\nu \in \{1,2,\ldots,rd_{\mathbf{x}}\}} A_\nu B_\nu \partial_\mu B_\nu \\
&- \sum_{\substack{\mathbf{k},\mathbf{q}\in \text{Q} \\ \nu \in \{1,2,\ldots,rd_{\mathbf{x}}\} \\ n,n' \in \{1,\ldots,\infty\} \\ \sigma \in \{\downarrow,\uparrow\}}} \frac{\beta}{4} \frac{\Omega_\nu(\mathbf{q})}{N_p} |g_{n'n\nu}(\mathbf{k},\mathbf{q})|^2 \left(\operatorname{sech}^2(\beta\xi_{n,\sigma,\mathbf{k}}/2) - \operatorname{sech}^2(\beta\xi_{n',\sigma,\mathbf{k}+\mathbf{q}}/2)\right) \left[\frac{\text{B}_\beta(\Omega_\nu(\mathbf{q})) - \text{B}_\beta(\xi_{n',\sigma,\mathbf{k}+\mathbf{q}} - \xi_{n,\sigma,\mathbf{k}})}{\left(\Omega_\nu(\mathbf{q}) + \xi_{n,\sigma,\mathbf{k}} - \xi_{n',\sigma,\mathbf{k}+\mathbf{q}}\right)^2} + \frac{1}{4} \frac{\beta \operatorname{csch}(\beta\Omega_\nu(\mathbf{q})/2)^2}{\Omega_\nu(\mathbf{q}) + \xi_{n,\sigma,\mathbf{k}} - \xi_{n',\sigma,\mathbf{k}+\mathbf{q}}}\right] \\
&+ \mathcal{O}(g^4)
\end{aligned}$$

and partial derivative

$$\partial_\mu B_\nu = \frac{1}{\sqrt{N_p}} \frac{\beta}{4} \sum_{\substack{\mathbf{k} \in \mathrm{Q} \\ n \in \{1,2,\ldots,\infty\} \\ \sigma \in \{\downarrow,\uparrow\}}} g_{nn\nu}(\mathbf{k}, 0) \operatorname{sech}^2\left(\beta \xi_{n,\sigma,\mathbf{k}}/2\right) \tag{25.40}$$

Proof 25.24 We use Equation (25.19) and note that we obtain with Lemma (9.63) and the chain-rule the identity

$$\partial_\mu \mathrm{F}_\beta(\xi_{n,\sigma,\bullet}) = \frac{\beta}{4} \operatorname{sech}^2\left(\beta \xi_{n,\sigma,\bullet}/2\right) \tag{25.41}$$

25.2.3.4. Temperature-Derivative of the Interaction Energy

Since this contribution only becomes relevant for crystals with more than one atom in the unit-cell (which we are not considering here, for simplicity), we omit a final, perfectly simplified expression and simply point out that one obtains an expression by taking the temperature-derivative of Equation (25.20).

26. Superconductivity

General Remarks

Apart from the toy-model for BCS-theory in section 30.2, we will introduce two formalisms for superconductivity.

1. The Eliashberg-Theory (ET for short),
2. The Path-Integral-Formalism for ([G]eneralized) [E]liashberg-[T]heory (GET / ET for short).

The strength and beauty in the path-integral-approach lies in the fact that it is carried out analogously to BCS-theory and reproduces the already established behavior for the order-parameters as a function of temperature. Further it reproduces and even opens the possibility to generalize Eliashberg-Theory in the appropriate limits. The path-integral-formalism can be considered as a generalization / unification of these theories. Another folklore-statement that is being reproduced is that superconductivity originates from an attractive interaction[1] that is mediated through phonons.

Fact 26.1 For "Eliashberg-theory" (to be introduced below), we consider the Hamiltonian from Definition 8.36, i.e. a system of electrons and phonons with only electron-phonon-interactions

$$H = \sum_{\substack{\mathbf{k}\in Q \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\dots,\infty\}}} \epsilon_{m\sigma}(\mathbf{k}) c^\dagger_{m\sigma}(\mathbf{k}) c_{m\sigma}(\mathbf{k}) + \sum_{\substack{\mathbf{q}\in Q \\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} \Omega_\nu(\mathbf{q}) b^\dagger_\nu(\mathbf{q}) b_\nu(\mathbf{q}) + \sum_{\substack{\mathbf{k},\mathbf{q}\in Q \\ \sigma\in\{\uparrow,\downarrow\} \\ \nu\in\{1,\dots,rd_{\mathbf{x}}\} \\ m,n\in\{1,\dots,\infty\}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\sqrt{N_p}} c^\dagger_{m\sigma}(\mathbf{k}+\mathbf{q}) c_{n\sigma}(\mathbf{k}) \left(b_\nu(\mathbf{q}) + b^\dagger_\nu(-\mathbf{q})\right) \tag{26.1}$$

Remark 26.1.1 The concept of "superconductivity" also extends to generalizations of this Hamiltonian. E.g. Hamiltonians that include more interactions, as in Defintions 8.39 and 8.40.

26.1. Phononic Eliashberg-Theory in the Operator-Formalism

26.1.1. An Operator-Expectation-Value like no Other

Fact 26.2 For normal-state systems, we introduced an expectation-value w.r.t. a density matrix in Definition 9.8. Then we introduced the natural density matrix in the natural ensemble in Equation (10.6) as *the* density matrix that we need to use in equilibrium systems in which no symmetries are being broken spontaneously, and we realized, that in hybrid ensembles one needs to have a generalization as in Equation (10.11). It was exactly *this* density

[1] Note however that contrary to the folklore, this interaction is attractive *not only* close to the Fermi-surface, but for all energies. But it will turn later out, that only those electronic energies close to the Fermi-surface and hence only those interactions will contribute to the emergence of superconductivity, cf. Theorem 26.70.

matrix, that allowed us to conlcude the translational invariance of the Green-functions and their (anti)-periodicity in Theorem 13.2. It was also *this* density matrix, that allowed us to draw *all* of the conclusions in Chapter 14.

Now we need to introduce the concept of spontaneous symmetry breaking, which is basically impossible to do properly (i.e. mathematically "clean") in the operator-formalism. (In contrast: In the path-integral description it will come quite natural from saddle-point-approximations.)

Hypothesis 26.3 For an operator in second quantization $A \equiv A(c, c^\dagger, b, b^\dagger)$ and for *low enough temperatures*[2], i.e. $0 < T < T_{\text{SC}}$ we assume the existence of a mapping

$$A \mapsto \langle A \rangle_{\text{SC}} \in \mathbb{C} \tag{26.2}$$

which we call *the expectation-value in the [S]uper-[C]onducting state*, and we assume that for this expectation-value "the U(1) symmetry is spontaneously broken". We further *assume* ...

1. that this mapping is compatible with linearity and scalar-multiplication, i.e. for scalars $a, b \in \mathbb{C}$ and operators A, B we have

$$\langle aA + bB \rangle_{\text{SC}} = a \langle A \rangle_{\text{SC}} + b \langle B \rangle_{\text{SC}} \tag{26.3}$$

2. that this mapping obeys

$$\langle A \rangle_{\text{SC}}^* = \left\langle A^\dagger \right\rangle_{\text{SC}} \tag{26.4}$$

Remark 26.3.1 Notice again that both requirements are relatively easy to prove in the normal state (cf. e.g. Lemma 9.9), for which one has the density in Equation (10.11), but it is *a priori* not clear why it would also hold in the superconducting state, since we do not know a priori whether the superconducting state is eligible to be treated in the density-formalism. In fact one rarely (never?) sees a density for the "superconducting state" in the literature. It is the authors opinion, that the *only* way of describing superconductors "appropriately" is through the field integral formalism.

Remark 26.3.2 Now we come into the problematic situation that we need to explain the implications of the vague statement "broken U(1) symmetry" above, which happens to be *completely natural* to see in the field integral formalism, but *it seems like stating arbitrary facts* in the operator-formalism. It is also in the field-integral formalism, where it is justified that we look at the so-called "Gorkov-Green-function" (to be introduced below) and why we obtain generalizations of the Bethe-Salpeter-equation (TBReferenced , cf. Theorem 15.16) (due to the effective action formalism!), but it seems *almost random* to do these things if one works in the operator-formalism.

[2]Subject to a given material; This temperature is material-specific and may be zero Kelvin.

26.1.2. Eliashbergs Preparations

Definition 26.4 We define[3] the *single-band Gorkov-Green-function* as

$$\widehat{\mathscr{G}}_{\substack{m \\ \text{Gorkov}}}(\tau, \mathbf{k}; \tau' \mathbf{k}') = -\frac{1}{\hbar} \begin{pmatrix} \left\langle \mathrm{T}_\tau \, c_{m,\uparrow}(\tau, \mathbf{k}) c^\dagger_{m,\uparrow}(\tau', \mathbf{k}') \right\rangle_{\mathrm{SC}} & \left\langle \mathrm{T}_\tau \, c_{m,\uparrow}(\tau, \mathbf{k}) c_{m,\downarrow}(\tau', -\mathbf{k}') \right\rangle_{\mathrm{SC}} \\ \left\langle \mathrm{T}_\tau \, c^\dagger_{m,\downarrow}(\tau, -\mathbf{k}) c^\dagger_{m,\uparrow}(\tau', \mathbf{k}') \right\rangle_{\mathrm{SC}} & \left\langle \mathrm{T}_\tau \, c^\dagger_{m,\downarrow}(\tau, -\mathbf{k}) c_{m,\downarrow}(\tau', -\mathbf{k}') \right\rangle_{\mathrm{SC}} \end{pmatrix} \tag{26.5}$$

Remark 26.4.1 Notice that inside the time-ordering-operator, the exchange of two fermionic operators yields a minus sign.

Remark 26.4.2 The off-diagonal components are usually called *Gorkov's anomalous Green-functions*.

Remark 26.4.3 Gorkov's anomalous Green-functions are only non-zero in the superconducting phase[4]. Evaluating these expressions w.r.t. the thermal state yields zero[5].

Fact 26.5 What we mean, with a "broken U(1) symmetry", is that the off-diagonal components of this expectation-value are not neccessarily equal to zero. All the other symmetries of the underlying action (and therefore, due to section 26.2, also of the underlying Green-function) are preserved. We have in particular ...

- that this Green-function is diagonal in the momentum-indices, i.e. it is spatial-translation symmetric

$$\widehat{\mathscr{G}}_{\substack{m \\ \text{Gorkov}}}(\tau, \mathbf{k}; \tau' \mathbf{k}') \equiv \delta_{\mathbf{k},\mathbf{k}'} \widehat{\mathscr{G}}_{\substack{m\mathbf{k} \\ \text{Gorkov}}}(\tau, \tau') \tag{26.6}$$

- that this Green-function depends only on time-differences, i.e. the system is time-translation symmetric, i.e.

$$\widehat{\mathscr{G}}_{\substack{m\mathbf{k} \\ \text{Gorkov}}}(\tau, \tau') = \widehat{\mathscr{G}}_{\substack{m\mathbf{k} \\ \text{Gorkov}}}(\tau - \tau', 0) = \widehat{\mathscr{G}}_{\substack{m\mathbf{k} \\ \text{Gorkov}}}(0, \tau' - \tau) \equiv \widehat{\mathscr{G}}_{\substack{m\mathbf{k} \\ \text{Gorkov}}}(\tau - \tau') \tag{26.7}$$

- that this Green-function obeys the anti-periodicity relation that one has in the normal state: It holds for all wavevectors $\mathbf{k} \in \mathrm{Q}$ and bands $m \in \{1, 2, 3, \ldots, \infty\}$ the identity

$$\forall \tau \in (-\hbar\beta, 0): \quad \widehat{\mathscr{G}}_{\substack{m\mathbf{k} \\ \text{Gorkov}}}(\tau + \hbar\beta) = -\widehat{\mathscr{G}}_{\substack{m\mathbf{k} \\ \text{Gorkov}}}(\tau) \tag{26.8}$$

[3] Notice that we are following the prefactor-convention of 03-Marsiglio, Eqs. (43-44), and [7] page 519 Equations (14.158), or Polaron-Physics 07, p. 16 in contrast to [32] page 635, Eq. (10.31). Notice further that our Equations are in harmony with Allens long article on pages 8 and 33 and Equation (7.2) in particular.

[4] Quoting [32] p. 635:

A basic feature of the BCS ground state (...) is that it is composed of a superposition of electronic states containing a different number of electrons. Such a formulation is possible in a grand canonical ensemble.

[5] Easy to prove, but also quoting [38] p. 77:

The expectation value of two creation or annihilation operators is zero in a state of definite particle number.

Remark 26.5.1 We again emphasize: A priori it is not clear why these relations would hold. When we re-derive the Eliashberg-equations later on in the path-integral formalism (when we introduce a so-called "Hubbard-Stratanovich-transformation" and apply a so-called "saddle-point-approximation") we will realise that the preservation of translational invariance and antiperiodicity is a natural consequence of breaking the $U(1)$-symmetry but no other symmetry. Strictly speaking this assumption was a leap of faith when Eliashberg derived his equations (because the functional integral formalism was not invented / discovered back then).

26.1.3. Gorkovs Generalized Hermiticity Relation

Diagonal Components

Notation 26.6 We write

$$\widehat{\mathscr{G}}_{\substack{m \\ 11 \\ \text{Gorkov}}}(\tau, \mathbf{k}) \equiv \mathscr{G}_{\substack{m \\ \text{Gorkov}}}(\tau, \mathbf{k}) \tag{26.9}$$

Lemma 26.7 For a spin-degenerate system, it follows that

$$\widehat{\mathscr{G}}_{\substack{m \\ 22 \\ \text{Gorkov}}}(\tau, \mathbf{k}) \equiv -\mathscr{G}_{\substack{m \\ \text{Gorkov}}}(-\tau, -\mathbf{k}) \tag{26.10}$$

Proof 26.7

For this purpose we TEMPORARILY define for $\sigma \in \{\uparrow, \downarrow\}$ the spin-resolved auxiliary Green-function

$$\mathscr{G}_{\substack{m\sigma \\ \text{aux-Gorkov}}}(\tau, \mathbf{k}) \equiv -\frac{1}{\hbar}\left\langle \mathrm{T}_\tau\, c_{m,\sigma}(\tau, \mathbf{k}) c^\dagger_{m,\sigma}(0, \mathbf{k})\right\rangle_{\mathrm{SC}}, \qquad \text{such that} \qquad \mathscr{G}_{\substack{m\uparrow \\ \text{aux-Gorkov}}} = \mathscr{G}_{\substack{m \\ \text{Gorkov}}}.$$

Step 1: Use the translation-invariance in time. The "2,2"-component of Equation (26.11) gives

$$\begin{aligned}\widehat{\mathscr{G}}_{\substack{m \\ 22 \\ \text{Gorkov}}}(\tau, \mathbf{k}) &= -\frac{1}{\hbar}\left\langle \mathrm{T}_\tau\, c^\dagger_{m,\downarrow}(\tau, -\mathbf{k}) c_{m,\downarrow}(0, -\mathbf{k})\right\rangle_{\mathrm{SC}} \\ &\overset{\text{Eq. (26.11)}}{=} -\frac{1}{\hbar}\left\langle \mathrm{T}_\tau\, c^\dagger_{m,\downarrow}(0, -\mathbf{k}) c_{m,\downarrow}(-\tau, -\mathbf{k})\right\rangle_{\mathrm{SC}} = \dots\end{aligned}$$

Step 2: Exchange inside the time-ordering. Exchanging the two fermionic operators inside T_τ yields a minus sign, hence

$$\widehat{\mathscr{G}}_{\substack{m \\ 22 \\ \text{Gorkov}}}(\tau, \mathbf{k}) = \dots = +\frac{1}{\hbar}\left\langle \mathrm{T}_\tau\, c_{m,\downarrow}(-\tau, -\mathbf{k}) c^\dagger_{m,\downarrow}(0, -\mathbf{k})\right\rangle_{\mathrm{SC}} = -\mathscr{G}_{\substack{m\downarrow \\ \text{aux-Gorkov}}}(-\tau, -\mathbf{k}).$$

Step 3: Spin-degeneracy. By assumption (cf. also Lemma 26.13) the system is spin-degenerate, i.e. the spin-rotation symmetry is *not* broken in the superconducting state. Hence we have $\mathscr{G}_{\substack{m\downarrow \\ \text{aux-Gorkov}}} = \mathscr{G}_{\substack{m\uparrow \\ \text{aux-Gorkov}}} = \mathscr{G}_{\substack{m \\ \text{Gorkov}}}$, and therefore

$$\widehat{\mathscr{G}}_{\substack{m \\ 22 \\ \text{Gorkov}}}(\tau,\mathbf{k}) = \ldots = -\mathscr{G}_{\substack{m\downarrow \\ \text{aux-Gorkov}}}(-\tau,-\mathbf{k}) = -\mathscr{G}_{\substack{m \\ \text{Gorkov}}}(-\tau,-\mathbf{k}).$$

Off Diagonal Components

Corollary 26.8 The translation invariance implies

$$\widehat{\mathscr{G}}_{\substack{m \\ \text{Gorkov}}}(\tau,0,\mathbf{k}) \equiv \widehat{\mathscr{G}}_{\substack{m \\ \text{Gorkov}}}(\tau,\mathbf{k}) \equiv \widehat{\mathscr{G}}_{\substack{m \\ \text{Gorkov}}}(0,-\tau,\mathbf{k}) \tag{26.11}$$

Proof 26.8 Follows immediately from repeated application of Equation (26.7).

Remark 26.8.1 Notice that Equation (26.11) yields e.g. for the "2,1"-component of the Gorkov'matrix

$$\left\langle \mathrm{T}_\tau\, c^\dagger_{m,\downarrow}(\tau,-\mathbf{k}) c^\dagger_{m,\uparrow}(0,\mathbf{k}) \right\rangle_{\mathrm{SC}} = \left\langle \mathrm{T}_\tau\, c^\dagger_{m,\downarrow}(0,-\mathbf{k}) c^\dagger_{m,\uparrow}(-\tau,\mathbf{k}) \right\rangle_{\mathrm{SC}} \tag{26.12}$$

which yields in particular for $\tau > 0$ the identity

$$\left\langle c^\dagger_{m,\downarrow}(\tau,-\mathbf{k}) c^\dagger_{m,\uparrow}(0,\mathbf{k}) \right\rangle_{\mathrm{SC}} = \left\langle c^\dagger_{m,\downarrow}(0,-\mathbf{k}) c^\dagger_{m,\uparrow}(-\tau,\mathbf{k}) \right\rangle_{\mathrm{SC}} \tag{26.13}$$

which is a highly non-trivial identity / assumption.

Notation 26.9 We now introduce the anomalous Gor'kov Green-function as

$$\widehat{\mathscr{G}}_{\substack{m \\ 12 \\ \text{Gorkov}}}(\tau,\mathbf{k}) \equiv \mathscr{F}_m(\tau,\mathbf{k}) \tag{26.14}$$

Before we prove the one relation that nobody in the literature seems to be able to write down properly, we need to recall the fact that for creation and annihilation-operators, we find their hermitian adjoints as $[c(\tau)]^\dagger = c^\dagger(-\tau)$, etc.

Lemma 26.10 We will prove now that

$$\widehat{\mathscr{G}}_{\substack{m \\ 21 \\ \text{Gorkov}}}(\tau,\mathbf{k}) = \widehat{\mathscr{G}}^*_{\substack{m \\ 12 \\ \text{Gorkov}}}(\tau,\mathbf{k}) = \mathscr{F}^*_m(\tau,\mathbf{k}) \equiv \mathscr{F}^\dagger_m(\tau,\mathbf{k}) \tag{26.15}$$

Proof 26.10

In order to prove this, we just use the very definitions

Case 1: $\tau > 0$

When we can omit the time-ordering operator and we obtain

$$\begin{aligned}\hat{\mathscr{G}}_{\substack{m\\21\\\text{Gorkov}}}(\tau,\mathbf{k}) &= -\frac{1}{\hbar}\langle \mathrm{T}_\tau\, c^\dagger_{m,\downarrow}(\tau,-\mathbf{k})c^\dagger_{m,\uparrow}(0,\mathbf{k})\rangle_{\mathrm{SC}}\\ &= -\frac{1}{\hbar}\langle c^\dagger_{m,\downarrow}(\tau,-\mathbf{k})c^\dagger_{m,\uparrow}(0,\mathbf{k})\rangle_{\mathrm{SC}}\\ &\overset{\text{Eq. (26.13)}}{=} -\frac{1}{\hbar}\langle c^\dagger_{m,\downarrow}(0,-\mathbf{k})c^\dagger_{m,\uparrow}(-\tau,\mathbf{k})\rangle_{\mathrm{SC}}\\ &= \Big[-\frac{1}{\hbar}\langle c_{m,\uparrow}(+\tau,\mathbf{k})c_{m,\downarrow}(0,-\mathbf{k})\rangle_{\mathrm{SC}}\Big]^\dagger\\ &= \Big[\hat{\mathscr{G}}_{\substack{m\\12\\\text{Gorkov}}}(\tau,\mathbf{k})\Big]^\dagger\end{aligned}$$

Case 2: $\tau < 0$

Analogous. TBDone.

Note on Case 1. For a complex number, $[\,\cdot\,]^\dagger$ means complex conjugation; the fourth equation sign uses

$$[c^\dagger_{m,\downarrow}(0,-\mathbf{k})c^\dagger_{m,\uparrow}(-\tau,\mathbf{k})]^\dagger = c_{m,\uparrow}(\tau,\mathbf{k})c_{m,\downarrow}(0,-\mathbf{k})$$

(with $[c^\dagger(-\tau)]^\dagger = c(\tau)$) and the second requirement of the Hypothesis, $\langle A\rangle^*_{\mathrm{SC}} = \langle A^\dagger\rangle_{\mathrm{SC}}$. Since $\tau > 0$, the time-ordering in $\mathscr{F}_m(\tau,\mathbf{k})$ is trivial as well.

Case 2 written out. For $\tau < 0$ the time-ordering puts the operator at time 0 to the left and produces a minus sign. With the time-translation invariance (by $-\tau$) and the same steps as in Case 1 we find

$$\begin{aligned}\hat{\mathscr{G}}_{\substack{m\\21\\\text{Gorkov}}}(\tau,\mathbf{k}) &= +\frac{1}{\hbar}\langle c^\dagger_{m,\uparrow}(0,\mathbf{k})c^\dagger_{m,\downarrow}(\tau,-\mathbf{k})\rangle_{\mathrm{SC}} = +\frac{1}{\hbar}\langle c^\dagger_{m,\uparrow}(-\tau,\mathbf{k})c^\dagger_{m,\downarrow}(0,-\mathbf{k})\rangle_{\mathrm{SC}}\\ &= \Big[+\frac{1}{\hbar}\langle c_{m,\downarrow}(0,-\mathbf{k})c_{m,\uparrow}(\tau,\mathbf{k})\rangle_{\mathrm{SC}}\Big]^* = \Big[-\frac{1}{\hbar}\langle \mathrm{T}_\tau\, c_{m,\uparrow}(\tau,\mathbf{k})c_{m,\downarrow}(0,-\mathbf{k})\rangle_{\mathrm{SC}}\Big]^* = \mathscr{F}^*_m(\tau,\mathbf{k}).\end{aligned}$$

Fact 26.11 We recall[6] from the last subsection, the *single-band Gorkov-Green-function* as

$$\hat{\mathscr{G}}_{\substack{m\\\text{Gorkov}}}(\tau,\mathbf{k}) = -\frac{1}{\hbar}\begin{pmatrix}\big\langle \mathrm{T}_\tau\, c_{m,\uparrow}(\tau,\mathbf{k})c^\dagger_{m,\uparrow}(0,\mathbf{k})\big\rangle_{\mathrm{SC}} & \big\langle \mathrm{T}_\tau\, c_{m,\uparrow}(\tau,\mathbf{k})c_{m,\downarrow}(0,-\mathbf{k})\big\rangle_{\mathrm{SC}}\\ \big\langle \mathrm{T}_\tau\, c^\dagger_{m,\downarrow}(\tau,-\mathbf{k})c^\dagger_{m,\uparrow}(0,\mathbf{k})\big\rangle_{\mathrm{SC}} & \big\langle \mathrm{T}_\tau\, c^\dagger_{m,\downarrow}(\tau,-\mathbf{k})c_{m,\downarrow}(0,-\mathbf{k})\big\rangle_{\mathrm{SC}}\end{pmatrix} \equiv \begin{pmatrix}\mathscr{G}_{\substack{m\\\text{Gorkov}}}(\tau,\mathbf{k}) & \mathscr{F}_m(\tau,\mathbf{k})\\ \mathscr{F}^\dagger_m(\tau,\mathbf{k}) & -\mathscr{G}_{\substack{m\\\text{Gorkov}}}(-\tau,-\mathbf{k})\end{pmatrix}$$

[6] Notice that we are following the prefactor-convention of [34], Eqs. (43-44), and Coleman page 519 Equations (14.158), or [24], p. 16 in contrast to Mahan3rd page 635, Eq. (10.31). Notice further that our Equations are in harmony with Allens long article on pages 8 and 33 and Equation (7.2) in particular.

26.1.4. Gorkov-Green-Functions in the Matsubara-Formalism

Lemma 26.12 In the Matsubara-representation one has the equation

$$\widehat{\mathscr{G}}_{\substack{m\\ \text{Gorkov}}}(\mathrm{i}\omega_n, \mathbf{k}) = \begin{pmatrix} \mathscr{G}_{\substack{m\\ \text{Gorkov}}}(\mathrm{i}\omega_n, \mathbf{k}) & \mathscr{F}_m(\mathrm{i}\omega_n, \mathbf{k}) \\ \mathscr{F}_m^\dagger(\mathrm{i}\omega_n, \mathbf{k}) & -\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(-\mathrm{i}\omega_n, -\mathbf{k}) \end{pmatrix} \tag{26.16}$$

Proof 26.12

Starting from the definition

$$\widehat{\mathscr{G}}_{\substack{m\\ \text{Gorkov}}}(\tau, \mathbf{k}) = \begin{pmatrix} \mathscr{G}_m(\tau, \mathbf{k}) & \mathscr{F}_m(\tau, \mathbf{k}) \\ \mathscr{F}_m^\dagger(\tau, \mathbf{k}) & -\mathscr{G}_m(-\tau, -\mathbf{k}) \end{pmatrix}$$

we compute the Matsubara-component of this function. For reasons that are difficult to motivate in advance, it is advantegous to use the definition from Theorem 1.7 in this calculation

$$\widehat{\mathscr{G}}_{\substack{m\\ \text{Gorkov}}}(\mathrm{i}\omega_n, \mathbf{k}) = \frac{1}{2}\int_{-\hbar\beta}^{\hbar\beta} \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\omega_n\tau} \begin{pmatrix} \mathscr{G}_m(\tau, \mathbf{k}) & \mathscr{F}_m(\tau, \mathbf{k}) \\ \mathscr{F}_m^\dagger(\tau, \mathbf{k}) & -\mathscr{G}_m(-\tau, -\mathbf{k}) \end{pmatrix}$$

Now the only component that requires further calculations is the lower right component of this matrix. By changing variables as $\tau \mapsto -\tau$ we compute

$$\begin{aligned} -\left(\widehat{\mathscr{G}}_{\substack{m\\ \text{Gorkov}}}(\mathrm{i}\omega_n, \mathbf{k})\right)_{2,2} &= \frac{1}{2}\int_{-\hbar\beta}^{\hbar\beta} \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\omega_n\tau}\mathscr{G}_m(-\tau, -\mathbf{k}) \\ &= \frac{1}{2}\int_{+\hbar\beta}^{-\hbar\beta} \mathrm{d}\tau\, \mathrm{e}^{-\mathrm{i}\omega_n\tau}\mathscr{G}_m(+\tau, -\mathbf{k})\cdot(-1) \\ &= \frac{1}{2}\int_{-\hbar\beta}^{+\hbar\beta} \mathrm{d}\tau\, \mathrm{e}^{-\mathrm{i}\omega_n\tau}\mathscr{G}_m(+\tau, -\mathbf{k}) \\ &= \mathscr{G}_m(-\mathrm{i}\omega_n, -\mathbf{k}) \end{aligned}$$

Combining this with the very definition, we obtain the desired equation.

Remark 26.12.1 We want to emphasize at this point, that $\mathscr{F}_m^\dagger(\mathrm{i}\omega_n, \mathbf{k})$ refers to the Matsubara-representation of the mapping $\tau \mapsto \mathscr{F}_m^\dagger(\tau, \mathbf{k})$, and *not* the hermitian conjugate of $\mathscr{F}_m(\mathrm{i}\omega_n, \mathbf{k})$. In order to emphasize it once more:

$$\mathscr{F}_m^\dagger(\mathrm{i}\omega_n, \mathbf{k}) \neq \left[\mathscr{F}_m(\mathrm{i}\omega_n, \mathbf{k})\right]^*. \tag{26.17}$$

In fact, the correct identity can be concluded easily with Equation (1.12) to be

$$\mathscr{F}_m^\dagger(\mathrm{i}\omega_n, \mathbf{k}) = \left[\mathscr{F}_m(-\mathrm{i}\omega_n, \mathbf{k})\right]^*, \tag{26.18}$$

but we shall refrain from using this identity for the derivation of processing of the Gorkov-Green-function.

Lemma 26.13 Assuming a spin-degenerate and inversion-symmetric system, we obtain for the Green-function in the non-superconducting state

$$\begin{aligned} \hat{\mathscr{G}}^{-1}_{\substack{0,m \\ \text{Gorkov}}}(\mathrm{i}\omega_n, \mathbf{k}) &= \mathrm{i}\hbar\omega_n\sigma_0 - \left(\epsilon_m(\mathbf{k}) - \mu\right)\sigma_3 \\ \iff \quad \hat{\mathscr{G}}_{\substack{0,m \\ \text{Gorkov}}}(\mathrm{i}\omega_n, \mathbf{k}) &= \begin{pmatrix} \dfrac{1}{\mathrm{i}\hbar\omega_n - \left(\epsilon_m(\mathbf{k}) - \mu\right)} & 0 \\ 0 & \dfrac{1}{\mathrm{i}\hbar\omega_n + \left(\epsilon_m(\mathbf{k}) - \mu\right)} \end{pmatrix}, \end{aligned} \tag{26.19}$$

whereas we introduced $\epsilon_m(\mathbf{k}) = \epsilon_{m,\uparrow}(\pm\mathbf{k}) = \epsilon_{m,\downarrow}(\pm\mathbf{k})$.

Proof 26.13 Recall from Theorem 13.6 that

$$\mathscr{G}_m(\mathrm{i}\omega_n, \mathbf{k}) = \frac{1}{\hbar}\frac{1}{\mathrm{i}\omega_n - \left(\epsilon_m(\mathbf{k}) - \mu\right)/\hbar}$$

and

$$\begin{aligned} -\mathscr{G}_m(-\mathrm{i}\omega_n, -\mathbf{k}) &= \frac{-1}{\hbar}\frac{1}{-\mathrm{i}\omega_n - \left(\epsilon_m(-\mathbf{k}) - \mu\right)/\hbar} \\ &= \frac{1}{\hbar}\frac{1}{\mathrm{i}\omega_n + \left(\epsilon_m(-\mathbf{k}) - \mu\right)/\hbar} \end{aligned}$$

Thus we obtain

$$\mathscr{G}^{-1}_m(\mathrm{i}\omega_n, \mathbf{k}) = \hbar\left(\mathrm{i}\omega_n - \left(\epsilon_m(\mathbf{k}) - \mu\right)/\hbar\right)$$

and

$$-\hat{\mathscr{G}}^{-1}_m(-\mathrm{i}\omega_n, -\mathbf{k}) = \hbar\left(\mathrm{i}\omega_n + \left(\epsilon_m(-\mathbf{k}) - \mu\right)/\hbar\right)$$

and using the Pauli-matrices and the theorem about inversion-symmetric and spin-degenerate band-structures we obtain

$$\hat{\mathscr{G}}^{-1}_{\substack{0,m \\ \text{Gorkov}}}(\mathrm{i}\omega_n, \mathbf{k}) = \mathrm{i}\hbar\omega_n\sigma_0 - \left(\epsilon_m(\mathbf{k}) - \mu\right)\sigma_3 \tag{26.20}$$

proving the lemma.

Notation 26.14 We write for *the Dyson-equation* (cf. Remark 16.46.1) *of the Gorkov-Green-function in the superconducting state*

$$\hat{\mathscr{G}}^{-1}_{\substack{m\\ \text{Gorkov}}}(\mathrm{i}\omega_n,\mathbf{k}) = \hat{\mathscr{G}}^{-1}_{\substack{0m\\ \text{Gorkov}}}(\mathrm{i}\omega_n,\mathbf{k}) - \hat{\Sigma}_{\substack{m\\ \text{Gorkov}}}(\mathrm{i}\omega_n,\mathbf{k}) \tag{26.21}$$

whereas $\hat{\mathscr{G}}_{\substack{0m\\ \text{Gorkov}}}$ represents the Gorkov-Green-function in the non-superconducting state and absence of electron-phonon-interactions.

Remark 26.14.1 Notice further, that this equation can be rewritten in several ways, e.g. as

$$\hat{\mathscr{G}}^{-1} = \hat{\mathscr{G}}_0^{-1} - \hat{\Sigma} \iff \hat{\mathscr{G}}_0^{-1} = \hat{\mathscr{G}}^{-1} + \hat{\Sigma} \iff \hat{\mathscr{G}}_0^{-1}\hat{\mathscr{G}} = 1 + \hat{\Sigma}\hat{\mathscr{G}} \iff \hat{\mathscr{G}} = \hat{\mathscr{G}}_0 + \hat{\mathscr{G}}_0\hat{\Sigma}\hat{\mathscr{G}} \tag{26.22}$$

whereas we lifted the multitude of arguments to lighten the notation.

Remark 26.14.2 Notice that just as the anti-periodicity of the Gorkov-Green-function, the existence (not to mention the computability) of the self-energy is a priori not clear.

Corollary 26.15 This gives for the Dyson-equation in the superconducting state the set of equations (for each component)

$$\begin{aligned}
\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(k) &= +\mathscr{G}_{\substack{0m\\ \text{Gorkov}}}(k) &&+ \mathscr{G}_{\substack{0m\\ \text{Gorkov}}}(k) && \left[\Sigma^m_{11}(k)\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(k) && + \Sigma^m_{12}(k)\mathscr{F}^\dagger_m(k)\right]\\
\mathscr{F}_m(k) &= &&+ \mathscr{G}_{\substack{0m\\ \text{Gorkov}}}(k) && \left[\Sigma^m_{11}(k)\mathscr{F}_m(k) && - \Sigma^m_{12}(k)\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(-k)\right]\\
\mathscr{F}^\dagger_m(k) &= &&- \mathscr{G}_{\substack{0m\\ \text{Gorkov}}}(-k) && \left[\Sigma^m_{21}(k)\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(k) && - \Sigma^m_{22}(k)\mathscr{F}^\dagger_m(k)\right]\\
-\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(-k) &= -\mathscr{G}_{\substack{0m\\ \text{Gorkov}}}(-k) &&- \mathscr{G}_{\substack{0m\\ \text{Gorkov}}}(-k) && \left[\Sigma^m_{21}(k)\mathscr{F}_m(k) && - \Sigma^m_{22}(k)\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(-k)\right]
\end{aligned} \tag{26.23}$$

Correction note. The sign in front of Σ_{22} in the third line is wrong. Since $(\hat{\mathscr{G}}_0)_{22}(k) = -\mathscr{G}_{\substack{0m\\ \text{Gorkov}}}(-k)$ and $(\hat{\Sigma}\hat{\mathscr{G}})_{21} = \Sigma_{21}\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(k) + \Sigma_{22}\mathscr{F}^\dagger_m(k)$ (cf. the second row, first column of the matrix in the proof), the correct third line reads

$$\mathscr{F}^\dagger_m(k) = -\mathscr{G}_{\substack{0m\\ \text{Gorkov}}}(-k)\left[\Sigma^m_{21}(k)\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(k) + \Sigma^m_{22}(k)\mathscr{F}^\dagger_m(k)\right].$$

The other three lines are correct. Here $k \equiv (\mathrm{i}\omega_n, \mathbf{k})$ and $-k \equiv (-\mathrm{i}\omega_n, -\mathbf{k})$.

Proof 26.15 We use Equation (26.22) and introduce the self-energy

$$\hat{\Sigma}_{\substack{m\\ \text{Gorkov}}}(k) = \begin{pmatrix} \Sigma^m_{11}(k) & \Sigma^m_{12}(k) \\ \Sigma^m_{21}(k) & \Sigma^m_{22}(k) \end{pmatrix} \tag{26.24}$$

This yields for the product

$$\begin{aligned}\left(\widehat{\mathscr{G}}_0\widehat{\Sigma}\widehat{\mathscr{G}}\right)(k) &= \widehat{\mathscr{G}}_0(k)\begin{pmatrix}\Sigma^m_{11}(k) & \Sigma^m_{12}(k)\\ \Sigma^m_{21}(k) & \Sigma^m_{22}(k)\end{pmatrix}\begin{pmatrix}\mathscr{G}^{\ m}_{\text{Gorkov}}(k) & \mathscr{F}_m(k)\\ \mathscr{F}^*_m(k) & -\mathscr{G}^{\ m}_{\text{Gorkov}}(-k)\end{pmatrix}\\ &= \widehat{\mathscr{G}}_0(k)\begin{pmatrix}\Sigma^m_{11}(k)\mathscr{G}^{\ m}_{\text{Gorkov}}(k)+\Sigma^m_{12}(k)\mathscr{F}^*_m(k) & \Sigma^m_{11}(k)\mathscr{F}_m(k)-\Sigma^m_{12}(k)\mathscr{G}^{\ m}_{\text{Gorkov}}(-k)\\ \Sigma^m_{21}(k)\mathscr{G}^{\ m}_{\text{Gorkov}}(k)+\Sigma^m_{22}(k)\mathscr{F}^*_m(k) & \Sigma^m_{21}(k)\mathscr{F}_m(k)-\Sigma^m_{22}(k)\mathscr{G}^{\ m}_{\text{Gorkov}}(-k)\end{pmatrix}\\ &= \begin{pmatrix}\mathscr{G}_0(k) & 0\\ 0 & -\mathscr{G}_0(-k)\end{pmatrix}\begin{pmatrix}\Sigma^m_{11}(k)\mathscr{G}^{\ m}_{\text{Gorkov}}(k)+\Sigma^m_{12}(k)\mathscr{F}^*_m(k) & \Sigma^m_{11}(k)\mathscr{F}_m(k)-\Sigma^m_{12}(k)\mathscr{G}^{\ m}_{\text{Gorkov}}(-k)\\ \Sigma^m_{21}(k)\mathscr{G}^{\ m}_{\text{Gorkov}}(k)+\Sigma^m_{22}(k)\mathscr{F}^*_m(k) & \Sigma^m_{21}(k)\mathscr{F}_m(k)-\Sigma^m_{22}(k)\mathscr{G}^{\ m}_{\text{Gorkov}}(-k)\end{pmatrix}\end{aligned}$$

whereas we used Equation (26.19). Using now Equation (26.22) yields the desired result.

Correction note. In the Matsubara-representation the lower left entry of $\widehat{\mathscr{G}}$ is $\mathscr{F}^\dagger_m(k)$ and not $\mathscr{F}^*_m(k)$ (cf. the Remark after Lemma 26.12); every $\mathscr{F}^*_m(k)$ in this proof has to be read as $\mathscr{F}^\dagger_m(k)$. Carrying out the last matrix product gives

$$\left(\widehat{\mathscr{G}}_0\widehat{\Sigma}\widehat{\mathscr{G}}\right)(k) = \begin{pmatrix}\mathscr{G}_0(k)\left[\Sigma^m_{11}\mathscr{G}^{\ m}_{\text{Gorkov}}(k)+\Sigma^m_{12}\mathscr{F}^\dagger_m(k)\right] & \mathscr{G}_0(k)\left[\Sigma^m_{11}\mathscr{F}_m(k)-\Sigma^m_{12}\mathscr{G}^{\ m}_{\text{Gorkov}}(-k)\right]\\ -\mathscr{G}_0(-k)\left[\Sigma^m_{21}\mathscr{G}^{\ m}_{\text{Gorkov}}(k)+\Sigma^m_{22}\mathscr{F}^\dagger_m(k)\right] & -\mathscr{G}_0(-k)\left[\Sigma^m_{21}\mathscr{F}_m(k)-\Sigma^m_{22}\mathscr{G}^{\ m}_{\text{Gorkov}}(-k)\right]\end{pmatrix}$$

(all Σ's evaluated at k). Adding $\widehat{\mathscr{G}}_0(k) = \mathrm{diag}(\mathscr{G}_0(k), -\mathscr{G}_0(-k))$ and comparing with $\widehat{\mathscr{G}}(k)$ entry by entry gives the four lines of the Corollary, with the corrected sign in the third line.

26.1.5. Derivation of the Self-Energy-Expressions in the Superconducting State

The main-result of this subsection is the following Theorem.

Theorem 26.16 With the equation of motion technique, one obtains the individual components of the Dyson-equation as

$$\mathscr{G}^{\ n}_{\text{Gorkov}}(\mathrm{i}\omega_{n_1},\mathbf{k}) = \mathscr{G}^{\ 0,n}_{\text{Gorkov}}(\mathrm{i}\omega_{n_1},\mathbf{k})\left[1+\sum_{\substack{\omega_{n_2}\in\Omega_{-1}\\ \mathbf{k}'\in\mathrm{Q}\\ n'\in\{1,\dots,\infty\}\\ \nu'\in\{1,\dots,rd_{\mathbf{x}}\}}}\frac{-|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{N_p}\left(+\frac{1}{\beta}\right)\mathscr{D}^{\ 0,\nu'}_{\mathbf{k}-\mathbf{k}'}(\mathrm{i}(\omega_{n_1}-\omega_{n_2}))\left[\mathscr{G}^{\ n'}_{\text{Gorkov}}(\mathrm{i}\omega_{n_2},\mathbf{k}')\mathscr{G}^{\ n}_{\text{Gorkov}}(\mathrm{i}\omega_{n_1},\mathbf{k})-\mathscr{F}^\dagger_n(\mathrm{i}\omega_{n_1},\mathbf{k})\mathscr{F}_{n'}(\mathrm{i}\omega_{n_2},\mathbf{k}')\right]\right] \tag{26.25}$$

$$\mathscr{F}_n(\mathrm{i}\omega_{n_2},\mathbf{k}) = \mathscr{G}^{\ 0,n}_{\text{Gorkov}}(\mathrm{i}\omega_{n_2},\mathbf{k})\frac{-1}{\beta}\sum_{\substack{\omega_{n_1}\in\Omega_{-1}\\ \mathbf{k}'\in\mathrm{Q}\\ \nu'\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ n'\in\{1,2,\dots\}}}\frac{|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{N_p}\mathscr{D}^{\ 0,\nu'}_{\mathbf{k}-\mathbf{k}'}(\mathrm{i}(\omega_{n_2}-\omega_{n_1}))\left[\mathscr{F}_{n'\mathbf{k}'}(\mathrm{i}\omega_{n_1})\mathscr{G}_{n-\mathbf{k}}(-\mathrm{i}\omega_{n_2})+\mathscr{F}_{n\mathbf{k}}(\mathrm{i}\omega_{n_2})\mathscr{G}_{n'\mathbf{k}'}(\mathrm{i}\omega_{n_1})\right] \tag{26.26}$$

$$\mathscr{F}^\dagger_n(\mathrm{i}\omega_{n_1},\mathbf{k}) = -\mathscr{G}^{\ 0,n}_{\text{Gorkov}}(-\mathrm{i}\omega_{n_1},-\mathbf{k})\sum_{\substack{\omega_{n_2}\in\Omega_{-1}\\ \mathbf{k}'\in\mathrm{Q}\\ n'\in\{1,\dots,\infty\}\\ \nu'\in\{1,\dots,rd_{\mathbf{x}}\}}}\frac{|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{\beta N_p}\mathscr{D}^{\ 0,\nu'}_{\mathbf{k}-\mathbf{k}'}(\mathrm{i}(\omega_{n_1}-\omega_{n_2}))\left[\mathscr{F}^\dagger_{n'}(\mathrm{i}\omega_{n_2},\mathbf{k}')\mathscr{G}^{\ n}_{\text{Gorkov}}(\mathrm{i}\omega_{n_1},\mathbf{k})+\mathscr{G}^{\ n'}_{\text{Gorkov}}(-\mathrm{i}\omega_{n_2},-\mathbf{k}')\mathscr{F}^\dagger_n(\mathrm{i}\omega_{n_1},\mathbf{k})\right] \tag{26.27}$$

$$-\mathscr{G}_{\underset{\text{Gorkov}}{n}}(-\mathrm{i}\omega_{n_1},-\mathbf{k}) = -\mathscr{G}_{\underset{\text{Gorkov}}{0,n}}(-\mathrm{i}\omega_{n_1},-\mathbf{k})\left[1+\sum_{\substack{\omega_{n_2}\in\Omega_{-1}\\ \mathbf{k}'\in Q\\ n'\in\{1,\dots,\infty\}\\ \nu'\in\{1,\dots,rd_{\mathbf{x}}\}}}\frac{|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{\beta N_p}\mathscr{D}_{\underset{\mathbf{k}-\mathbf{k}'}{0,\nu'}}(\mathrm{i}(\omega_{n_1}-\omega_{n_2}))\left[\mathscr{F}^\dagger_{n'}(\mathrm{i}\omega_{n_2},\mathbf{k}')\mathscr{F}_n(\mathrm{i}\omega_{n_1},\mathbf{k})-\mathscr{G}_{\underset{\text{Gorkov}}{n'}}(-\mathrm{i}\omega_{n_2},-\mathbf{k}')\mathscr{G}_{\underset{\text{Gorkov}}{n}}(-\mathrm{i}\omega_{n_1},-\mathbf{k})\right]\right] \tag{26.28}$$

Note. In the second equation the external frequency is called ω_{n_2} and the summation frequency ω_{n_1}; after relabeling $\omega_{n_1}\leftrightarrow\omega_{n_2}$ (and using $\mathscr{D}_0(\mathrm{i}\omega)=\mathscr{D}_0(-\mathrm{i}\omega)$) all four equations have the external frequency ω_{n_1}. All four equations hold in the approximation of Theorem 26.24, i.e. neglecting vertex corrections and the terms with zero phonon momentum $\mathbf{k}'=\mathbf{k}$.

This theorem is proven throughout the subsection.

(Equation (26.25) is Theorem 26.25, the second equation is the Corollary at the end of Preparation 2/4, and Equations (26.27) and (26.28) are proven at the end of Preparation 3/4 and 4/4.)

Corollary 26.17 We obtain for the individual compdonents of the self-energy the identities

$$\underset{n}{\Sigma_{11}}(k) = \sum_{\substack{\mathrm{i}\omega_{n_2}\in\Omega_{-1}\\ \mathbf{k}'\in Q\\ n'\in\{1,2,3,\dots\}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}}}\frac{-|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{\beta N_p}\mathscr{D}_{\underset{\mathbf{k}-\mathbf{k}'}{0,\nu'}}\left(\mathrm{i}(\omega_{n_1}-\omega_{n_2})\right)\mathscr{G}_{n'}(\mathrm{i}\omega_{n_2},\mathbf{k}') \tag{26.29}$$

and

$$\underset{n}{\Sigma_{12}}(k) = \sum_{\substack{\mathrm{i}\omega_{n_2}\in\Omega_{-1}\\ \mathbf{k}'\in Q\\ n'\in\{1,2,3,\dots\}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}}}\frac{+|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{\beta N_p}\mathscr{D}_{\underset{\mathbf{k}-\mathbf{k}'}{0,\nu'}}\left(\mathrm{i}(\omega_{n_1}-\omega_{n_2})\right)\mathscr{F}_{n'}(\mathrm{i}\omega_{n_2},\mathbf{k}') \tag{26.30}$$

$$\underset{n}{\Sigma_{21}}(k) = \sum_{\substack{\omega_{n_2}\in\Omega_{-1}\\ \mathbf{k}'\in Q\\ n'\in\{1,2,3,\dots\}\\ \nu'\in\{1,2,\dots,rd_{\mathbf{x}}\}}}\frac{+|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{\beta N_p}\mathscr{D}_{\underset{\mathbf{k}-\mathbf{k}'}{0,\nu'}}\left(\mathrm{i}(\omega_{n_1}-\omega_{n_2})\right)\mathscr{F}^\dagger_{n'}(\mathrm{i}\omega_{n_2},\mathbf{k}') \tag{26.31}$$

$$\underset{n}{\Sigma_{22}}(k) = \sum_{\substack{\omega_{n_2}\in\Omega_{-1}\\ \mathbf{k}'\in Q\\ n'\in\{1,2,3,\dots\}\\ \nu'\in\{1,2,\dots,rd_{\mathbf{x}}\}}}\frac{+|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{\beta N_p}\mathscr{D}_{\underset{\mathbf{k}-\mathbf{k}'}{0,\nu'}}\left(\mathrm{i}(\omega_{n_1}-\omega_{n_2})\right)\mathscr{G}_{\underset{\text{Gorkov}}{n'}}(-\mathrm{i}\omega_{n_2},-\mathbf{k}') \tag{26.32}$$

with $k\equiv(\mathrm{i}\omega_{n_1},\mathbf{k})$. In the first two equations the summation runs over $\omega_{n_2}\in\Omega_{-1}$ and ν' (not ν), and $\mathscr{G}_{n'}$ means $\mathscr{G}_{\underset{\text{Gorkov}}{n'}}$. Since $(\widehat{\mathscr{G}}_{n'})_{22}(\mathrm{i}\omega,\mathbf{k}')=-\mathscr{G}_{\underset{\text{Gorkov}}{n'}}(-\mathrm{i}\omega,-\mathbf{k}')$, all four components can be collected in the matrix identity

$$\widehat{\Sigma}_{\underset{\text{Gorkov}}{n}}(\mathrm{i}\omega_{n_1},\mathbf{k}) = -\frac{1}{\beta N_p}\sum_{\substack{\omega_{n_2}\in\Omega_{-1}\\ \mathbf{k}'\in Q\\ n'\in\{1,2,3,\dots\}\\ \nu'\in\{1,2,\dots,rd_{\mathbf{x}}\}}}|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2\mathscr{D}_{\underset{\mathbf{k}-\mathbf{k}'}{0,\nu'}}\left(\mathrm{i}(\omega_{n_1}-\omega_{n_2})\right)\sigma_3\widehat{\mathscr{G}}_{\underset{\text{Gorkov}}{n'}}(\mathrm{i}\omega_{n_2},\mathbf{k}')\sigma_3. \tag{26.33}$$

Proof 26.17 We combine Equation (26.23) with Equations (26.25) - (26.28) which yields the desired result.

Details (why "reading off" is unique). Denote by $\widehat{M}_n(\mathrm{i}\omega_{n_1}, \mathbf{k})$ the right-hand side of Equation (26.33). Writing out $\widehat{\mathscr{G}}_0 \widehat{M} \widehat{\mathscr{G}}$ as in the proof of Corollary 26.15 (with Σ_{ij} replaced by M_{ij}), one checks entry by entry that the four equations of the Theorem are exactly the four entries of

$$\underset{\text{Gorkov}}{\widehat{\mathscr{G}}_{\,n}} = \underset{\text{Gorkov}}{\widehat{\mathscr{G}}_{0,n}} + \underset{\text{Gorkov}}{\widehat{\mathscr{G}}_{0,n}} \widehat{M}_n \underset{\text{Gorkov}}{\widehat{\mathscr{G}}_{\,n}},$$

e.g. $M_{11}\mathscr{G} + M_{12}\mathscr{F}^\dagger$ reproduces the bracket of Equation (26.25), and $M_{21}\mathscr{G} + M_{22}\mathscr{F}^\dagger$ the bracket of Equation (26.27). If $\widehat{\mathscr{G}}_0$ and $\widehat{\mathscr{G}}$ are invertible, multiplying from the left with $\widehat{\mathscr{G}}_0^{-1}$ and from the right with $\widehat{\mathscr{G}}^{-1}$ gives $\widehat{M} = \widehat{\mathscr{G}}_0^{-1} - \widehat{\mathscr{G}}^{-1} = \widehat{\Sigma}$ by Equation (26.21). Hence the self-energy is uniquely determined and equals Equation (26.33). (Comparing only one scalar equation, e.g. the 1, 1-component, would not determine Σ_{11} and Σ_{12} separately.)

Preparation 0/4: Commutators and Equations of Motion for Creation- and Annihilation-Operators

Lemma 26.18 One finds for the imaginary-time-evolution of an operator X the Heisenberg-equation of motion

$$\partial_\tau X_{\mathrm{H}}(\xi\tau) = -\frac{\xi}{\hbar}\left[H - \mu N, X\right]_{\mathrm{H}}(\xi\tau) + \xi\left(\partial_\tau X\right)_{\mathrm{H}}(\xi\tau) \tag{26.34}$$

Correction note. The commutator has the wrong order. With $X_{\mathrm{H}}(\xi\tau) = \mathrm{e}^{\xi\tau(H-\mu N)/\hbar} X \mathrm{e}^{-\xi\tau(H-\mu N)/\hbar}$ the correct equation (which is also the last line of the proof below, and the version used in all later proofs) reads

$$\partial_\tau X_{\mathrm{H}}(\xi\tau) = -\frac{\xi}{\hbar}\left[X, H - \mu N\right]_{\mathrm{H}}(\xi\tau) + \xi\left(\partial_\tau X\right)_{\mathrm{H}}(\xi\tau) = +\frac{\xi}{\hbar}\left[H - \mu N, X\right]_{\mathrm{H}}(\xi\tau) + \xi\left(\partial_\tau X\right)_{\mathrm{H}}(\xi\tau).$$

Proof 26.18

Recalling that $U(\xi\tau, 0) = \exp -\frac{1}{\hbar}\xi\tau\widetilde{H} = \exp -\xi(\tau - 0)\widetilde{H}/\hbar$, with $\widetilde{H} = H - \mu N$ we obtain analogously the auxiliary identities

$$\frac{\mathrm{d}}{\mathrm{d}\tau}U(\xi\tau, 0) = -\frac{\xi}{\hbar}\widetilde{H}U(\xi\tau, 0)$$
$$\frac{\mathrm{d}}{\mathrm{d}\tau}U(0, \xi\tau) = \frac{\xi}{\hbar}U(0, \xi\tau)\widetilde{H}$$

Remark: There are more identities like this, but we only need these here. Then it follows

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\tau}X_{\mathrm{H}}(\xi\tau) &= \frac{\mathrm{d}}{\mathrm{d}t}U(0,\xi\tau)X(\xi\tau)U(\xi\tau,0)\\
&= \left(\frac{\mathrm{d}}{\mathrm{d}\tau}U(0,\xi\tau)\right)X(\xi\tau)U(\xi\tau,0) + U(0,\xi\tau)\left(\frac{\mathrm{d}}{\mathrm{d}\tau}X(\xi\tau)\right)U(\xi\tau,0) + U(0,\xi\tau)X(\xi\tau)\left(\frac{\mathrm{d}}{\mathrm{d}\tau}U(\xi\tau,0)\right)\\
&= \frac{\xi}{\hbar}U(0,\xi\tau)\widetilde{H}X(\xi\tau)U(\xi\tau,0) + U(0,\xi\tau)\left(\frac{\mathrm{d}}{\mathrm{d}\tau}X(\xi\tau)\right)U(\xi\tau,0) + U(0,\xi\tau)X(\xi\tau)\left(-\frac{\xi}{\hbar}\widetilde{H}U(\xi\tau,0)\right)\\
&= \frac{\xi}{\hbar}U(0,\xi\tau)\left(\widetilde{H}X(\xi\tau) - X(\xi\tau)\widetilde{H}\right)U(\xi\tau,0) + U(0,\xi\tau)\left(\frac{\mathrm{d}}{\mathrm{d}t}X(\xi\tau)\right)U(\xi\tau,0)\\
&= \frac{\xi}{\hbar}U(0,\xi\tau)\left[\widetilde{H},X(\xi\tau)\right]U(\xi\tau,0) + U(0,\xi\tau)\left(\frac{\mathrm{d}}{\mathrm{d}\tau}X(\xi\tau)\right)U(\xi\tau,0)\\
&= -\frac{\xi}{\hbar}\left[X,\widetilde{H}\right]_{\mathrm{H}}(\xi\tau) + U(0,\xi\tau)\left(\frac{\mathrm{d}}{\mathrm{d}\tau}X(\xi\tau)\right)U(\xi\tau,0)
\end{aligned}
$$

Note. The two $\frac{\mathrm{d}}{\mathrm{d}t}$ should read $\frac{\mathrm{d}}{\mathrm{d}\tau}$, and $U(0,\xi\tau)\big(\frac{\mathrm{d}}{\mathrm{d}\tau}X(\xi\tau)\big)U(\xi\tau,0) = \xi(\partial_\tau X)_{\mathrm{H}}(\xi\tau)$ (chain rule). The last line is correct; it proves the corrected version of the Lemma.

Lemma 26.19 One finds the identities

$$
\begin{aligned}
\partial_\tau b_\nu(\xi\tau,\bullet) &= -\xi\omega_\nu(\bullet)b_\nu(\xi\tau,\bullet) - \xi\sum_{\substack{\mathbf{k}\in\mathrm{Q}\\ \sigma\in\{\uparrow,\downarrow\}\\ m,n\in\{1,\ldots,\infty\}}}\frac{g_{mn\nu}(\mathbf{k},-\bullet)}{\hbar\sqrt{N_p}}c^\dagger_{m\sigma}(\xi\tau,\mathbf{k}-\bullet)c_{n\sigma}(\xi\tau,\mathbf{k})\\
\partial_\tau b^\dagger_\nu(\xi\tau,-\bullet) &= +\xi\omega_\nu(-\bullet)b^\dagger_\nu(\xi\tau,-\bullet) + \xi\sum_{\substack{\mathbf{k}\in\mathrm{Q}\\ \sigma\in\{\uparrow,\downarrow\}\\ m,n\in\{1,\ldots,\infty\}}}\frac{g_{mn\nu}(\mathbf{k},-\bullet)}{\hbar\sqrt{N_p}}c^\dagger_{m\sigma}(\xi\tau,\mathbf{k}-\bullet)c_{n\sigma}(\xi\tau,\mathbf{k})
\end{aligned}
$$

for $\xi\in\{-1,+1\}$.

Proof 26.19 We compute the equation of motion for the annihilation-operators using the Heisenberg-equation of motion (26.34) for arbitrary $\bullet\in\mathrm{Q}$ with H from Equation (26.1)(in the corrected form $-\frac{\xi}{\hbar}[X,H-\mu N]_{\mathrm{H}}$, and with $\Omega_\nu(\mathbf{q})\equiv\hbar\omega_\nu(\mathbf{q})$ in Equation (26.1); b_ν, $b^\dagger_\nu$ commute with N, which gives the "+0")

$$
\begin{aligned}
\partial_\tau b_\nu(\xi\tau,\bullet) &= -\frac{\xi}{\hbar}[b_\nu(\bullet),H-\mu N]_{\mathrm{H}}(\xi\tau)\\
&= -\xi\sum_{\substack{\mathbf{q}'\in\mathrm{Q}\\ \nu'\in\{1,\ldots,rd_{\mathbf{x}}\}}}\omega_{\nu'}(\mathbf{q}')[b_\nu(\bullet),b^\dagger_{\nu'}(\mathbf{q}')b_{\nu'}(\mathbf{q}')]_{\mathrm{H}}(\xi\tau) \quad + \quad 0\\
&\quad -\xi\sum_{\substack{\mathbf{k}',\mathbf{q}'\in\mathrm{Q}\\ \sigma'\in\{\uparrow,\downarrow\}\\ \nu'\in\{1,\ldots,rd_{\mathbf{x}}\}\\ m',n'\in\{1,\ldots,\infty\}}}\frac{g_{m'n'\nu'}(\mathbf{k}',\mathbf{q}')}{\hbar\sqrt{N_p}}c^\dagger_{m'\sigma'}(\xi\tau,\mathbf{k}'+\mathbf{q}')c_{n'\sigma'}(\xi\tau,\mathbf{k}')\left([b_\nu(\bullet),b^\dagger_{\nu'}(-\mathbf{q}')]_{\mathrm{H}}(\xi\tau) \quad + 0\right)\\
&= \ldots
\end{aligned}
$$

Now we use Equation (10.4) and Lemma 7.17, i.e.

$$[A, BC] = [A, B]_\zeta C + \zeta B[A, C]_\zeta \tag{26.35}$$

to simplify the second and third row as

$$\begin{aligned}[b_\nu(\bullet), b^\dagger_{\nu'}(\mathbf{q}')b_{\nu'}(\mathbf{q}')] &= \delta_{\nu,\nu'}\delta_{\bullet,\mathbf{q}'}b_{\nu'}(\mathbf{q}')\\ [b_\nu(\bullet), b^\dagger_{\nu'}(-\mathbf{q}')] &= \delta_{\nu,\nu'}\delta_{\bullet,-\mathbf{q}'}\end{aligned}$$

such that we obtain

$$\ldots = -\xi\omega_\nu(\bullet)b_\nu(\xi\tau,\bullet) - \xi \sum_{\substack{\mathbf{k}'\in Q\\ \sigma'\in\{\uparrow,\downarrow\}\\ m',n'\in\{1,\ldots,\infty\}}} \frac{g_{m'n'\nu}(\mathbf{k}',-\bullet)}{\hbar\sqrt{N_p}} c^\dagger_{m'\sigma'}(\xi\tau,\mathbf{k}'-\bullet)c_{n'\sigma'}(\xi\tau,\mathbf{k}')$$

replacing now the summation indices (i.e. dropping the primes), we obtain the desired result.
In the same fashion we obtain

$$\begin{aligned}\partial_\tau b^\dagger_\nu(\xi\tau,-\bullet) &= -\frac{\xi}{\hbar}[b^\dagger_\nu(-\bullet), H-\mu N]_{\mathrm{H}}(\xi\tau)\\ &= -\xi \sum_{\substack{\mathbf{q}'\in Q\\ \nu'\in\{1,\ldots,rd_{\mathbf{x}}\}}} \omega_{\nu'}(\mathbf{q}')[b^\dagger_\nu(-\bullet), b^\dagger_{\nu'}(\mathbf{q}')b_{\nu'}(\mathbf{q}')]_{\mathrm{H}}(\xi\tau) \quad + \quad 0\\ &\quad - \xi \sum_{\substack{\mathbf{k}',\mathbf{q}'\in Q\\ \sigma'\in\{\uparrow,\downarrow\}\\ \nu'\in\{1,\ldots,rd_{\mathbf{x}}\}\\ m',n'\in\{1,\ldots,\infty\}}} \frac{g_{m'n'\nu'}(\mathbf{k}',\mathbf{q}')}{\hbar\sqrt{N_p}} c^\dagger_{m'\sigma'}(\xi\tau,\mathbf{k}'+\mathbf{q}')c_{n'\sigma'}(\xi\tau,\mathbf{k}')\left([b^\dagger_\nu(-\bullet), b_{\nu'}(+\mathbf{q}')]_{\mathrm{H}}(\xi\tau) \quad + \quad 0\right)\\ &= \ldots\end{aligned}$$

Now we use again Equation (10.4) and Lemma 7.17

$$\begin{aligned}[b^\dagger_\nu(-\bullet), b^\dagger_{\nu'}(\mathbf{q}')b_{\nu'}(\mathbf{q}')] &= -\delta_{\nu,\nu'}\delta_{-\bullet,\mathbf{q}'}b^\dagger_{\nu'}(\mathbf{q}')\\ [b^\dagger_\nu(-\bullet), b_{\nu'}(\mathbf{q}')] &= -\delta_{\nu,\nu'}\delta_{-\bullet,\mathbf{q}'}\end{aligned}$$

(notice that the extra minus sign appears due to the commutation-relations), such that we obtain

$$\ldots = +\xi\omega_\nu(-\bullet)b^\dagger_\nu(\xi\tau,-\bullet) + \xi \sum_{\substack{\mathbf{k}'\in Q\\ \sigma'\in\{\uparrow,\downarrow\}\\ m',n'\in\{1,\ldots,\infty\}}} \frac{g_{m'n'\nu}(\mathbf{k}',-\bullet)}{\hbar\sqrt{N_p}} c^\dagger_{m'\sigma'}(\xi\tau,\mathbf{k}'-\bullet)c_{n'\sigma'}(\xi\tau,\mathbf{k}')$$

using now the inversion-symmetry of ω and dropping the primes we obtain the desired result.

Remark 26.19.1 Notice that we used in the proof that $\omega_\nu(\mathbf{q}) = \omega_\nu(-\mathbf{q})$, and hence used the time-reversal-symmetry of the crystal.

Remark 26.19.2 Notice further, that the $\xi\tau$ dependence of the operators on the right-hand side of the equations can be simplified to refer to the operator-*pair* $c^\dagger c$.

Preparation 1/4: Equations of Motion for the normal, spin-up Green-Function

Lemma 26.20 One finds for the Gorkov-Green-function

$$\begin{aligned}&\left(\partial_\tau + \frac{\epsilon_n(\mathbf{k}) - \mu}{\hbar}\right) \mathscr{G}_{\substack{n \\ \text{Gorkov}}}(\tau, \mathbf{k}) \\ &= -\frac{1}{\hbar}\delta(\tau) + \sum_{\substack{\mathbf{k}' \in \mathrm{Q} \\ n' \in \{1,\dots,\infty\} \\ \nu' \in \{1,\dots,rd_{\mathbf{x}}\}}} \frac{g_{nn'\nu'}(\mathbf{k}', \mathbf{k}-\mathbf{k}')}{\hbar^2\sqrt{N}_p} \left\langle \mathrm{T}_\tau\, c_{n',\uparrow}(\tau, \mathbf{k}') c^\dagger_{n,\uparrow}(\mathbf{k}, 0) \left(b_{\nu'}(\tau, \mathbf{k}-\mathbf{k}') + b^\dagger_{\nu'}(\tau, \mathbf{k}'-\mathbf{k})\right)\right\rangle_{\mathrm{SC}}\end{aligned} \tag{26.36}$$

Proof 26.20 Recall from Lemma 13.5 that the equation of motion for the Green-function in imaginary time reads

$$\partial_\tau \mathscr{G}_{\substack{n \\ \text{Gorkov}}}(\tau, \mathbf{k}) = -\frac{1}{\hbar}\delta(\tau) - \frac{1}{\hbar}\left\langle \mathrm{T}_\tau \left[\frac{H - \mu N}{\hbar},\, c_{n,\uparrow}(\mathbf{k})\right]_{\mathrm{H}}(\tau) c^\dagger_{n,\uparrow}(\mathbf{k}, 0)\right\rangle_{\mathrm{SC}} \tag{26.37}$$

whereas N refers to the total electronic occupation-number operator. We now compute the commutator for the EPW-system as

$$\begin{aligned}[\frac{H - \mu N}{\hbar}, c_{n\uparrow}(\mathbf{k})] = &\sum_{\substack{\mathbf{k}' \in \mathrm{Q} \\ \sigma' \in \{\uparrow,\downarrow\} \\ n' \in \{1,\dots,\infty\}}} \frac{1}{\hbar}\left(\epsilon_{n'}(\mathbf{k}') - \mu\right) [c^\dagger_{n'\sigma'}(\mathbf{k}') c_{n'\sigma'}(\mathbf{k}'), c_{n\uparrow}(\mathbf{k})] \\ &+ \sum_{\substack{\mathbf{q}', \mathbf{k}' \in \mathrm{Q} \\ \sigma' \in \{\uparrow,\downarrow\} \\ \nu' \in \{1,\dots,rd_{\mathbf{x}}\} \\ n', m' \in \{1,\dots,\infty\}}} \frac{g_{m'n'\nu'}(\mathbf{k}', \mathbf{q}')}{\hbar\sqrt{N_p}} [c^\dagger_{m'\sigma'}(\mathbf{k}' + \mathbf{q}') c_{n'\sigma'}(\mathbf{k}') \left(b_{\nu'}(\mathbf{q}') + b^\dagger_{\nu'}(-\mathbf{q}')\right), c_{n\uparrow}(\mathbf{k})] \\ &= \dots\end{aligned}$$

Now we evaluate the individual commutators. For the first line we have

$$[c^\dagger_{n'\sigma'}(\mathbf{k}') c_{n'\sigma'}(\mathbf{k}'), c_{n\uparrow}(\mathbf{k})] = -[c_{n\uparrow}(\mathbf{k}), c^\dagger_{n'\sigma'}(\mathbf{k}') c_{n'\sigma'}(\mathbf{k}')] = -\delta_{n',n}\delta_{\sigma',\uparrow}\delta_{\mathbf{k}',\mathbf{k}} c_{n'\sigma'}(\mathbf{k}') \tag{26.38}$$

and

$$[c^\dagger_{m'\sigma'}(\mathbf{k}'+\mathbf{q}')c_{n'\sigma'}(\mathbf{k}')\left(b_{\nu'}(\mathbf{q}')+b^\dagger_{\nu'}(-\mathbf{q}')\right), c_{n\uparrow}(\mathbf{k})] = -[c_{n\uparrow}(\mathbf{k}), c^\dagger_{m'\sigma'}(\mathbf{k}'+\mathbf{q}')c_{n'\sigma'}(\mathbf{k}')]\left(b_{\nu'}(\mathbf{q}')+b^\dagger_{\nu'}(-\mathbf{q}')\right)$$
$$= -\delta_{m',n}\delta_{\sigma',\uparrow}\delta_{\mathbf{k}'+\mathbf{q}',\mathbf{k}}c_{n'\sigma'}(\mathbf{k}')\left(b_{\nu'}(\mathbf{q}')+b^\dagger_{\nu'}(-\mathbf{q}')\right)$$

whereas we used Lemma 7.17 in both cases, and thus we obtain, after terminating the sums over $\mathbf{q}'$, m' and σ', the equation

$$\ldots = -\left(\frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\right)c_{n\uparrow}(\mathbf{k}) - \sum_{\substack{\mathbf{k}'\in \mathrm{Q}\\ \nu'\in\{1,\ldots,rd_{\mathbf{x}}\}\\ n'\in\{1,\ldots,\infty\}}} \frac{g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')}{\hbar\sqrt{N_p}}\left(b_{\nu'}(\mathbf{k}-\mathbf{k}')+b^\dagger_{\nu'}(\mathbf{k}'-\mathbf{k})\right)c_{n'\uparrow}(\mathbf{k}')$$

Plugging this into the equation of motion, Equation (26.37), yields

$$\partial_\tau \mathscr{G}_{\substack{n\\ \mathrm{Gorkov}}}(\tau,\mathbf{k}) = -\delta(\tau)/\hbar + \frac{\epsilon_n(\mathbf{k})-\mu}{\hbar^2}\left\langle \mathrm{T}_\tau\, c_{n\uparrow}(\tau,\mathbf{k})c^\dagger_{n\uparrow}(0,\mathbf{k})\right\rangle_{\mathrm{SC}}$$
$$+ \sum_{\substack{\mathbf{k}'\in \mathrm{Q}\\ \nu'\in\{1,\ldots,rd_{\mathbf{x}}\}\\ n'\in\{1,\ldots,\infty\}}} \frac{g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')}{\hbar^2\sqrt{N_p}}\left\langle \mathrm{T}_\tau\left(b_{\nu'}(\tau,\mathbf{k}-\mathbf{k}')+b^\dagger_{\nu'}(\tau,\mathbf{k}'-\mathbf{k})\right)c_{n'\uparrow}(\tau,\mathbf{k}')c^\dagger_{n\uparrow}(\mathbf{k},0)\right\rangle_{\mathrm{SC}}$$

which can be simplified to

$$\left(\partial_\tau + \frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\right)\mathscr{G}_{\substack{n\\ \mathrm{Gorkov}}}(\tau,\mathbf{k})$$
$$= -\delta(\tau)/\hbar + \sum_{\substack{\mathbf{k}'\in \mathrm{Q}\\ \nu'\in\{1,\ldots,rd_{\mathbf{x}}\}\\ n'\in\{1,\ldots,\infty\}}} \frac{g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')}{\hbar^2\sqrt{N_p}}\left\langle \mathrm{T}_\tau\left(b_{\nu'}(\tau,\mathbf{k}-\mathbf{k}')+b^\dagger_{\nu'}(\tau,\mathbf{k}'-\mathbf{k})\right)c_{n'\uparrow}(\tau,\mathbf{k}')c^\dagger_{n\uparrow}(\mathbf{k},0)\right\rangle_{\mathrm{SC}} \tag{26.39}$$

Definition 26.21 We define *the auxiliary-Green-function* for $\tau,\tau'\in(0,\hbar\beta)$

$$\mathscr{G}_{\substack{\mathrm{aux}\\ n,n',\nu'}}(\tau,\tau',\mathbf{k},\mathbf{k}') = -\frac{1}{\hbar}\left\langle \mathrm{T}_\tau\, c_{n',\uparrow}(\tau',\mathbf{k}')c^\dagger_{n,\uparrow}(0,\mathbf{k})\left(b_{\nu'}(\tau,\mathbf{k}-\mathbf{k}')+b^\dagger_{\nu'}(\tau,\mathbf{k}'-\mathbf{k})\right)\right\rangle_{\mathrm{SC}} \tag{26.40}$$

Remark 26.21.1 Notice that this Green-function has, just like a "regular" Green-function the unit of $1/\text{Energy}\times$ Time.

Remark 26.21.2 Notice that Equation (26.36) can now be rewritten as

$$\left(\partial_\tau + \frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\right)\mathscr{G}_{\substack{n\\ \mathrm{Gorkov}}}(\tau,\mathbf{k}) = -\frac{1}{\hbar}\delta(\tau) - \sum_{\substack{\mathbf{k}'\in \mathrm{Q}\\ n'\in\{1,\ldots,\infty\}\\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\}}} \frac{g_{nn'\nu}(\mathbf{k}',\mathbf{k}-\mathbf{k}')}{\hbar\sqrt{N_p}}\mathscr{G}_{\substack{\mathrm{aux}\\ n,n',\nu}}(\tau,\tau,\mathbf{k},\mathbf{k}') \tag{26.41}$$

Lemma 26.22 For $\mathbf{k} \neq \mathbf{k}'$ we obtain the equations for the first partial derivative

$$\partial_\tau \mathscr{G}^{\text{aux}}_{n,n',\nu'}(\tau,\tau',\mathbf{k},\mathbf{k}') = +\frac{\omega_{\nu'}(\mathbf{k}-\mathbf{k}')}{\hbar}\left\langle \mathrm{T}_\tau \left(b_{\nu'}(\tau,\mathbf{k}-\mathbf{k}') - b^\dagger_{\nu'}(\tau,\mathbf{k}'-\mathbf{k})\right) c_{n',\uparrow}(\tau',\mathbf{k}')c^\dagger_{n,\uparrow}(0,\mathbf{k})\right\rangle_{\text{SC}} \tag{26.42}$$

and for the second partial derivative[7]

$$\begin{aligned}&\left(\partial_\tau^2 - \omega^2_{\nu'}(\mathbf{k}-\mathbf{k}')\right)\mathscr{G}^{\text{aux}}_{n,n',\nu'}(\tau,\tau',\mathbf{k},\mathbf{k}')\\ &= \frac{-2\omega_{\nu'}(\mathbf{k}-\mathbf{k}')}{\hbar}\sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ m,m'\in\{1,\dots,\infty\}\\ \sigma\in\{\uparrow,\downarrow\}}}\frac{g_{mm'\nu'}(\mathbf{q},\mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}}\left\langle \mathrm{T}_\tau\, c^\dagger_{m,\sigma}(\tau,\mathbf{q}+\mathbf{k}'-\mathbf{k})c_{m',\sigma}(\tau,\mathbf{q})c_{n',\uparrow}(\tau',\mathbf{k}')c^\dagger_{n,\uparrow}(0,\mathbf{k})\right\rangle_{\text{SC}}\end{aligned} \tag{26.43}$$

Proof 26.22 Notice first that Equation (26.40) can be expanded as

$$\begin{aligned}\mathscr{G}^{\text{aux}}_{\nu',n,n'}(\tau,\tau',\mathbf{k},\mathbf{k}') = -\frac{1}{\hbar}\Big[&+\theta(\tau')\left\langle \left(b_{\nu'}(\tau,\mathbf{k}-\mathbf{k}') + b^\dagger_{\nu'}(\tau,\mathbf{k}'-\mathbf{k})\right) c_{n',\uparrow}(\tau',\mathbf{k}')c^\dagger_{n,\uparrow}(0,\mathbf{k})\right\rangle_{\text{SC}}\\ &-\theta(-\tau')\left\langle \left(b_{\nu'}(\tau,\mathbf{k}-\mathbf{k}') + b^\dagger_{\nu'}(\tau,\mathbf{k}'-\mathbf{k})\right) c^\dagger_{n,\uparrow}(0,\mathbf{k})c_{n',\uparrow}(\tau',\mathbf{k}')\right\rangle_{\text{SC}}\Big].\end{aligned} \tag{26.44}$$

Correction note. Equation (26.44) is not literally the time-ordered product: it orders only the two fermionic operators and always puts the phonon operators to the very left. In the interacting system $b_{\mathrm{H}}(\tau)$ and $c_{\mathrm{H}}(\tau')$ do *not* commute for $\tau \neq \tau'$, so for $\tau < \tau'$ or $\tau < 0$ the position of the phonon operator matters. What is true (and all that is needed) is the following: the τ-derivative of the full time-ordered product produces, besides $\langle \mathrm{T}_\tau(\partial_\tau A)\dots\rangle$, only terms of the form $\delta(\tau-\tau')[A(\tau), c_{n'\uparrow}(\tau,\mathbf{k}')]$ and $\delta(\tau)[A(0), c^\dagger_{n\uparrow}(0,\mathbf{k})]$ with $A = b_{\nu'}(\mathbf{k}-\mathbf{k}')+b^\dagger_{\nu'}(\mathbf{k}'-\mathbf{k})$. These equal-time commutators vanish, since phonon and electron operators commute at equal times. Hence $\partial_\tau\langle \mathrm{T}_\tau\, c'c^\dagger A(\tau)\rangle = \langle \mathrm{T}_\tau\, c'c^\dagger\partial_\tau A(\tau)\rangle$, and the result of the computation below is correct.

Since the time-ordering-operator decomposese into the bosonic and fermionic part and it is sufficient[8] to focus on the bosonic part. Thus taking the derivative w.r.t. τ yields doesn't involve any δ-functions. One finds by straightforward computation with Equation (26.44) that[9]

$$\begin{aligned}\partial_\tau\mathscr{G}^{\text{aux}}_{\nu',n,n'}(\tau,\tau',\mathbf{k},\mathbf{k}') = &-\frac{1}{\hbar}\left\langle \mathrm{T}_\tau\left(\partial_\tau b_{\nu'}(\tau,\mathbf{k}-\mathbf{k}')\right) c_{n',\uparrow}(\tau',\mathbf{k}')c^\dagger_{n,\uparrow}(0,\mathbf{k})\right\rangle_{\text{SC}}\\ &-\frac{1}{\hbar}\left\langle \mathrm{T}_\tau\left(\partial_\tau b^\dagger_{\nu'}(\tau,\mathbf{k}'-\mathbf{k})\right) c_{n',\uparrow}(\tau'\pm\epsilon,\mathbf{k}')c^\dagger_{n,\uparrow}(0,\mathbf{k})\right\rangle_{\text{SC}} = \dots\end{aligned}$$

and then by using Lemma 26.19 we obtain

[7] Note that this is in perfect harmony with Marsiglios article, except that he has typos in ω and g.

[8] Maybe this should be added as a corollary. Cf. definition 8.14.

[9] Notice that the order doesn't matter cause within T_τ it has even statistics.

$$
\begin{aligned}
&\dots \\
&= -\frac{1}{\hbar}\left\langle \mathrm{T}_\tau\, c_{n',\uparrow}(\tau',\mathbf{k}')c^\dagger_{n,\uparrow}(0,\mathbf{k})\Big[-\omega_{\nu'}(\mathbf{k}-\mathbf{k}')b_{\nu'}(\tau,\mathbf{k}-\mathbf{k}') - \sum_{\substack{\widetilde{\mathbf{k}}\in\mathrm{Q}\\ \widetilde{\sigma}\in\{\uparrow,\downarrow\}\\ \widetilde{m},\widetilde{n}\in\{1,\dots,\infty\}}} \frac{g_{\widetilde{m}\widetilde{n}\nu'}(\widetilde{\mathbf{k}},\mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}} c^\dagger_{\widetilde{m}\widetilde{\sigma}}(\tau,\widetilde{\mathbf{k}}+\mathbf{k}'-\mathbf{k})c_{\widetilde{n}\widetilde{\sigma}}(\tau,\widetilde{\mathbf{k}})\Big]\right\rangle \\
&- \frac{1}{\hbar}\left\langle \mathrm{T}_\tau\, c_{n',\uparrow}(\tau',\mathbf{k}')c^\dagger_{n,\uparrow}(0,\mathbf{k})\Big[\omega_{\nu'}(\mathbf{k}'-\mathbf{k})b^\dagger_{\nu'}(\tau,\mathbf{k}'-\mathbf{k}) + \sum_{\substack{\widetilde{\mathbf{k}}\in\mathrm{Q}\\ \widetilde{\sigma}\in\{\uparrow,\downarrow\}\\ \widetilde{m},\widetilde{n}\in\{1,\dots,\infty\}}} \frac{g_{\widetilde{m}\widetilde{n}\nu'}(\widetilde{\mathbf{k}},\mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}} c^\dagger_{\widetilde{m}\widetilde{\sigma}}(\tau,\widetilde{\mathbf{k}}+\mathbf{k}'-\mathbf{k})c_{\widetilde{n}\widetilde{\sigma}}(\tau,\widetilde{\mathbf{k}})\Big]\right\rangle_{\mathrm{SC}} \\
&= \dots
\end{aligned}
$$

and see that the contributions containing the electron-phonon-coupling g cancel out and we obtain

$$
\begin{aligned}
\partial_\tau \mathscr{G}^{\mathrm{aux}}_{\nu',n,n'}(\tau,\tau',\mathbf{k},\mathbf{k}') &= +\frac{\omega_{\nu'}(\mathbf{k}-\mathbf{k}')}{\hbar}\left\langle \mathrm{T}_\tau\, b_{\nu'}(\tau,\mathbf{k}-\mathbf{k}')c_{n',\uparrow}(\tau',\mathbf{k}')c^\dagger_{n,\uparrow}(0,\mathbf{k})\right\rangle_{\mathrm{SC}} \\
&\quad - \frac{\omega_{\nu'}(\mathbf{k}'-\mathbf{k})}{\hbar}\left\langle \mathrm{T}_\tau\, b^\dagger_{\nu'}(\tau,\mathbf{k}'-\mathbf{k})c_{n',\uparrow}(\tau',\mathbf{k}')c^\dagger_{n,\uparrow}(0,\mathbf{k})\right\rangle_{\mathrm{SC}} \\
&= \frac{\omega_{\nu'}(\mathbf{k}-\mathbf{k}')}{\hbar}\left\langle \mathrm{T}_\tau\, \left(b_{\nu'}(\tau,\mathbf{k}-\mathbf{k}') - b^\dagger_{\nu'}(\tau,\mathbf{k}'-\mathbf{k})\right) c_{n',\uparrow}(\tau',\mathbf{k}')c^\dagger_{n,\uparrow}(0,\mathbf{k})\right\rangle_{\mathrm{SC}}
\end{aligned}
$$

whereas we used the inversion-symmetry $\omega_\nu(+\bullet) = \omega_\nu(-\bullet)$ in the last equation-sign and hence we obtain the desired result. For the second derivative we obtain

$$
\begin{aligned}
\partial^2_\tau \mathscr{G}^{\mathrm{aux}}_{\nu',n,n'}(\tau,\tau',\mathbf{k},\mathbf{k}') &= \frac{\omega_{\nu'}(\mathbf{k}-\mathbf{k}')}{\hbar}\left\langle \mathrm{T}_\tau\, \partial_\tau \left(b_{\nu'}(\tau,\mathbf{k}-\mathbf{k}') - b^\dagger_{\nu'}(\tau,\mathbf{k}'-\mathbf{k})\right) c_{n',\uparrow}(\tau',\mathbf{k}')c^\dagger_{n,\uparrow}(0,\mathbf{k})\right\rangle_{\mathrm{SC}} \\
&= \mathrm{I} + \mathrm{II} \\
&= \dots
\end{aligned}
\tag{26.45}
$$

using now Lemma 26.19 again we obtain for the individual contributions

$$
\begin{aligned}
\mathrm{I} = \frac{\omega_{\nu'}(\mathbf{k}-\mathbf{k}')}{\hbar}\Bigg\langle \mathrm{T}_\tau \Big[&-\omega_{\nu'}(\mathbf{k}-\mathbf{k}')b_{\nu'}(\tau,\mathbf{k}-\mathbf{k}') \\
&- \sum_{\substack{\widetilde{\mathbf{k}}\in\mathrm{Q}\\ \widetilde{\sigma}\in\{\uparrow,\downarrow\}\\ \widetilde{m},\widetilde{n}\in\{1,\dots,\infty\}}} \frac{g_{\widetilde{m}\widetilde{n}\nu'}(\widetilde{\mathbf{k}},\mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}} c^\dagger_{\widetilde{m}\widetilde{\sigma}}(\tau,\widetilde{\mathbf{k}}+\mathbf{k}'-\mathbf{k})c_{\widetilde{n}\widetilde{\sigma}}(\tau,\widetilde{\mathbf{k}})\Big] c_{n',\uparrow}(\tau',\mathbf{k}')c^\dagger_{n,\uparrow}(0,\mathbf{k})\Bigg\rangle_{\mathrm{SC}}
\end{aligned}
$$

and

$$\mathrm{II} = -\frac{\omega_{\nu'}(\mathbf{k}-\mathbf{k}')}{\hbar}\Bigg\langle \mathrm{T}_\tau\Bigg[+\omega_{\nu'}(\mathbf{k}'-\mathbf{k})b^\dagger_{\nu'}(\tau,\mathbf{k}'-\mathbf{k}) + \sum_{\substack{\widetilde{\mathbf{k}}\in\mathrm{Q}\\ \widetilde{\sigma}\in\{\uparrow,\downarrow\}\\ \widetilde{m},\widetilde{n}\in\{1,\dots,\infty\}}} \frac{g_{\widetilde{m}\widetilde{n}\nu'}(\widetilde{\mathbf{k}},\mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}} c^\dagger_{\widetilde{m}\widetilde{\sigma}}(\tau,\widetilde{\mathbf{k}}+\mathbf{k}'-\mathbf{k})c_{\widetilde{n}\widetilde{\sigma}}(\tau,\widetilde{\mathbf{k}})\Bigg]c_{n',\uparrow}(\tau',\mathbf{k}')c^\dagger_{n,\uparrow}(0,\mathbf{k})\Bigg\rangle_{\mathrm{SC}}$$

and collecting the individual contributions we obtain

$$\begin{aligned}\partial_\tau^2 \mathscr{G}^{\mathrm{aux}}_{\nu',n,n'}(\tau,\tau',\mathbf{k},\mathbf{k}') &= \omega^2_{\nu'}(\mathbf{k}-\mathbf{k}')\mathscr{G}^{\mathrm{aux}}_{\nu',n,n'}(\tau,\tau',\mathbf{k},\mathbf{k}') \\ &\quad - \frac{2\omega_{\nu'}(\mathbf{k}-\mathbf{k}')}{\hbar}\sum_{\substack{\widetilde{\mathbf{k}}\in\mathrm{Q}\\ \widetilde{\sigma}\in\{\uparrow,\downarrow\}\\ \widetilde{m},\widetilde{n}\in\{1,\dots,\infty\}}} \frac{g_{\widetilde{m}\widetilde{n}\nu'}(\widetilde{\mathbf{k}},\mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}}\left\langle \mathrm{T}_\tau\, c^\dagger_{\widetilde{m}\widetilde{\sigma}}(\tau,\widetilde{\mathbf{k}}+\mathbf{k}'-\mathbf{k})c_{\widetilde{n}\widetilde{\sigma}}(\tau,\widetilde{\mathbf{k}})c_{n',\uparrow}(\tau',\mathbf{k}')c^\dagger_{n,\uparrow}(0,\mathbf{k})\right\rangle_{\mathrm{SC}}\end{aligned} \tag{26.46}$$

Now rearranging terms and relabelling the summation-indices we obtain

$$\begin{aligned}&\left(\partial_\tau^2 - \omega^2_{\nu'}(\mathbf{k}-\mathbf{k}')\right)\mathscr{G}^{\mathrm{aux}}_{\nu',n,n'}(\tau,\tau',\mathbf{k},\mathbf{k}') \\ &= \frac{-2\omega_{\nu'}(\mathbf{k}-\mathbf{k}')}{\hbar}\sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ mm'\in\{1,\dots,\infty\}\\ \sigma\in\{\uparrow,\downarrow\}}} \frac{g_{mm'\nu'}(\mathbf{q},\mathbf{k}'-\mathbf{k})}{\hbar N_p}\left\langle \mathrm{T}_\tau\, c^\dagger_{m,\sigma}(\tau,\mathbf{q}+\mathbf{k}'-\mathbf{k})c_{m',\sigma}(\tau,\mathbf{q})c_{n',\uparrow}(\tau',\mathbf{k}')c^\dagger_{n,\uparrow}(0,\mathbf{k})\right\rangle_{\mathrm{SC}}\end{aligned}$$

Correction note. In the last equation the denominator has to be $\hbar\sqrt{N_p}$ (as in the line before and in the Lemma), not $\hbar N_p$. In the expression for II the factor $\omega_{\nu'}(\mathbf{k}'-\mathbf{k})$ equals $\omega_{\nu'}(\mathbf{k}-\mathbf{k}')$; then $\mathrm{I}+\mathrm{II} = -\frac{\omega^2}{\hbar}\langle \mathrm{T}_\tau(b+b^\dagger)c'c^\dagger\rangle - \frac{2\omega}{\hbar}\sum\ldots = \omega^2\mathscr{G}_{\mathrm{aux}} - \frac{2\omega}{\hbar}\sum\ldots$, as stated.

Remark 26.22.1 Notice that we used $\omega_\nu(\mathbf{q}) = \omega_\nu(-\mathbf{q})$, and hence used the time-reversal-symmetry of the crystal.

Corollary 26.23 It follows for the equal-time Green-function[10] the equation

$$\mathscr{G}^{\mathrm{aux}}_{n,n',\nu'}(\tau,\tau,\mathbf{k},\mathbf{k}') = -\oint\!\!\!\!\!\!\sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ \tau'\in[0,\hbar\beta]\\ m,m'\in\{1,\dots,\infty\}\\ \sigma\in\{\uparrow,\downarrow\}}} \mathscr{D}^{0,\nu}_{\mathbf{k}-\mathbf{k}'}(\tau-\tau')\frac{g_{mm'\nu'}(\mathbf{q},\mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}}\left\langle \mathrm{T}_\tau\, c^\dagger_{m,\sigma}(\tau',\mathbf{q}+\mathbf{k}'-\mathbf{k})c_{m',\sigma}(\tau',\mathbf{q})c_{n',\uparrow}(\tau,\mathbf{k}')c^\dagger_{n,\uparrow}(0,\mathbf{k})\right\rangle_{\mathrm{SC}}$$

Note. The phonon propagator carries the mode index ν', i.e. $\mathscr{D}^{0,\nu'}_{\mathbf{k}-\mathbf{k}'}$. The Corollary needs (i) $\omega_{\nu'}(\mathbf{k}-\mathbf{k}') > 0$, which is the reason for the assumption $\mathbf{k} \neq \mathbf{k}'$ in Lemma 26.22 (for acoustic modes $\omega_\nu(\mathbf{0}) = 0$ and $\mathscr{D}_0$ does not exist),

[10] Notice that Marsiglio has exchanged values for the couplings and he has no global minus-sign, which is because we defined our auxiliary-Green-function with a global minus-sign, which is more consistent with the usual definition of Green-functions.

and (ii) that $\tau' \mapsto \mathscr{G}_{\text{aux}}(\tau', \tau, \ldots)$ is $\hbar\beta$-periodic (bosonic in the phonon time), so that the boundary terms of the two integrations by parts in the proof cancel. In the normal state (ii) follows from the cyclicity of the trace; in the superconducting state it is part of the assumptions of the Fact on the Gorkov-Green-function.

Proof 26.23

First, we exchange[11] the roles of τ and τ' in the equations (26.42) and (26.43). This yields for the two equations

$$\partial_{\tau'} \mathscr{G}_{\substack{\text{aux}\\ \nu',n,n'}}(\tau', \tau, \mathbf{k}, \mathbf{k}') = +\frac{\omega_{\nu'}(\mathbf{k}-\mathbf{k}')}{\hbar} \left\langle \mathrm{T}_\tau \left(b_{\nu'}(\tau', \mathbf{k}-\mathbf{k}') - b^\dagger_{\nu'}(\tau', \mathbf{k}'-\mathbf{k}) \right) c_{n',\uparrow}(\tau, \mathbf{k}') c^\dagger_{n,\uparrow}(0, \mathbf{k}) \right\rangle_{\text{SC}}$$

$$\begin{aligned} &\left(\partial^2_{\tau'} - \omega^2_{\nu'}(\mathbf{k}-\mathbf{k}')\right) \mathscr{G}_{\substack{\text{aux}\\ \nu',n,n'}}(\tau', \tau, \mathbf{k}, \mathbf{k}') \\ &= \frac{-2\omega_{\nu'}(\mathbf{k}-\mathbf{k}')}{\hbar} \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ m,m'\in\{1,\ldots,\infty\} \\ \sigma\in\{\uparrow,\downarrow\}}} \frac{g_{mm'\nu'}(\mathbf{q}, \mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}} \left\langle \mathrm{T}_\tau\, c^\dagger_{m,\sigma}(\tau', \mathbf{q}+\mathbf{k}'-\mathbf{k}) c_{m',\sigma}(\tau', \mathbf{q}) c_{n',\uparrow}(\tau, \mathbf{k}') c^\dagger_{n,\uparrow}(0, \mathbf{k}) \right\rangle_{\text{SC}} \end{aligned} \tag{26.47}$$

Therefore, we start with equation (26.47) which is

$$\begin{aligned} &\left(\partial^2_{\tau'} - \omega^2_{\nu'}(\mathbf{k}-\mathbf{k}')\right) \mathscr{G}_{\substack{\text{aux}\\ \nu',n,n'}}(\tau', \tau, \mathbf{k}, \mathbf{k}') \\ &= \frac{-2\omega_{\nu'}(\mathbf{k}-\mathbf{k}')}{\hbar} \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ m,m'\in\{1,\ldots,\infty\} \\ \sigma\in\{\uparrow,\downarrow\}}} \frac{g_{mm'\nu'}(\mathbf{q}, \mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}} \left\langle \mathrm{T}_\tau\, c^\dagger_{m,\sigma}(\tau', \mathbf{q}+\mathbf{k}'-\mathbf{k}) c_{m',\sigma}(\tau', \mathbf{q}) c_{n',\uparrow}(\tau, \mathbf{k}') c^\dagger_{n,\uparrow}(0, \mathbf{k}) \right\rangle_{\text{SC}} \end{aligned}$$

we multiply both sides with $\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau - \tau')$, integrate τ' from 0 to $\hbar\beta$, perform two integration by parts and using the Equation (13.23) from Theorem 13.11.

$$\left(\partial^2_{\tau} - \omega^2_{\nu'}(\mathbf{k}-\mathbf{k}')\right) \mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau - \tau') = 2\omega_{\nu'}(\mathbf{k}-\mathbf{k}')\delta(\tau-\tau')/\hbar$$

Notice that the left hand side of this has the unit $\frac{1}{\text{time}^2}\frac{1}{\text{Energy}\times\text{time}}$ in complete harmony with the r.h.s. of this equation. This yields

$$\begin{aligned} &\int_0^{\hbar\beta} \mathrm{d}\tau' \, \mathscr{G}_{\substack{\text{aux}\\ \nu',n,n'}}(\tau', \tau, \mathbf{k}, \mathbf{k}') \left(\partial^2_{\tau'} - \omega^2_{\nu'}(\mathbf{k}-\mathbf{k}')\right) \mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau - \tau') \\ &= \frac{+2\omega_{\nu'}(\mathbf{k}-\mathbf{k}')}{\hbar} \mathscr{G}_{\substack{\text{aux}\\ \nu',n,n'}}(\tau, \tau, \mathbf{k}, \mathbf{k}) \\ &= \int_0^{\hbar\beta} \mathrm{d}\tau' \, \mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau - \tau') \frac{-2\omega_{\nu'}(\mathbf{k}-\mathbf{k}')}{\hbar} \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ m,m'\in\{1,\ldots,\infty\} \\ \sigma\in\{\uparrow,\downarrow\}}} \frac{g_{mm'\nu'}(\mathbf{q}, \mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}} \left\langle \mathrm{T}_\tau\, c^\dagger_{m,\sigma}(\tau', \mathbf{q}+\mathbf{k}'-\mathbf{k}) c_{m',\sigma}(\tau', \mathbf{q}) c_{n',\uparrow}(\tau, \mathbf{k}') c^\dagger_{n,\uparrow}(0, \mathbf{k}) \right\rangle_{\text{SC}} \end{aligned} \tag{26.48}$$

[11] Notice that this has no influence on the time-ordering-operator which has the unconvenient notation of a τ in its index.

simplifying both sides gives then the final result

$$\mathscr{G}^{\text{aux}}_{\nu',n,n'}(\tau,\tau,\mathbf{k},\mathbf{k}') = \sum\!\!\!\!\!\!\int_{\substack{\mathbf{q}\in\mathrm{Q}\\ \tau'\in[0,\hbar\beta]\\ m,m'\in\{1,\dots,\infty\}\\ \sigma\in\{\uparrow,\downarrow\}}} (-1)\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\frac{g_{mm'\nu'}(\mathbf{q},\mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}}\left\langle \mathrm{T}_\tau\, c^\dagger_{m,\sigma}(\tau',\mathbf{q}+\mathbf{k}'-\mathbf{k})c_{m',\sigma}(\tau',\mathbf{q})c_{n',\uparrow}(\tau,\mathbf{k}')c^\dagger_{n,\uparrow}(0,\mathbf{k})\right\rangle \tag{26.49}$$

Notice that this equation has again the right units (1 / Energy x time x time on both sides).

Correction note. In the middle line of the equation before, the last argument is $\mathbf{k}'$, i.e. $\mathscr{G}_{\text{aux}}(\tau,\tau,\mathbf{k},\mathbf{k}')$, not $(\tau,\tau,\mathbf{k},\mathbf{k})$. For completeness, the step "two integrations by parts" reads

$$\int_0^{\hbar\beta}\mathrm{d}\tau'\,\mathscr{G}_{\text{aux}}(\tau',\tau)\big(\partial^2_{\tau'}-\omega^2\big)\mathscr{D}_0(\tau-\tau') = \int_0^{\hbar\beta}\mathrm{d}\tau'\,\mathscr{D}_0(\tau-\tau')\big(\partial^2_{\tau'}-\omega^2\big)\mathscr{G}_{\text{aux}}(\tau',\tau) + \Big[\mathscr{G}_{\text{aux}}\,\partial_{\tau'}\mathscr{D}_0 - \mathscr{D}_0\,\partial_{\tau'}\mathscr{G}_{\text{aux}}\Big]^{\tau'=\hbar\beta}_{\tau'=0},$$

where the boundary term vanishes because both functions are $\hbar\beta$-periodic in τ'. The first integral is evaluated with $(\partial^2_{\tau'}-\omega^2)\mathscr{D}_0(\tau-\tau') = 2\omega\,\delta(\tau-\tau')/\hbar$, the second one with Equation (26.47); dividing by $2\omega/\hbar \neq 0$ gives the result.

Remark 26.23.1 Notice that now the equation of motion (26.41) can be rewritten as

$$\begin{aligned}&\left(\partial_\tau + \frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\right)\mathscr{G}^{\ n}_{\text{Gorkov}}(\tau,\mathbf{k})\\ &= -\frac{1}{\hbar}\delta(\tau)\\ &+ \sum\!\!\!\!\!\!\int_{\substack{\mathbf{q},\mathbf{k}'\in\mathrm{Q}\\ \tau'\in(0,\hbar\beta)\\ \nu'\in\{1,\dots,rd_{\mathrm{x}}\}\\ m,m',n'\in\{1,\dots,\infty\}\\ \sigma\in\{\uparrow,\downarrow\}}} \frac{g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')g_{mm'\nu'}(\mathbf{q},\mathbf{k}'-\mathbf{k})}{\hbar^2 N_p}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\left\langle \mathrm{T}_\tau\, c^\dagger_{m,\sigma}(\tau',\mathbf{q}+\mathbf{k}'-\mathbf{k})c_{m',\sigma}(\tau',\mathbf{q})c_{n',\uparrow}(\tau,\mathbf{k}')c^\dagger_{n,\uparrow}(0,\mathbf{k})\right\rangle_{\text{SC}}\end{aligned} \tag{26.50}$$

Theorem 26.24 Neglecting vertex-corrections allows us to rewrite the equation of motion as

$$\begin{aligned}&\left(\partial_\tau + \frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\right)\mathscr{G}^{\ n}_{\text{Gorkov}}(\tau,\mathbf{k})\\ &= -\frac{1}{\hbar}\delta(\tau) + \sum\!\!\!\!\!\!\int_{\substack{\tau'\in(0,\hbar\beta)\\ \mathbf{k}'\in\mathrm{Q}\\ n'\in\{1,\dots,\infty\}\\ \nu'\in\{1,\dots,rd_{\mathrm{x}}\}}} \frac{|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{N_p}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\big[\mathscr{G}^{\ n}_{\text{Gorkov}}(\tau',\mathbf{k})\mathscr{G}^{\ n'}_{\text{Gorkov}}(\tau-\tau',+\mathbf{k}') - \mathscr{F}_{n'}(\tau-\tau',\mathbf{k})\mathscr{F}^\dagger_n(\tau',\mathbf{k})\big]\end{aligned} \tag{26.51}$$

Note on the approximations. The proof uses three ingredients, which should be stated explicitly: (a) the vertex-correction in Equation (15.19) is neglected (Migdal); (b) the decoupling is done with *normal* Nambu-contractions $\langle \mathrm{T}_\tau\,\eta\bar{\eta}\rangle$ only. This is exact once (a) is assumed, since the possible anomalous Nambu-contractions $\langle \mathrm{T}_\tau\,\eta_1\eta_1\rangle$, $\langle \mathrm{T}_\tau\,\eta_1\eta_2\rangle$, $\langle \mathrm{T}_\tau\,\eta_2\eta_2\rangle$ are $\langle c_\uparrow c_\uparrow\rangle$, $\langle c_\uparrow c^\dagger_\downarrow\rangle$, $\langle c^\dagger_\downarrow c^\dagger_\downarrow\rangle$, which vanish for spin-singlet pairing with conserved S_z. In addition

the Gorkov-Green-function is assumed to be band-diagonal, $\widehat{\mathscr{G}}_{n'n} = \delta_{n'n}\widehat{\mathscr{G}}_n$; (c) the terms (I,1) and (II,4) are dropped. Both have $\mathbf{k}' = \mathbf{k}$, i.e. zero phonon momentum. This is exactly the case that is excluded in Lemma 26.22 and Corollary 26.23. Physically, these are (static) Hartree-terms, since $\int \mathrm{d}\tau' \mathscr{D}_0(\tau - \tau') = \mathscr{D}_0(\mathrm{i}0)$ does not depend on τ; they shift $\epsilon_n(\mathbf{k}) - \mu$ by a frequency-independent amount and can be absorbed into the band energies.

Remark 26.24.1 Notice that both sides of this Equation have the (correct) unit Energy^{-1} × Time^{-2}.

Remark 26.24.2 Notice that the terms on the r.h.s. of this Equation are (II,3) and (I,2).

Proof 26.24 We combine the approximation of the Bethe-Salpether-equation with Remark 26.23.1: The Bethe-Salpeter-equation (15.19), in which one neglects the vertex-correction, reads

$$\mathscr{G}(i_1, i_2|i_1', i_2') \approx \mathscr{G}(i_1|i_1')\mathscr{G}(i_2|i_2') + \zeta\mathscr{G}(i_1|i_2')\mathscr{G}(i_2|i_1') \tag{26.52}$$

The left hand side of this equation is

$$\mathscr{G}(i_1, i_2|i_1', i_2') = \left(-\frac{1}{\hbar}\right)^2 \left\langle \mathrm{T}_\tau\, c_{i_1} c_{i_2} c_{i_2'}^\dagger c_{i_1'}^\dagger \right\rangle \tag{26.53}$$

Now, following Definition 44.8, we introduce the following notation

$$c_{m\sigma}^\dagger(\tau', \mathbf{q} + \mathbf{k}' - \mathbf{k}) = \begin{cases} \eta_{m,2}(\tau', -\mathbf{q} - \mathbf{k}' + \mathbf{k}) & \text{if } \sigma = \downarrow \\ \overline{\eta}_{m,1}(\tau', \mathbf{q} + \mathbf{k}' - \mathbf{k}) & \text{if } \sigma = \uparrow \end{cases} \tag{26.54}$$

and

$$c_{m'\sigma}(\tau, \mathbf{q}) = \begin{cases} \overline{\eta}_{m',2}(\tau, -\mathbf{q}) & \text{if } \sigma = \downarrow \\ \eta_{m',1}(\tau, \mathbf{q}) & \text{if } \sigma = \uparrow \end{cases} \tag{26.55}$$

and hence also $c_{n'\uparrow}(\tau, \mathbf{k}') \equiv \eta_{n',1}(\tau, \mathbf{k}')$, and $c_{n\uparrow}^\dagger(0, \mathbf{k}) \equiv \overline{\eta}_{n,1}(0, \mathbf{k})$.

This gives thus for the sum from Equation (26.50)

$$\begin{aligned} &\sum_{\sigma\in\{\downarrow,\uparrow\}} \left\langle \mathrm{T}_\tau\, c_{m,\sigma}^\dagger(\tau', \mathbf{q} + \mathbf{k}' - \mathbf{k}) c_{m',\sigma}(\tau', \mathbf{q}) c_{n',\uparrow}(\tau, \mathbf{k}') c_{n,\uparrow}^\dagger(0, \mathbf{k}) \right\rangle \\ &= \left\langle \mathrm{T}_\tau\, \eta_{m,2}(\tau', -\mathbf{q} - \mathbf{k}' + \mathbf{k}) \overline{\eta}_{m',2}(\tau', -\mathbf{q}) \eta_{n',1}(\tau, \mathbf{k}') \overline{\eta}_{n,1}(0, \mathbf{k}) \right\rangle \\ &\quad + \left\langle \mathrm{T}_\tau\, \overline{\eta}_{m,1}(\tau', +\mathbf{q} + \mathbf{k}' - \mathbf{k}) \eta_{m',1}(\tau', +\mathbf{q}) \eta_{n',1}(\tau, \mathbf{k}') \overline{\eta}_{n,1}(0, \mathbf{k}) \right\rangle \\ &= \left\langle \mathrm{T}_\tau\, \eta_{n',1}(\tau, \mathbf{k}') \eta_{m,2}(\tau', -\mathbf{q} - \mathbf{k}' + \mathbf{k}) \overline{\eta}_{m',2}(\tau', -\mathbf{q}) \overline{\eta}_{n,1}(0, \mathbf{k}) \right\rangle \\ &\quad + \left\langle \mathrm{T}_\tau\, \eta_{m',1}(\tau', +\mathbf{q}) \eta_{n',1}(\tau, \mathbf{k}') \overline{\eta}_{m,1}(\tau', +\mathbf{q} + \mathbf{k}' - \mathbf{k}) \overline{\eta}_{n,1}(0, \mathbf{k}) \right\rangle \\ &\equiv \mathrm{I} + \mathrm{II} \end{aligned} \tag{26.56}$$

Now we use the decoupling for the $\sigma = \downarrow$ contribution (for the first of the two consecutive lines)

$$
\begin{aligned}
\mathrm{I} &= \hbar^2 \mathscr{G}\left(i_1 = \left[n', 1, \tau, \mathbf{k}'\right], \quad i_2 = \left[m, 2, \tau', -\mathbf{q} - \mathbf{k}' + \mathbf{k}\right] \quad | \quad i_1' = \left[n, 1, 0, \mathbf{k}\right], \quad i_2' = \left[m', 2, \tau', -\mathbf{q}\right]\right) \\
&\approx \hbar^2 \underset{1,1}{\mathscr{G}_{n',n}}(\tau - 0; \mathbf{k}', \mathbf{k}) \underset{2,2}{\mathscr{G}_{m,m'}}(0; -\mathbf{q} - \mathbf{k}' + \mathbf{k}, -\mathbf{q}) \quad - \quad \hbar^2 \underset{1,2}{\mathscr{G}_{n',m'}}(\tau - \tau'; \mathbf{k}', -\mathbf{q}) \underset{2,1}{\mathscr{G}_{m,n}}(\tau'; -\mathbf{q} - \mathbf{k}' + \mathbf{k}, \mathbf{k}) \\
&= \hbar^2 \delta_{n,n'} \delta_{m,m'} \delta_{\mathbf{k},\mathbf{k}'} \underset{1,1}{\mathscr{G}_{n}}(\tau, \mathbf{k}) \underset{2,2}{\mathscr{G}_{m}}(0, -\mathbf{q}) \quad - \quad \hbar^2 \delta_{n',m'} \delta_{m,n} \delta_{\mathbf{k}',-\mathbf{q}} \underset{1,2}{\mathscr{G}_{n'}}(\tau - \tau', \mathbf{k}') \underset{2,1}{\mathscr{G}_{m}}(\tau', \mathbf{k}) \\
&= \hbar^2 - \delta_{n,n'} \delta_{m,m'} \delta_{\mathbf{k},\mathbf{k}'} \underset{\text{Gorkov}}{\mathscr{G}_{n}}(\tau, \mathbf{k}) \underset{\text{Gorkov}}{\mathscr{G}_{m}}(0, +\mathbf{q}) \quad - \quad \hbar^2 \delta_{n',m'} \delta_{m,n} \delta_{\mathbf{k}',-\mathbf{q}} \mathscr{F}_{n'}(\tau - \tau', \mathbf{k}') \mathscr{F}_{n}^{\dagger}(\tau', \mathbf{k})
\end{aligned}
$$

Note. In the last line, "$\hbar^2 - \delta$" means $-\hbar^2\delta$. The minus sign comes from the equal-time Nambu-function $(\widehat{\mathscr{G}}_m)_{22}(0, -\mathbf{q}) = -\frac{1}{\hbar}\langle c_{m\downarrow}^{\dagger}(\mathbf{q}) c_{m\downarrow}(\mathbf{q})\rangle_{\mathrm{SC}} = -\underset{\text{Gorkov}}{\mathscr{G}_{m}}(0^-, \mathbf{q})$. Here and below, the equal-time arguments "0" of the Hartree-terms mean 0^-, because the operator pair $c^{\dagger}(\tau')c(\tau')$ stays normal ordered inside T_{τ}.

whereas we used Definition 26.11 in the last equation. Now inserting this into the r.h.s. of Equation (26.50) yields (in addition to the delta-functions) two terms

$$
\begin{aligned}
(\mathrm{I}, 1) &= -1 \cdot \sum\!\!\!\!\!\!\int_{\substack{\tau' \in (0,\hbar\beta) \\ \mathbf{q},\mathbf{k}' \in \mathrm{Q} \\ m,m',n' \in \{1,\ldots,\infty\} \\ \nu' \in \{1,\ldots,rd_{\mathbf{x}}\}}} \frac{g_{nn'\nu'}(\mathbf{k}', \mathbf{k} - \mathbf{k}') g_{mm'\nu'}(\mathbf{q}, \mathbf{k}' - \mathbf{k})}{\hbar^2 N_p} \underset{\mathbf{k}-\mathbf{k}'}{\mathscr{D}_{0,\nu'}}(\tau - \tau') \delta_{n,n'} \delta_{m,m'} \delta_{\mathbf{k},\mathbf{k}'} \underset{\text{Gorkov}}{\mathscr{G}_{n}}(\tau, \mathbf{k}) \underset{\text{Gorkov}}{\mathscr{G}_{m}}(0, +\mathbf{q}) \hbar^2 \\
&= -1 \cdot \sum\!\!\!\!\!\!\int_{\substack{\tau' \in (0,\hbar\beta) \\ \mathbf{q} \in \mathrm{Q} \\ m \in \{1,\ldots,\infty\} \\ \nu' \in \{1,\ldots,rd_{\mathbf{x}}\}}} \frac{g_{nn\nu'}(\mathbf{k}', 0) g_{mm\nu'}(\mathbf{q}, 0)}{N_p \hbar^2} \underset{\mathbf{0}}{\mathscr{D}_{0,\nu'}}(\tau - \tau') \underset{\text{Gorkov}}{\mathscr{G}_{n}}(\tau, \mathbf{k}) \underset{\text{Gorkov}}{\mathscr{G}_{m}}(0, +\mathbf{q}) \hbar^2
\end{aligned}
\tag{26.57}
$$

Correction note. After terminating the sum over $\mathbf{k}'$ the first coupling is $g_{nn\nu'}(\mathbf{k}, 0)$, not $g_{nn\nu'}(\mathbf{k}', 0)$.

and the second term can be treated similarly, yielding

$$
\begin{aligned}
(\mathrm{I}, 2) &= -1 \cdot \sum\!\!\!\!\!\!\int_{\substack{\tau' \in (0,\hbar\beta) \\ \mathbf{q},\mathbf{k}' \in \mathrm{Q} \\ m,m',n' \in \{1,\ldots,\infty\} \\ \nu' \in \{1,\ldots,rd_{\mathbf{x}}\}}} \frac{g_{nn'\nu'}(\mathbf{k}', \mathbf{k} - \mathbf{k}') g_{mm'\nu'}(\mathbf{q}, \mathbf{k}' - \mathbf{k})}{\hbar^2 N_p} \underset{\mathbf{k}-\mathbf{k}'}{\mathscr{D}_{0,\nu'}}(\tau - \tau') \delta_{n',m'} \delta_{m,n} \delta_{\mathbf{k}',-\mathbf{q}} \mathscr{F}_{n'}(\tau - \tau', \mathbf{k}') \mathscr{F}_{n}^{\dagger}(\tau', \mathbf{k}) \hbar^2 \\
&= -1 \cdot \sum\!\!\!\!\!\!\int_{\substack{\tau' \in (0,\hbar\beta) \\ \mathbf{q} \in \mathrm{Q} \\ n' \in \{1,\ldots,\infty\} \\ \nu' \in \{1,\ldots,rd_{\mathbf{x}}\}}} \frac{g_{nn'\nu'}(-\mathbf{q}, \mathbf{k} + \mathbf{q}) g_{nn'\nu'}(\mathbf{q}, -\mathbf{q} - \mathbf{k})}{N_p \hbar^2} \underset{\mathbf{k}+\mathbf{q}}{\mathscr{D}_{0,\nu'}}(\tau - \tau') \mathscr{F}_{n'}(\tau - \tau', -\mathbf{q}) \mathscr{F}_{n}^{\dagger}(\tau', \mathbf{k}) \hbar^2 \\
&= -1 \cdot \sum\!\!\!\!\!\!\int_{\substack{\tau' \in (0,\hbar\beta) \\ \mathbf{q} \in \mathrm{Q} \\ n' \in \{1,\ldots,\infty\} \\ \nu' \in \{1,\ldots,rd_{\mathbf{x}}\}}} \frac{|g_{nn'\nu'}(\mathbf{q}, -\mathbf{q} - \mathbf{k})|^2}{N_p} \underset{\mathbf{k}+\mathbf{q}}{\mathscr{D}_{0,\nu'}}(\tau - \tau') \mathscr{F}_{n'}(\tau - \tau', -\mathbf{q}) \mathscr{F}_{n}^{\dagger}(\tau', \mathbf{k})
\end{aligned}
\tag{26.58}
$$

whereas we terminated the summations over m and m' in the second last equation-sign and we used the inversion-symmetry for the couplings in the last equation-sign. Now we do the same procedure for the other term in Equation (26.56), i.e. the second line, giving

$$
\begin{aligned}
\mathrm{II} &= \hbar^2 \mathscr{G}\left(i_1 = [m', 1, \tau', \mathbf{q}], \quad i_2 = [n', 1, \tau, \mathbf{k}'] \quad | \quad i_1' = [n, 1, 0, \mathbf{k}], \quad i_2' = [m, 1, \tau', +\mathbf{q} + \mathbf{k}' - \mathbf{k}]\right) \\
&\approx \hbar^2 \underset{\substack{1,1\\ \mathbf{q},\mathbf{k}}}{\mathscr{G}_{m',n}}(\tau' - 0) \underset{\substack{1,1\\ \mathbf{k}',+\mathbf{q}}}{\mathscr{G}_{n',m}}(\tau - \tau') \quad - \quad \hbar^2 \underset{\substack{1,1\\ \mathbf{q},+\mathbf{q}}}{\mathscr{G}_{m',m}}(0) \underset{\substack{1,1\\ \mathbf{k}',\mathbf{k}}}{\mathscr{G}_{n',n}}(\tau - 0) \\
&= \hbar^2 \delta_{m',n}\delta_{n',m}\delta_{\mathbf{q},\mathbf{k}}\delta_{\mathbf{q},\mathbf{k}'} \underset{\substack{1,1\\ \mathbf{k}}}{\mathscr{G}_{n}}(\tau') \underset{\substack{1,1\\ +\mathbf{k}'}}{\mathscr{G}_{m}}(\tau - \tau') \quad - \quad \hbar^2 \delta_{m',m}\delta_{n',n}\delta_{\mathbf{q},+\mathbf{q}}\delta_{\mathbf{k}',\mathbf{k}} \underset{\substack{1,1\\ +\mathbf{q}}}{\mathscr{G}_{m}}(0) \underset{\substack{1,1\\ \mathbf{k}}}{\mathscr{G}_{n}}(\tau - 0) \\
&= \hbar^2 \delta_{m',n}\delta_{n',m}\delta_{\mathbf{q},\mathbf{k}}\delta_{\mathbf{q},\mathbf{k}'} \mathscr{G}_{n,\mathrm{Gorkov}}(\tau', \mathbf{k}) \mathscr{G}_{m,\mathrm{Gorkov}}(\tau - \tau', +\mathbf{k}') \quad - \quad \hbar^2 \delta_{m',m}\delta_{n',n}\delta_{\mathbf{q},+\mathbf{q}}\delta_{\mathbf{k}',\mathbf{k}} \mathscr{G}_{m,\mathrm{Gorkov}}(0, +\mathbf{q}) \mathscr{G}_{n,\mathrm{Gorkov}}(\tau, \mathbf{k})
\end{aligned}
$$

Correction note (this resolves the "lost Kronecker-delta" below). Since $i_2' = [m, 1, \tau', \mathbf{q} + \mathbf{k}' - \mathbf{k}]$, the second momentum index of $\mathscr{G}(i_2|i_2')$ and of $\mathscr{G}(i_1|i_2')$ is $\mathbf{q} + \mathbf{k}' - \mathbf{k}$, not $+\mathbf{q}$. With translation invariance this gives

$$
\underset{\substack{1,1\\ \mathbf{k}',\mathbf{q}+\mathbf{k}'-\mathbf{k}}}{\mathscr{G}_{n',m}}(\tau - \tau') = \delta_{n',m}\delta_{\mathbf{q},\mathbf{k}} \mathscr{G}_{n',\mathrm{Gorkov}}(\tau - \tau', \mathbf{k}') \quad \text{and} \quad \underset{\substack{1,1\\ \mathbf{q},\mathbf{q}+\mathbf{k}'-\mathbf{k}}}{\mathscr{G}_{m',m}}(0) = \delta_{m',m}\delta_{\mathbf{k}',\mathbf{k}} \mathscr{G}_{m,\mathrm{Gorkov}}(0^-, \mathbf{q}).
$$

Hence the first term carries $\delta_{\mathbf{q},\mathbf{k}}$ twice (once from each factor), i.e. only *one* independent Kronecker-delta $\delta_{\mathbf{q},\mathbf{k}}$ and no $\delta_{\mathbf{q},\mathbf{k}'}$; the second term carries $\delta_{\mathbf{k}',\mathbf{k}}$ (the $\delta_{\mathbf{q},\mathbf{q}} = 1$ is trivial). The correct result is

$$
\mathrm{II} \approx \hbar^2 \delta_{m',n}\delta_{n',m}\delta_{\mathbf{q},\mathbf{k}} \mathscr{G}_{n,\mathrm{Gorkov}}(\tau', \mathbf{k}) \mathscr{G}_{n',\mathrm{Gorkov}}(\tau - \tau', \mathbf{k}') - \hbar^2 \delta_{m',m}\delta_{n',n}\delta_{\mathbf{k}',\mathbf{k}} \mathscr{G}_{m,\mathrm{Gorkov}}(0^-, \mathbf{q}) \mathscr{G}_{n,\mathrm{Gorkov}}(\tau, \mathbf{k}).
$$

In (II,3) below one therefore terminates only the sums over m, m' and $\mathbf{q}$, and the sum over $\mathbf{k}'$ survives, as in the second line of (II,3). Nothing is lost.

whereas we used Definition 26.11 in the last equation.

Now we insert this into Equation (26.50), giving two additional terms

$$
\begin{aligned}
(\mathrm{II},3) &= \sum_{\substack{\tau' \in (0,\hbar\beta)\\ \mathbf{q},\mathbf{k}' \in \mathrm{Q}\\ m,m',n' \in \{1,\dots,\infty\}\\ \nu' \in \{1,\dots,rd_{\mathbf{x}}\}}} \frac{g_{nn'\nu'}(\mathbf{k}', \mathbf{k} - \mathbf{k}') g_{mm'\nu'}(\mathbf{q}, \mathbf{k}' - \mathbf{k})}{\hbar^2 N_p} \mathscr{D}_{\mathbf{k}-\mathbf{k}',\nu'}(\tau - \tau') \delta_{m',n}\delta_{n',m}\delta_{\mathbf{q},\mathbf{k}}\delta_{\mathbf{q},\mathbf{k}'} \mathscr{G}_{n,\mathrm{Gorkov}}(\tau', \mathbf{k}) \mathscr{G}_{m,\mathrm{Gorkov}}(\tau - \tau', +\mathbf{k}') \hbar^2 \\
&= \sum_{\substack{\tau' \in (0,\hbar\beta)\\ \mathbf{k}' \in \mathrm{Q}\\ n' \in \{1,\dots,\infty\}\\ \nu' \in \{1,\dots,rd_{\mathbf{x}}\}}} \frac{g_{nn'\nu'}(\mathbf{k}', \mathbf{k} - \mathbf{k}') g_{n'n\nu'}(\mathbf{k}, \mathbf{k}' - \mathbf{k})}{N_p} \mathscr{D}_{\mathbf{k}-\mathbf{k}',\nu'}(\tau - \tau') \mathscr{G}_{n,\mathrm{Gorkov}}(\tau', \mathbf{k}) \mathscr{G}_{n',\mathrm{Gorkov}}(\tau - \tau', +\mathbf{k}') \\
&= \sum_{\substack{\tau' \in (0,\hbar\beta)\\ \mathbf{k}' \in \mathrm{Q}\\ n' \in \{1,\dots,\infty\}\\ \nu' \in \{1,\dots,rd_{\mathbf{x}}\}}} \frac{|g_{n'n\nu'}(\mathbf{k}, \mathbf{k}' - \mathbf{k})|^2}{N_p} \mathscr{D}_{\mathbf{k}-\mathbf{k}',\nu'}(\tau - \tau') \mathscr{G}_{n,\mathrm{Gorkov}}(\tau', \mathbf{k}) \mathscr{G}_{n',\mathrm{Gorkov}}(\tau - \tau', +\mathbf{k}')
\end{aligned}
\tag{26.59}
$$

whereas in the second last equation, we terminated the summations over m and m' and $\mathbf{q}$, and in the last equation we used the hermiticity of the couplings and something went wrong because we lost a Kronecker-delta. (Resolved: $\delta_{\mathbf{q},\mathbf{k}'}$ should have been $\delta_{\mathbf{q},\mathbf{k}}$, see the note above. The hermiticity $g_{n'n\nu'}(\mathbf{k}, \mathbf{k}' - \mathbf{k}) = g^*_{nn'\nu'}(\mathbf{k}', \mathbf{k} - \mathbf{k}')$, Lemma 8.37, gives $|g_{n'n\nu'}(\mathbf{k}, \mathbf{k}' - \mathbf{k})|^2 = |g_{nn'\nu'}(\mathbf{k}', \mathbf{k} - \mathbf{k}')|^2$, which is used in the last step below.). And for the other term we obtain

$$
\begin{aligned}
(\mathrm{II},4) &= -1 \cdot \sum\!\!\!\!\!\!\int_{\substack{\tau' \in (0,\hbar\beta) \\ \mathbf{q},\mathbf{k}' \in \mathrm{Q} \\ m,m',n' \in \{1,\ldots,\infty\} \\ \nu' \in \{1,\ldots,rd_{\mathbf{x}}\}}} \frac{g_{nn'\nu'}(\mathbf{k}', \mathbf{k}-\mathbf{k}') g_{mm'\nu'}(\mathbf{q}, \mathbf{k}'-\mathbf{k})}{\hbar^2 N_p} \underset{\mathbf{k}-\mathbf{k}'}{\mathscr{D}_{0,\nu'}}(\tau-\tau') \delta_{m',m}\delta_{n',n}\delta_{\mathbf{q},+\mathbf{q}}\delta_{\mathbf{k}',\mathbf{k}} \mathscr{G}_{\substack{m \\ \mathrm{Gorkov}}}(0,+\mathbf{q}) \mathscr{G}_{\substack{n \\ \mathrm{Gorkov}}}(\tau,\mathbf{k}) \\
&= -1 \cdot \sum\!\!\!\!\!\!\int_{\substack{\tau' \in (0,\hbar\beta) \\ \mathbf{q} \in \mathrm{Q} \\ m \in \{1,\ldots,\infty\} \\ \nu' \in \{1,\ldots,rd_{\mathbf{x}}\}}} \frac{g_{nn\nu'}(\mathbf{k}, 0) g_{mm\nu'}(\mathbf{q}, 0)}{N_p} \underset{0}{\mathscr{D}_{0,\nu'}}(\tau-\tau') \mathscr{G}_{\substack{m \\ \mathrm{Gorkov}}}(0,+\mathbf{q}) \mathscr{G}_{\substack{n \\ \mathrm{Gorkov}}}(\tau,\mathbf{k})
\end{aligned}
\tag{26.60}
$$

whereas we terminated the summations over m', n' and $\mathbf{k}'$ in the last equation.

Standard Eliashberg-theory now assumes $g(\mathbf{k}, 0) = 0$, i.e. restricting attention to systems with only one atom per unit cell.

Now we collect the non-vanishing contributions and obtain

$$
\begin{aligned}
&\left(\partial_\tau + \frac{\epsilon_n(\mathbf{k}) - \mu}{\hbar}\right) \mathscr{G}_{\substack{n \\ \mathrm{Gorkov}}}(\tau,\mathbf{k}) \\
&= -\frac{1}{\hbar}\delta(\tau) - \sum\!\!\!\!\!\!\int_{\substack{\tau' \in (0,\hbar\beta) \\ \mathbf{q} \in \mathrm{Q} \\ n' \in \{1,\ldots,\infty\} \\ \nu' \in \{1,\ldots,rd_{\mathbf{x}}\}}} \left(|g_{nn'\nu'}(-\mathbf{q}, \mathbf{k}+\mathbf{q})|^2/(N_p\hbar)\right) \underset{\mathbf{k}+\mathbf{q}}{\mathscr{D}_{0,\nu'}}(\tau-\tau') \mathscr{F}_{n'}(\tau-\tau', -\mathbf{q}) \mathscr{F}_n^\dagger(\tau', \mathbf{k}) \hbar^2 \\
&+ \sum\!\!\!\!\!\!\int_{\substack{\tau' \in (0,\hbar\beta) \\ \mathbf{k}' \in \mathrm{Q} \\ n' \in \{1,\ldots,\infty\} \\ \nu' \in \{1,\ldots,rd_{\mathbf{x}}\}}} \left(|g_{n'n\nu'}(\mathbf{k}, \mathbf{k}'-\mathbf{k})|^2/(N_p\hbar)\right) \underset{\mathbf{k}-\mathbf{k}'}{\mathscr{D}_{0,\nu'}}(\tau-\tau') \mathscr{G}_{\substack{n \\ \mathrm{Gorkov}}}(\tau',\mathbf{k}) \mathscr{G}_{\substack{n' \\ \mathrm{Gorkov}}}(\tau-\tau', +\mathbf{k}') \hbar^2 \\
&\overset{\mathbf{q}\mapsto-\mathbf{k}'}{=} -\frac{1}{\hbar}\delta(\tau) - \sum\!\!\!\!\!\!\int_{\substack{\tau' \in (0,\hbar\beta) \\ \mathbf{k}' \in \mathrm{Q} \\ n' \in \{1,\ldots,\infty\} \\ \nu' \in \{1,\ldots,rd_{\mathbf{x}}\}}} \left(|g_{nn'\nu'}(\mathbf{k}', \mathbf{k}-\mathbf{k}')|^2/(N_p\hbar)\right) \underset{\mathbf{k}-\mathbf{k}'}{\mathscr{D}_{0,\nu'}}(\tau-\tau') \mathscr{F}_{n'}(\tau-\tau', \mathbf{k}') \mathscr{F}_n^\dagger(\tau', \mathbf{k}) \hbar^2 \\
&+ \sum\!\!\!\!\!\!\int_{\substack{\tau' \in (0,\hbar\beta) \\ \mathbf{k}' \in \mathrm{Q} \\ n' \in \{1,\ldots,\infty\} \\ \nu' \in \{1,\ldots,rd_{\mathbf{x}}\}}} \left(|g_{n'n\nu'}(\mathbf{k}, \mathbf{k}'-\mathbf{k})|^2/(N_p\hbar)\right) \underset{\mathbf{k}-\mathbf{k}'}{\mathscr{D}_{0,\nu'}}(\tau-\tau') \mathscr{G}_{\substack{n \\ \mathrm{Gorkov}}}(\tau',\mathbf{k}) \mathscr{G}_{\substack{n' \\ \mathrm{Gorkov}}}(\tau-\tau', +\mathbf{k}') \hbar^2 \\
&= \ldots
\end{aligned}
\tag{26.61}
$$

and this gives then

$$
\begin{aligned}
\ldots &= -\frac{1}{\hbar}\delta(\tau) \\
&+ \sum\!\!\!\!\!\!\int_{\substack{\tau' \in (0,\hbar\beta) \\ \mathbf{k}' \in \mathrm{Q} \\ n' \in \{1,\ldots,\infty\} \\ \nu' \in \{1,\ldots,rd_{\mathbf{x}}\}}} \hbar^2 \left(|g_{nn'\nu'}(\mathbf{k}', \mathbf{k}-\mathbf{k}')|^2/(N_p\hbar)\right) \underset{\mathbf{k}-\mathbf{k}'}{\mathscr{D}_{0,\nu'}}(\tau-\tau') \left[\mathscr{G}_{\substack{n \\ \mathrm{Gorkov}}}(\tau',\mathbf{k}) \mathscr{G}_{\substack{n' \\ \mathrm{Gorkov}}}(\tau-\tau', +\mathbf{k}') - \mathscr{F}_{n'}(\tau-\tau', \mathbf{k}') \mathscr{F}_n^\dagger(\tau', \mathbf{k})\right]
\end{aligned}
\tag{26.62}
$$

Correction note. In the last two equations the prefactor has to be $|g|^2/N_p$, as in the final lines of (I,2) and (II,3), i.e. "$\hbar^2\,(|g|^2/(N_p\hbar))$" has to be replaced by $|g|^2/N_p$. The $\hbar^2$ from the decoupling cancels the $1/\hbar^2$ of Equation (26.50), and no further $1/\hbar$ appears. With this the result agrees with the Theorem, including the unit check of the Remark after it. In the last step one additionally uses $|g_{n'n\nu'}(\mathbf{k}, \mathbf{k}'-\mathbf{k})|^2 = |g_{nn'\nu'}(\mathbf{k}', \mathbf{k}-\mathbf{k}')|^2$ (hermiticity). Concerning "$g(\mathbf{k}, 0) = 0$": the dropped terms (I,1), (II,4) are the zero-phonon-momentum (Hartree) terms, cf. the

note (c) after the Theorem; for acoustic phonons $g(\mathbf{k},\mathbf{q}) \to 0$ for $\mathbf{q} \to 0$, and for optical phonons they give a static shift of $\epsilon_n(\mathbf{k}) - \mu$.

Theorem 26.25 Going to Matsubara-space gives the equation of motion for the Green-function as

$$\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_1},\mathbf{k}) = \mathscr{G}_{\substack{0,n\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_1},\mathbf{k})\left[1 + \sum_{\substack{\omega_{n_2}\in\Omega_{-1}\\ \mathbf{k}'\in\mathrm{Q}\\ n'\in\{1,\ldots,\infty\}\\ \nu'\in\{1,\ldots,rd_{\mathbf{x}}\}}} \frac{-|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{N_p}\left(+\frac{1}{\beta}\right)\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\mathrm{i}(\omega_{n_1}-\omega_{n_2}))\left[\mathscr{G}_{\substack{n'\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_2},\mathbf{k}')\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_1},\mathbf{k}) - \mathscr{F}_n^\dagger(\mathrm{i}\omega_{n_1},\mathbf{k})\mathscr{F}_{n'}(\mathrm{i}\omega_{n_2},\mathbf{k}')\right]\right] \tag{26.63}$$

Proof 26.25 We rewrite the equation of motion, i.e. Equation (26.68) in Matsubara-space. We start with the l.h.s. and obtain with Lemma 1.11 and Theorem 13.6

$$\begin{aligned}\left(\partial_\tau + \frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\right)\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(\tau,\mathbf{k}) &= \frac{1}{\hbar\beta}\sum_{\omega_{n_1}\in\Omega_{-1}}\left(-\mathrm{i}\omega_{n_1} + \frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\right)\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(\mathbf{k},\omega_{n_1})\mathrm{e}^{-\mathrm{i}\omega_{n_1}\tau}\\ &= \frac{1}{\hbar\beta}\sum_{\omega_{n_1}\in\Omega_{-1}}\left(-\hbar\mathscr{G}^{\,0}_{\substack{n\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_1},\mathbf{k})\right)^{-1}\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_1},\mathbf{k})\mathrm{e}^{-\mathrm{i}\omega_{n_1}\tau}\end{aligned}$$

On the r.h.s. we expand each term individually and obtain with Theorem 1.16

$$-\frac{1}{\hbar}\delta(\tau) = \frac{1}{\hbar\beta}\sum_{\omega_{n_1}\in\Omega_{-1}} -\frac{1}{\hbar}\mathrm{e}^{-\mathrm{i}\omega_{n_1}\tau} \tag{26.64}$$

for the delta-function and for the other term number (II,3):

$$\begin{aligned}\mathrm{II,3} &= +\frac{1}{(\hbar\beta)^3}\oint_{\substack{\mathbf{k}'\in\mathrm{Q}\\ \nu'\in\{1,\ldots,rd_{\mathbf{x}}\}\\ n'\in\{1,\ldots,\infty\}\\ \tau'\in(0,\hbar\beta)}}\frac{|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{\hbar^2 N_p}\hbar^2\sum_{\substack{\omega_{n_1},\omega_{n_2}\in\Omega_{-1}\\ \omega_{n_3}\in\Omega_1}}\mathrm{e}^{-\mathrm{i}\omega_{n_3}(\tau-\tau')+\mathrm{i}\omega_{n_1}(\tau'-\tau)-\mathrm{i}\omega_{n_2}\tau'}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\mathrm{i}\omega_{n_3})\mathscr{G}_{\substack{n'\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_1},\mathbf{k}')\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(\\ &= \ldots\end{aligned}$$

Now we collect the terms in τ' and perform the integration with Corollary 1.12

$$\int_0^{\hbar\beta}\mathrm{d}\tau'\,\mathrm{e}^{\mathrm{i}\tau'(\omega_{n_3}+\omega_{n_1}-\omega_{n_2})} = \hbar\beta\delta_{\omega_{n_3}+\omega_{n_1},\omega_{n_2}} \tag{26.65}$$

Noting further that

$$\mathrm{e}^{\mathrm{i}\tau\left(-\omega_{n_3}-\omega_{n_1}\right)}\Big|_{\omega_{n_3}+\omega_{n_1}=\omega_{n_2}\Leftrightarrow\omega_{n_3}=\omega_{n_2}-\omega_{n_1}} = \mathrm{e}^{-\mathrm{i}\tau\omega_{n_2}} \tag{26.66}$$

This allows us to terminate the summation over ω_{n_3} and continue as

$$\mathrm{I} = \ldots = \frac{\hbar^2}{\hbar\beta} \sum_{\substack{\omega_{n_1},\omega_{n_2}\in\Omega_{-1}\\ \mathbf{k}'\in\mathrm{Q}\\ n'\in\{1,\ldots,\infty\}\\ \nu'\in\{1,\ldots,rd_{\mathbf{x}}\}}} \left(\frac{|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{N_p}\right)\left(+\frac{1}{\hbar\beta}\right) \mathrm{e}^{-\mathrm{i}\omega_{n_2}\tau} \mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\mathrm{i}\omega_{n_2}+\mathrm{i}\omega_{n_1}) \mathscr{G}_{\substack{n'\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_1},\mathbf{k}') \mathscr{G}_{\substack{n\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_2},\mathbf{k})$$

Correction note. (i) The left-hand side is the term (II,3) (not "I"). (ii) The argument of the phonon propagator is $\mathrm{i}\omega_{n_3} = \mathrm{i}(\omega_{n_2} - \omega_{n_1})$, not $\mathrm{i}\omega_{n_2} + \mathrm{i}\omega_{n_1}$ (this is what the Kronecker-delta above says). (iii) The prefactor is $\frac{1}{(\hbar\beta)^2}\frac{|g|^2}{N_p}$, i.e. without the $\hbar^2$ in front: $\frac{1}{(\hbar\beta)^3}\cdot\frac{|g|^2}{\hbar^2 N_p}\hbar^2\cdot\hbar\beta = \frac{1}{(\hbar\beta)^2}\frac{|g|^2}{N_p}$. The final result of this proof uses the correct prefactor and the correct argument (after relabeling $\omega_{n_1}\leftrightarrow\omega_{n_2}$ and with $\mathscr{D}_0(\mathrm{i}\omega) = \mathscr{D}_0(-\mathrm{i}\omega)$). For the same reason "(II,3)" in the green-boxed sentence below is the term (I,2).

Now we shift our attention to the term II (still?) and obtain for the other term number 2 (still?):

$$\mathrm{I,2} = \frac{-1}{(\hbar\beta)^3} \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}'\in\mathrm{Q}\\ \nu'\in\{1,\ldots,rd_{\mathbf{x}}\}\\ n'\in\{1,\ldots,\infty\}\\ \tau'\in(0,\hbar\beta)}} \frac{|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{N_p\hbar^2}\hbar^2 \sum_{\substack{\omega_{n_1},\omega_{n_2}\in\Omega_{-1}\\ \omega_{n_3}\in\Omega_1}} \mathrm{e}^{-\mathrm{i}\omega_{n_3}(\tau-\tau')-\mathrm{i}\omega_{n_1}(\tau-\tau')-\mathrm{i}\omega_{n_2}\tau'} \mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\omega_{n_3}) \mathscr{F}_n^\dagger(\mathbf{k},\omega_{n_2}) \mathscr{F}_{n'}(\mathbf{k}',\omega_{n_1})$$

Now we collect the terms in τ' and perform the integration

$$\int_0^{\hbar\beta} \mathrm{d}\tau'\, \mathrm{e}^{\mathrm{i}\tau'(\omega_{n_3}+\omega_{n_1}-\omega_{n_2})} = \hbar\beta\delta_{\omega_{n_3},\omega_{n_2}-\omega_{n_1}} \tag{26.67}$$

Noting further that

$$\mathrm{e}^{\mathrm{i}\tau(-\omega_{n_3}-\omega_{n_1})} = \mathrm{e}^{-\mathrm{i}\tau(-\omega_{n_1}+\omega_{n_2})-\omega_{n_1}\tau\mathrm{i}} = \mathrm{e}^{-\mathrm{i}\tau\omega_{n_2}}$$

which gives the result

$$\mathrm{I,2} = \ldots = \frac{-1}{\hbar\beta} \sum_{\substack{\omega_{n_1},\omega_{n_2}\in\Omega_{-1}\\ n'\in\{1,\ldots,\infty\}\\ \nu'\in\{1,\ldots,rd_{\mathbf{x}}\}\\ \mathbf{k}'\in\mathrm{Q}}} \hbar^2 \left(\frac{|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{\hbar^2 N_p}\right)\left(\frac{1}{\hbar\beta}\right) \mathrm{e}^{-\mathrm{i}\omega_{n_2}\tau} \mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\omega_{n_2}-\omega_{n_1}) \mathscr{F}_n^\dagger(\mathrm{i}\omega_{n_2},\mathbf{k}) \mathscr{F}_{n'}(\mathrm{i}\omega_{n_1},\mathbf{k}')$$

Note. Here and in the next equation $\mathscr{D}_0(\omega_{n_2}-\omega_{n_1})$ means $\mathscr{D}_0(\mathrm{i}(\omega_{n_2}-\omega_{n_1}))$. In the first line of (I,2) the Matsubara-functions are $\mathscr{D}_0(\mathrm{i}\omega_{n_3})$, $\mathscr{F}_n^\dagger(\mathrm{i}\omega_{n_2},\mathbf{k})$, $\mathscr{F}_{n'}(\mathrm{i}\omega_{n_1},\mathbf{k}')$. The equation labelled (26.68) at the beginning of the proof should be the equation of Theorem 26.24; Equation (26.68) is the result.

Combining the results gives the final result

$$
\begin{aligned}
&+\frac{1}{\hbar\beta}\sum_{\omega_{n_1}\in\Omega_{-1}}\left(-\hbar\mathscr{G}_{\substack{0,n\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_1},\mathbf{k})\right)^{-1}\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_1},\mathbf{k})\mathrm{e}^{-i\omega_{n_1}\tau}\\
&=\frac{1}{\hbar\beta}\sum_{\omega_{n_1}\in\Omega_{-1}}-\frac{1}{\hbar}\mathrm{e}^{-i\omega_{n_1}\tau}\\
&+\frac{1}{\hbar\beta}\sum_{\substack{\omega_{n_1},\omega_{n_2}\in\Omega_{-1}\\ n'\in\{1,\dots,\infty\}\\ \nu'\in\{1,\dots,rd_{\mathbf{x}}\}\\ \mathbf{k}'\in\mathrm{Q}}}\hbar^2\left(\frac{|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{\hbar^2N_p}\right)\left(+\frac{1}{\hbar\beta}\right)\mathrm{e}^{-\mathrm{i}\omega_{n_2}\tau}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\mathrm{i}\omega_{n_2}+\mathrm{i}\omega_{n_1})\mathscr{G}_{\substack{n'\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_1},\mathbf{k}')\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_2},\mathbf{k})\\
&-\frac{1}{\hbar\beta}\sum_{\substack{\omega_{n_1},\omega_{n_2}\in\Omega_{-1}\\ n'\in\{1,\dots,\infty\}\\ \nu'\in\{1,\dots,rd_{\mathbf{x}}\}\\ \mathbf{k}'\in\mathrm{Q}}}\hbar^2\left(\frac{|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{\hbar^2N_p}\right)\left(\frac{1}{\hbar\beta}\right)\mathrm{e}^{-\mathrm{i}\omega_{n_2}\tau}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\omega_{n_2}-\omega_{n_1})\mathscr{F}_n^\dagger(\mathrm{i}\omega_{n_2},\mathbf{k})\mathscr{F}_{n'}(\mathrm{i}\omega_{n_1},\mathbf{k}')
\end{aligned}
$$

now relabeling $\omega_{n_1}\leftrightarrow\omega_{n_2}$ and comparing coefficients gives the desired result.

Going to Matsubara-space gives the equation of motion for the Green-function as

$$
\begin{aligned}
&\left(-\hbar\mathscr{G}_{\substack{0,n\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_1},\mathbf{k})\right)^{-1}\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_1},\mathbf{k})\\
&=-\frac{1}{\hbar}+\sum_{\substack{\omega_{n_2}\in\Omega_{-1}\\ \mathbf{k}'\in\mathrm{Q}\\ n'\in\{1,\dots,\infty\}\\ \nu'\in\{1,\dots,rd_{\mathbf{x}}\}}}\hbar^2\frac{|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{\hbar^2N_p}\left(+\frac{1}{\hbar\beta}\right)\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\mathrm{i}(\omega_{n_1}-\omega_{n_2}))\left[\mathscr{G}_{\substack{n'\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_2},\mathbf{k}')\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_1},\mathbf{k})-\mathscr{F}_n^\dagger(\mathrm{i}\omega_{n_1},\mathbf{k})\mathscr{F}_{n'}(\mathrm{i}\omega_{n_2},\mathbf{k}')\right]
\end{aligned}
\tag{26.68}
$$

which can be rewritten as

$$
\begin{aligned}
&\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_1},\mathbf{k})\\
&=\mathscr{G}_{\substack{0,n\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_1},\mathbf{k})\left[1+\sum_{\substack{\omega_{n_2}\in\Omega_{-1}\\ \mathbf{k}'\in\mathrm{Q}\\ n'\in\{1,\dots,\infty\}\\ \nu'\in\{1,\dots,rd_{\mathbf{x}}\}}}\frac{-|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{N_p}\left(+\frac{1}{\beta}\right)\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\mathrm{i}(\omega_{n_1}-\omega_{n_2}))\left[\mathscr{G}_{\substack{n'\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_2},\mathbf{k}')\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_1},\mathbf{k})-\mathscr{F}_n^\dagger(\mathrm{i}\omega_{n_1},\mathbf{k})\mathscr{F}_{n'}(\mathrm{i}\omega_{n_2},\mathbf{k}')\right]\right]
\end{aligned}
\tag{26.69}
$$

[Cf. continuation on TBDigitalized for SC. page 1]

Preparation 2/4: Equations of Motion for the other anomalous Green-Function

Fact 26.26 The equation of motion for the anomalous Green-function in imaginary time reads

$$
\left(\partial_\tau+\frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\right)\mathscr{F}_n(\tau,\mathbf{k})=\sum_{\substack{\mathbf{k}'\in\mathrm{Q}\\ n'\in\{1,2,3,\dots\}\\ \nu'\in\{1,2,\dots,rd_{\mathbf{x}}\}}}\frac{g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')}{\hbar^2N_p}\left\langle\mathrm{T}_\tau\, c_{n'\uparrow}(\tau,\mathbf{k}')c_{n\downarrow}(0,-\mathbf{k})\left(b_{\nu'}(\tau,\mathbf{k}-\mathbf{k}')+b_{\nu'}^\dagger(\tau,\mathbf{k}'-\mathbf{k})\right)\right\rangle
\tag{26.70}
$$

Correction note. The denominator has to be $\hbar^2\sqrt{N_p}$ (as in Lemma 26.20), not $\hbar^2 N_p$: the commutator $[(H-\mu N)/\hbar, c_{n\uparrow}(\mathbf{k})]$ is the same as in the proof of Lemma 26.20 and contains $g/(\hbar\sqrt{N_p})$. The expectation value is $\langle\ldots\rangle_{\mathrm{SC}}$. Contrary to the 1, 1-component, no $\delta(\tau)$ appears, since $\{c_{n\uparrow}(\mathbf{k}), c_{n\downarrow}(-\mathbf{k})\} = 0$.

Proof 26.26 We compute the equation of motion for the anomalous Green-function in the 1,2-component of the Green-function. We obtain analogous to the Lemma in the 1,1-component

$$\begin{aligned}\partial_\tau \mathscr{F}_n(\tau,\mathbf{k}) &= \partial_\tau\left(-\frac{1}{\hbar}\right)\left\langle \mathrm{T}_\tau\, c_{n\uparrow}(\tau,\mathbf{k})c_{n\downarrow}(0,-\mathbf{k})\right\rangle \\ &= \frac{1}{\hbar}\left\langle \left[c_{n,\uparrow}(\mathbf{k}), \frac{H-\mu N}{\hbar}\right]_{\mathrm{H}} c_{n,\downarrow}(0,-\mathbf{k})\right\rangle\end{aligned} \tag{26.71}$$

This gives, using the same calculation as before, an equation analogous to "filled square equation"

$$\left(\partial_\tau + \frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\right)\mathscr{F}_n(\tau,\mathbf{k}) = \sum_{\substack{\mathbf{k}'\in\mathrm{Q}\\ n'\in\{1,2,3,\ldots\}\\ \nu'\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} \frac{g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')}{\hbar^2 N_p}\left\langle \mathrm{T}_\tau\, c_{n'\uparrow}(\tau,\mathbf{k}')c_{n\downarrow}(0,-\mathbf{k})\left(b_{\nu'}(\tau,\mathbf{k}-\mathbf{k}')+b^\dagger_{\nu'}(\tau,\mathbf{k}'-\mathbf{k})\right)\right\rangle \tag{26.72}$$

Notation 26.27 We introduce

$$\mathscr{G}^{\mathrm{aux2}}_{\nu' nn'}(\tau,\tau',\mathbf{k},\mathbf{k}') = -\frac{1}{\hbar}\left\langle \mathrm{T}_\tau\left(b_{\nu'}(\tau,\mathbf{k}-\mathbf{k}')-b^\dagger_{\nu'}(\tau,\mathbf{k}'-\mathbf{k})\right)c_{n'\uparrow}(\tau',\mathbf{k})c_{n\downarrow}(0,-\mathbf{k})\right\rangle \tag{26.73}$$

Correction note. For the following Remark and Lemma to hold, the definition has to read (with + between the phonon operators, momentum $\mathbf{k}'$ in the third operator, exactly analogous to Equation (26.40))

$$\mathscr{G}^{\mathrm{aux2}}_{\nu' nn'}(\tau,\tau',\mathbf{k},\mathbf{k}') = -\frac{1}{\hbar}\left\langle \mathrm{T}_\tau\left(b_{\nu'}(\tau,\mathbf{k}-\mathbf{k}')+b^\dagger_{\nu'}(\tau,\mathbf{k}'-\mathbf{k})\right)c_{n'\uparrow}(\tau',\mathbf{k}')c_{n\downarrow}(0,-\mathbf{k})\right\rangle_{\mathrm{SC}}.$$

Remark 26.27.1 Notice that this allows us to rewrite the equation of motion as

$$\left(\partial_\tau + \frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\right)\mathscr{F}_n(\tau,\mathbf{k}) = -\sum_{\substack{\mathbf{k}'\in\mathrm{Q}\\ n'\in\{1,2,3,\ldots\}\\ \nu'\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} \frac{g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')}{\hbar N_p}\mathscr{G}^{\mathrm{aux2}}_{\nu' nn'}(\tau,\tau,\mathbf{k},\mathbf{k}') \tag{26.74}$$

Correction note. The denominator has to be $\hbar\sqrt{N_p}$, not $\hbar N_p$ (from $\frac{g}{\hbar^2\sqrt{N_p}}\langle\ldots\rangle_{\mathrm{SC}} = \frac{g}{\hbar^2\sqrt{N_p}}(-\hbar)\mathscr{G}_{\mathrm{aux2}}$).

Lemma 26.28 We obtain

$$\partial_\tau \mathscr{G}^{\mathrm{aux2}}_{\nu' nn'}(\tau,\tau',\mathbf{k},\mathbf{k}') = \frac{\omega_{\nu'}(\mathbf{k}-\mathbf{k}')}{\hbar}\left\langle \mathrm{T}_\tau\left(b_{\nu'}(\tau,\mathbf{k}-\mathbf{k}')-b^\dagger_{\nu'}(\tau,\mathbf{k}'-\mathbf{k})\right)c_{n'\uparrow}(\tau',\mathbf{k}')c_{n\downarrow}(0,-\mathbf{k})\right\rangle \tag{26.75}$$

and

$$\left(\partial_\tau^2 - \omega_{\nu'}^2(\mathbf{k}-\mathbf{k}')\partial_\tau \mathscr{G}^{\text{aux2}}_{\nu' nn'}\right) = \dots \tag{26.76}$$

Completion. The second equation reads (the bracket on the left-hand side closes before $\mathscr{G}_{\text{aux2}}$, and there is no ∂_τ in front of $\mathscr{G}_{\text{aux2}}$)

$$\begin{aligned}&\left(\partial_\tau^2 - \omega_{\nu'}^2(\mathbf{k}-\mathbf{k}')\right)\mathscr{G}^{\text{aux2}}_{\nu' nn'}(\tau,\tau',\mathbf{k},\mathbf{k}')\\ &= \frac{-2\omega_{\nu'}(\mathbf{k}-\mathbf{k}')}{\hbar}\sum_{\substack{\mathbf{q}\in Q\\ m,m'\in\{1,\dots,\infty\}\\ \sigma\in\{\uparrow,\downarrow\}}}\frac{g_{mm'\nu'}(\mathbf{q},\mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}}\left\langle \mathrm{T}_\tau\, c^\dagger_{m,\sigma}(\tau,\mathbf{q}+\mathbf{k}'-\mathbf{k})c_{m',\sigma}(\tau,\mathbf{q})c_{n'\uparrow}(\tau',\mathbf{k}')c_{n\downarrow}(0,-\mathbf{k})\right\rangle_{\text{SC}}.\end{aligned} \tag{26.77}$$

Proof 26.28 Follows analogously as in the proof of Lemma TBReferenced.

(Lemma 26.22: the phonon operators enter in the same combination $b_{\nu'}(\tau,\mathbf{k}-\mathbf{k}')+b^\dagger_{\nu'}(\tau,\mathbf{k}'-\mathbf{k})$, and the equal-time commutators with $c_{n'\uparrow}$ and $c_{n\downarrow}$ vanish. Only the two fermionic "spectator" operators change, $c^\dagger_{n\uparrow}(0,\mathbf{k}) \to c_{n\downarrow}(0,-\mathbf{k})$. The same argument as in Corollary 26.23 then gives the next Remark.)

Remark 26.28.1 This allows us to rewrite the equation of motion as

$$\left(\partial_\tau + \frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\right)\mathscr{F}_n(\tau,\mathbf{k}) = \sum_{\substack{\tau'\in(0,\hbar\beta)\\ \mathbf{q},\mathbf{k}'\in Q\\ \nu'\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ m,m',n'\in\{1,2,3,\dots\}\\ \sigma\in\{\downarrow,\uparrow\}}}\frac{g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')g_{mm'\nu'}(\mathbf{q},\mathbf{k}'-\mathbf{k})}{\hbar^2 N_p}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\left\langle \mathrm{T}_\tau\, c^\dagger_{m,\sigma}(\tau',\mathbf{q}+\mathbf{k}'-\mathbf{k})c_{m'\sigma}(\tau',\mathbf{q})c_{n'\uparrow}(\tau,\mathbf{k}')c_{n\downarrow}(0,-\mathbf{k})\right\rangle \tag{26.78}$$

Notation 26.29 Now we obtain for the individual creation- and annihilation-operators

- for the first one

$$c^\dagger_{m,\sigma}(\tau',\mathbf{q}+\mathbf{k}'-\mathbf{k}) = \begin{cases}\overline{\eta}_{m,1}(\tau',\mathbf{q}+\mathbf{k}'-\mathbf{k}), & \sigma=\uparrow\\ \eta_{m,2}(\tau',-\mathbf{q}-\mathbf{k}'+\mathbf{k}), & \sigma=\downarrow\end{cases} \tag{26.79}$$

- for the second one

$$c_{m',\sigma}(\tau',\mathbf{q}) = \begin{cases}\eta_{m',1}(\tau',\mathbf{q}), & \sigma=\uparrow\\ \overline{\eta}_{m',2}(\tau',-\mathbf{q}), & \sigma=\downarrow\end{cases} \tag{26.80}$$

- for the third one

$$c_{n'\uparrow}(\tau,\mathbf{k}') = \eta_{n'1}(\tau,\mathbf{k}') \tag{26.81}$$

- for the fourth one

$$c_{n\downarrow}(0,-\mathbf{k}) = \overline{\eta}_{n,2}(0,+\mathbf{k}) \tag{26.82}$$

Note. This is the operator version of Definition 44.8: $\eta_{n,1}(\tau,\mathbf{k}) = c_{n\uparrow}(\tau,\mathbf{k})$, $\eta_{n,2}(\tau,\mathbf{k}) = c^\dagger_{n\downarrow}(\tau,-\mathbf{k})$, $\overline{\eta}_{n,1}(\tau,\mathbf{k}) = c^\dagger_{n\uparrow}(\tau,\mathbf{k})$, $\overline{\eta}_{n,2}(\tau,\mathbf{k}) = c_{n\downarrow}(\tau,-\mathbf{k})$. With it, $(\widehat{\mathscr{G}}_n)_{ij}(\tau-\tau',\mathbf{k})\delta_{\mathbf{k},\mathbf{k}'} = -\frac{1}{\hbar}\langle \mathrm{T}_\tau\, \eta_{n,i}(\tau,\mathbf{k})\overline{\eta}_{n,j}(\tau',\mathbf{k}')\rangle_{\mathrm{SC}}$ for all $i,j\in\{1,2\}$, and $\langle \mathrm{T}_\tau\, \eta_{i_1}\eta_{i_2}\overline{\eta}_{i'_2}\overline{\eta}_{i'_1}\rangle_{\mathrm{SC}} \approx \hbar^2\left[\widehat{\mathscr{G}}(i_1|i'_1)\widehat{\mathscr{G}}(i_2|i'_2) - \widehat{\mathscr{G}}(i_1|i'_2)\widehat{\mathscr{G}}(i_2|i'_1)\right]$ (Theorem 15.16 without vertex-correction).

Corollary 26.30 We obtain the equation of motion for $\mathscr{F}_n$ therefore reads now

$$\left(\partial_\tau + \frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\right)\mathscr{F}_n(\tau,\mathbf{k}) = \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}'\in\mathrm{Q}\\ \tau'\in(0,\hbar\beta)\\ \nu'\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ n'\in\{1,2,\dots\}}} \frac{|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{N_p}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\Big[\mathscr{F}_{n'\mathbf{k}'}(\tau-\tau')\mathscr{G}_{n-\mathbf{k}}(-\tau') + \mathscr{F}_{n\mathbf{k}}(\tau')\mathscr{G}_{n'-\mathbf{k}'}(\tau-\tau')\Big] \tag{26.83}$$

Correction note. In the second term the momentum is $+\mathbf{k}'$, i.e. $\mathscr{G}_{\substack{n'\\ \mathrm{Gorkov}}}(\tau-\tau',+\mathbf{k}')$: it comes from $\widehat{\mathscr{G}}(i_2|i'_2) = (\widehat{\mathscr{G}}_{n'})_{11}(\tau-\tau',\mathbf{k}')$ (box 3 of the proof). For an inversion-symmetric, spin-degenerate system $\mathscr{G}_{\substack{n\\ \mathrm{Gorkov}}}(\tau,-\mathbf{k}) = \mathscr{G}_{\substack{n\\ \mathrm{Gorkov}}}(\tau,\mathbf{k})$, so the value is the same. As in Theorem 26.24, the zero-phonon-momentum terms (boxes 1 and 4 below) are dropped. Written with the Gorkov-matrix,

$$\left(\partial_\tau + \tfrac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\right)\mathscr{F}_n(\tau,\mathbf{k}) = \sum\!\!\!\!\!\!\int_{\mathbf{k}',\tau',\nu',n'} \tfrac{|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{N_p}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\Big[\mathscr{G}_{\substack{n'\\ \mathrm{Gorkov}}}(\tau-\tau',\mathbf{k}')\mathscr{F}_n(\tau',\mathbf{k}) - \mathscr{F}_{n'}(\tau-\tau',\mathbf{k}')(\widehat{\mathscr{G}}_n)_{22}(\tau',\mathbf{k})\Big],$$

using $(\widehat{\mathscr{G}}_n)_{22}(\tau',\mathbf{k}) = -\mathscr{G}_{\substack{n\\ \mathrm{Gorkov}}}(-\tau',-\mathbf{k})$ (Lemma 26.7).

Proof 26.30 Now we approximate the resulting expression using the Bethe-Salpeter-equation again, whereas the first line corresponds to the "spin down" contribution and the second one to the "spin up" contribution, resulting in:

$$\begin{aligned}
\mathrm{CORR} &= \langle \eta_{m,2}(\tau',-\mathbf{q}-\mathbf{k}'+\mathbf{k})\overline{\eta}_{m',2}(\tau',-\mathbf{q})\eta_{n'1}(\tau,\mathbf{k}')\overline{\eta}_{n,2}(0,+\mathbf{k})\rangle_{\mathrm{SC}}\\
&+ \langle \overline{\eta}_{m,1}(\tau',+\mathbf{q}+\mathbf{k}'-\mathbf{k})\eta_{m',1}(\tau',+\mathbf{q})\eta_{n'1}(\tau,\mathbf{k}')\overline{\eta}_{n,2}(0,+\mathbf{k})\rangle_{\mathrm{SC}}\\
&= \langle \eta_{n'1}(\tau,\mathbf{k}')\eta_{m,2}(\tau',-\mathbf{q}-\mathbf{k}'+\mathbf{k})\overline{\eta}_{m',2}(\tau',-\mathbf{q})\overline{\eta}_{n,2}(0,+\mathbf{k})\rangle_{\mathrm{SC}}\\
&+ \langle \eta_{m',1}(\tau',+\mathbf{q})\eta_{n'1}(\tau,\mathbf{k}')\overline{\eta}_{m,1}(\tau',+\mathbf{q}+\mathbf{k}'-\mathbf{k})\overline{\eta}_{n,2}(0,+\mathbf{k})\rangle_{\mathrm{SC}}\\
&= \hbar^2\mathscr{G}\left(i_1=[n',1,\tau,\mathbf{k}'],i_2=[m,2,\tau',-\mathbf{q}-\mathbf{k}'+\mathbf{k}],i'_1=[n,2,0,\mathbf{k}],i'_2=[m',2,\tau',-\mathbf{q}]\right)\\
&+ \hbar^2\mathscr{G}\left(i_1=[m',1,\tau',\mathbf{q}],i_2=[n',1,\tau,\mathbf{k}'],i'_1=[n,2,0,\mathbf{k}],i'_2=[m,1,\tau',\mathbf{q}+\mathbf{k}'-\mathbf{k}]\right)\\
&= \mathrm{I}+\mathrm{II}
\end{aligned} \tag{26.84}$$

Now we get two terms each

$$\begin{aligned}
\mathrm{I} &= \hbar^2\widehat{\mathscr{G}}(i_1,i'_1)\widehat{\mathscr{G}}(i_2,i'_2) - \hbar^2\widehat{\mathscr{G}}(i_1,i'_2)\widehat{\mathscr{G}}(i_2,i'_1)\\
&= \hbar^2\widehat{\mathscr{G}}_{\substack{n',n\\ 1,2\\ \mathbf{k}',\mathbf{k}}}(\tau-0)\widehat{\mathscr{G}}_{\substack{m',m\\ 2,2\\ -\mathbf{q},-\mathbf{q}-\mathbf{k}'+\mathbf{k}}}(0) - \hbar^2\widehat{\mathscr{G}}_{\substack{n',m'\\ 1,2\\ \mathbf{k}',-\mathbf{q}}}(\tau-\tau')\widehat{\mathscr{G}}_{\substack{m,n\\ 2,2\\ +\mathbf{k},-\mathbf{q}-\mathbf{k}'+\mathbf{k}}}(\tau') = \dots
\end{aligned} \tag{26.85}$$

and the other term gives

$$\begin{aligned} \mathrm{II} &= \hbar^2 \widehat{\mathscr{G}}(i_1, i_1') \widehat{\mathscr{G}}(i_2, i_2') - \hbar^2 \widehat{\mathscr{G}}(i_1, i_2') \widehat{\mathscr{G}}(i_2, i_1') \\ &= \hbar^2 \underset{\substack{1,2\\ \mathbf{q},\mathbf{k}}}{\widehat{\mathscr{G}}_{m',n}}(\tau' - 0) \underset{\substack{1,1\\ -\mathbf{k}',\mathbf{q}+\mathbf{k}'-\mathbf{k}}}{\widehat{\mathscr{G}}^{\,n',m}}(\tau - \tau') - \hbar^2 \underset{\substack{1,1\\ \mathbf{q},\mathbf{q}+\mathbf{k}'-\mathbf{k}}}{\widehat{\mathscr{G}}^{\,m',m}}(0) \underset{\substack{1,2\\ \mathbf{k}',\mathbf{k}}}{\widehat{\mathscr{G}}_{n',n}}(\tau - 0) = \dots \end{aligned} \tag{26.86}$$

Now we use the definition of the Gorkov-Green-functions and the fact that translational invariance is preserved

$$\begin{aligned} \mathrm{I} &= \hbar^2 \delta_{n',n} \delta_{m',m} \delta_{\mathbf{k}',\mathbf{k}} \underset{1,2}{\widehat{\mathscr{G}}_{n\mathbf{k}'}}(\tau) \underset{2,2}{\widehat{\mathscr{G}}_{m\mathbf{q}}}(0) - \hbar^2 \delta_{n',m'} \delta_{n,m} \delta_{\mathbf{k}',-\mathbf{q}} \underset{1,2}{\widehat{\mathscr{G}}_{n'\mathbf{k}'}}(\tau - \tau') \underset{2,2}{\widehat{\mathscr{G}}_{n\mathbf{k}}}(\tau') \\ &= \hbar^2 \delta_{n',n} \delta_{m',m} \delta_{\mathbf{k}',\mathbf{k}} \mathscr{F}_{n\mathbf{k}'}(\tau)(-1) \mathscr{G}_{m\mathbf{q}}(0) - \hbar^2 \delta_{n',m'} \delta_{n,m} \delta_{\mathbf{k}',-\mathbf{q}} \mathscr{F}_{n'\mathbf{k}'}(\tau - \tau')(-1) \mathscr{G}_{n\mathbf{k}}(-\tau') \end{aligned} \tag{26.87}$$

and the other term gives

$$\begin{aligned} \mathrm{II} &= \hbar^2 \delta_{m',n} \delta_{n',m} \delta_{\mathbf{q},\mathbf{k}} \underset{1,2}{\widehat{\mathscr{G}}_{n\mathbf{k}}}(\tau') \underset{1,1}{\widehat{\mathscr{G}}_{n'\mathbf{q}}}(\tau - \tau') - \hbar^2 \delta_{m,m'} \delta_{n,n'} \delta_{\mathbf{k},\mathbf{k}'} \underset{1,1}{\widehat{\mathscr{G}}_{m\mathbf{q}}}(0) \underset{1,2}{\widehat{\mathscr{G}}_{n\mathbf{k}'}}(\tau) \\ &= \hbar^2 \delta_{m',n} \delta_{n',m} \delta_{\mathbf{q},\mathbf{k}} \mathscr{F}_{n\mathbf{k}}(\tau') \mathscr{G}_{n'\mathbf{k}'}(\tau - \tau') - \hbar^2 \delta_{m,m'} \delta_{n,n'} \delta_{\mathbf{k},\mathbf{k}'} \mathscr{G}_{m\,\mathbf{q}}(0) \mathscr{F}_{n\mathbf{k}'}(\tau') \end{aligned} \tag{26.88}$$

Correction note (index typos in I and II; the final boxes 1–4 are correct).

- In I:
$$\widehat{\mathscr{G}}(i_2|i_2') = (\widehat{\mathscr{G}}) \underset{\substack{2,2\\ \mathbf{k}-\mathbf{k}'-\mathbf{q},-\mathbf{q}}}{{}^{m,m'}}(0) = \delta_{mm'} \delta_{\mathbf{k}\mathbf{k}'} (\widehat{\mathscr{G}}_m)_{22}(0, -\mathbf{q}) = -\delta_{mm'} \delta_{\mathbf{k}\mathbf{k}'} \mathscr{G}^{\,m}_{\mathrm{Gorkov}}(0^-, \mathbf{q}),$$
$$\widehat{\mathscr{G}}(i_2|i_1') = (\widehat{\mathscr{G}}) \underset{\substack{2,2\\ \mathbf{k}-\mathbf{k}'-\mathbf{q},\mathbf{k}}}{{}^{m,n}}(\tau') = -\delta_{mn} \delta_{\mathbf{k}',-\mathbf{q}} \mathscr{G}^{\,n}_{\mathrm{Gorkov}}(-\tau', -\mathbf{k}).$$
So the last factor of I is $\mathscr{G}^{\,n}_{\mathrm{Gorkov}}(-\tau', -\mathbf{k})$, not $\mathscr{G}_{n\mathbf{k}}(-\tau')$ (box 2 has it correctly).
- In II: $\widehat{\mathscr{G}}(i_2|i_2') = (\widehat{\mathscr{G}}) \underset{\substack{1,1\\ \mathbf{k}',\mathbf{q}+\mathbf{k}'-\mathbf{k}}}{{}^{n',m}}(\tau - \tau') = \delta_{n'm} \delta_{\mathbf{q}\mathbf{k}} \mathscr{G}^{\,n'}_{\mathrm{Gorkov}}(\tau - \tau', \mathbf{k}')$ (first momentum $+\mathbf{k}'$, not $-\mathbf{k}'$; afterwards $\widehat{\mathscr{G}}_{n'\mathbf{k}'}$, not $\widehat{\mathscr{G}}_{n'\mathbf{q}}$), and $\widehat{\mathscr{G}}(i_2|i_1') = (\widehat{\mathscr{G}})_{\underset{1,2}{n',n}}(\tau) = \delta_{n'n} \delta_{\mathbf{k}'\mathbf{k}} \mathscr{F}_n(\tau, \mathbf{k})$. So the last factor of II is $\mathscr{F}_n(\tau, \mathbf{k})$, not $\mathscr{F}_{n\mathbf{k}'}(\tau')$ (box 4 has it correctly).
- In box 3 (second line) the last factor is $\mathscr{G}_{n'\mathbf{k}'}(\tau - \tau')$; the step "the other symmetry" is the hermiticity $g_{n'nv'}(\mathbf{k}, \mathbf{k}' - \mathbf{k}) = g^*_{nn'v'}(\mathbf{k}', \mathbf{k} - \mathbf{k}')$ (Lemma 8.37), and "symmetry" in box 2 is the inversion symmetry $g_{nn'v'}(-\mathbf{k}', \mathbf{k}' - \mathbf{k}) = g^*_{nn'v'}(\mathbf{k}', \mathbf{k} - \mathbf{k}')$ (Lemma 8.38).
- "r.h.s. $(\star\star\star)$" refers to the right-hand side of the Remark after Lemma 26.28; the $\hbar^2$ of the decoupling cancels the $1/\hbar^2$ there, which is why the boxes carry $1/N_p$.

Therefore we obtain

$$\begin{aligned} \text{r.h.s.}(\star\star\star) &= \sum\!\!\!\!\!\!\int_{\substack{\mathbf{q},\mathbf{k}' \in \mathrm{Q}\\ \tau' \in (0,\hbar\beta)\\ \nu' \in \{1,2,\dots,rd_{\mathbf{x}}\}\\ m,m',n' \in \{1,2,\dots\}}} \frac{g_{nn'v'}(\mathbf{k}', \mathbf{k} - \mathbf{k}') g_{mm'v'}(\mathbf{q}, \mathbf{k}' - \mathbf{k})}{\hbar^2 N_p} \underset{\mathbf{k}-\mathbf{k}'}{\mathscr{D}_{0,v'}}(\tau - \tau')\,(1 + 2 + 3 + 4) \\ &\equiv \sum_{i=1}^{4} \boxed{i} \end{aligned} \tag{26.89}$$

Then we get

$$\begin{aligned}
\boxed{1} &= -\sum\!\!\!\!\!\!\int_{\substack{\mathbf{q},\mathbf{k}'\in \mathrm{Q}\\ \tau'\in(0,\hbar\beta)\\ \nu'\in\{1,2,\ldots,rd_{\mathbf{x}}\}\\ m,m',n'\in\{1,2,\ldots\}}} \frac{g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')g_{mm'\nu'}(\mathbf{q},\mathbf{k}'-\mathbf{k})}{N_p}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\delta_{n',n}\delta_{m',m}\delta_{\mathbf{k}',\mathbf{k}}\mathscr{F}_{n\mathbf{k}'}(\tau)\mathscr{G}_{m\mathbf{q}}(0)\\
&\overset{\text{kill } n',m',\mathbf{k}'}{=} -\sum\!\!\!\!\!\!\int_{\substack{\mathbf{q}\in \mathrm{Q}\\ \tau'\in(0,\hbar\beta)\\ \nu'\in\{1,2,\ldots,rd_{\mathbf{x}}\}\\ m\in\{1,2,\ldots\}}} \frac{g_{nn\nu'}(\mathbf{k},0)g_{mm\nu'}(\mathbf{q},0)}{N_p}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{0}}}(\tau-\tau')\mathscr{F}_{n\mathbf{k}}(\tau)\mathscr{G}_{m\mathbf{q}}(0)
\end{aligned} \tag{26.90}$$

and

$$\begin{aligned}
\boxed{2} &= \sum\!\!\!\!\!\!\int_{\substack{\mathbf{q},\mathbf{k}'\in \mathrm{Q}\\ \tau'\in(0,\hbar\beta)\\ \nu'\in\{1,2,\ldots,rd_{\mathbf{x}}\}\\ m,m',n'\in\{1,2,\ldots\}}} \frac{g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')g_{mm'\nu'}(\mathbf{q},\mathbf{k}'-\mathbf{k})}{N_p}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\delta_{n',m'}\delta_{n,m}\delta_{\mathbf{k}',-\mathbf{q}}\mathscr{F}_{n'\mathbf{k}'}(\tau-\tau')\mathscr{G}_{n-\mathbf{k}}(-\tau')\\
&\overset{\text{kill } m,m',\mathbf{q}}{=} \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}'\in \mathrm{Q}\\ \tau'\in(0,\hbar\beta)\\ \nu'\in\{1,2,\ldots,rd_{\mathbf{x}}\}\\ n'\in\{1,2,\ldots\}}} \frac{g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')g_{nn'\nu'}(-\mathbf{k}',-\mathbf{k}+\mathbf{k}')}{N_p}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\mathscr{F}_{n'\mathbf{k}'}(\tau-\tau')\mathscr{G}_{n-\mathbf{k}}(-\tau')\\
&\overset{\text{symmetry}}{=} \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}'\in \mathrm{Q}\\ \tau'\in(0,\hbar\beta)\\ \nu'\in\{1,2,\ldots,rd_{\mathbf{x}}\}\\ n'\in\{1,2,\ldots\}}} \frac{|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{N_p}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\mathscr{F}_{n'\mathbf{k}'}(\tau-\tau')\mathscr{G}_{n-\mathbf{k}}(-\tau')
\end{aligned} \tag{26.91}$$

and

$$\begin{aligned}
\boxed{3} &= \sum\!\!\!\!\!\!\int_{\substack{\mathbf{q},\mathbf{k}'\in \mathrm{Q}\\ \tau'\in(0,\hbar\beta)\\ \nu'\in\{1,2,\ldots,rd_{\mathbf{x}}\}\\ m,m',n'\in\{1,2,\ldots\}}} \frac{g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')g_{mm'\nu'}(\mathbf{q},\mathbf{k}'-\mathbf{k})}{N_p}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\delta_{m',n}\delta_{n',m}\delta_{\mathbf{k},\mathbf{q}}\mathscr{F}_{n\mathbf{k}}(\tau')\mathscr{G}_{n'\mathbf{k}'}(\tau-\tau')\\
&\overset{\text{kill } m,m',\mathbf{q}}{=} \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}'\in \mathrm{Q}\\ \tau'\in(0,\hbar\beta)\\ \nu'\in\{1,2,\ldots,rd_{\mathbf{x}}\}\\ n'\in\{1,2,\ldots\}}} \frac{g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')g_{n'n\nu'}(\mathbf{k},\mathbf{k}'-\mathbf{k})}{N_p}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\mathscr{F}_{n\mathbf{k}}(\tau')\mathscr{G}_{n'\mathbf{k}}(\tau-\tau')\\
&\overset{\text{the other symmetry}}{=} \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}'\in \mathrm{Q}\\ \tau'\in(0,\hbar\beta)\\ \nu'\in\{1,2,\ldots,rd_{\mathbf{x}}\}\\ n'\in\{1,2,\ldots\}}} \frac{|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{N_p}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\mathscr{F}_{n\mathbf{k}}(\tau')\mathscr{G}_{n'\mathbf{k}'}(\tau-\tau')
\end{aligned} \tag{26.92}$$

and

$$\begin{aligned}
\boxed{4} &= -\sum\!\!\!\!\!\!\int_{\substack{\mathbf{q},\mathbf{k}'\in \mathrm{Q}\\ \tau'\in(0,\hbar\beta)\\ \nu'\in\{1,2,\ldots,rd_{\mathbf{x}}\}\\ m,m',n'\in\{1,2,\ldots\}}} \frac{g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')g_{mm'\nu'}(\mathbf{q},\mathbf{k}'-\mathbf{k})}{N_p}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\delta_{n',n}\delta_{m',m}\delta_{\mathbf{k}',\mathbf{k}}\mathscr{F}_{n\mathbf{k}'}(\tau)\mathscr{G}_{m\mathbf{q}}(0)\\
&\overset{\text{kill } n',m',\mathbf{k}'}{=} -\sum\!\!\!\!\!\!\int_{\substack{\mathbf{q}\in \mathrm{Q}\\ \tau'\in(0,\hbar\beta)\\ \nu'\in\{1,2,\ldots,rd_{\mathbf{x}}\}\\ m\in\{1,2,\ldots\}}} \frac{g_{nn\nu'}(\mathbf{k},0)g_{mm\nu'}(\mathbf{q},0)}{N_p}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{0}}}(\tau-\tau')\mathscr{F}_{n\mathbf{k}}(\tau)\mathscr{G}_{m\mathbf{q}}(0)
\end{aligned} \tag{26.93}$$

now we do the "usual thing" and neglect the terms $\boxed{1}$ and $\boxed{4}$, which means that we neglect contributions from optical phonons. (More precisely: boxes 1 and 4 are the zero-phonon-momentum (Hartree) terms $\mathbf{k}' = \mathbf{k}$, which are excluded anyway by the assumption $\mathbf{k} \neq \mathbf{k}'$ of Lemma 26.22; they vanish for acoustic phonons, $g(\mathbf{k}, \mathbf{q} \to 0) \to 0$, and for optical phonons they are a static shift of $\epsilon_n(\mathbf{k}) - \mu$, cf. note (c) after Theorem 26.24.) The equation of motion for $\mathscr{F}_n$ therefore reads now

$$\left(\partial_\tau + \frac{\epsilon_n(\mathbf{k}) - \mu}{\hbar}\right) \mathscr{F}_n(\tau, \mathbf{k}) = \oint\!\!\!\sum_{\substack{\mathbf{k}' \in \mathrm{Q} \\ \tau' \in (0,\hbar\beta) \\ \nu' \in \{1,2,\ldots,rd_{\mathbf{x}}\} \\ n' \in \{1,2,\ldots\}}} \frac{|g_{nn'\nu'}(\mathbf{k}', \mathbf{k} - \mathbf{k}')|^2}{N_p} \mathscr{D}_{\substack{0,\nu' \\ \mathbf{k}-\mathbf{k}'}}(\tau - \tau') \Big[\mathscr{F}_{n'\mathbf{k}'}(\tau - \tau')\mathscr{G}_{n-\mathbf{k}}(-\tau') + \mathscr{F}_{n\mathbf{k}}(\tau')\mathscr{G}_{n'-\mathbf{k}'}(\tau - \tau')\Big] \tag{26.94}$$

Corollary 26.31 Going to Matsubara-space, we obtain

$$\mathscr{F}_n(\mathrm{i}\omega_{n_2}, \mathbf{k}) = \mathscr{G}_{\substack{0,n \\ \text{Gorkov}}}(\mathrm{i}\omega_{n_2}, \mathbf{k}) \frac{-1}{\beta} \sum_{\substack{\omega_{n_1} \in \Omega_{-1} \\ \mathbf{k}' \in \mathrm{Q} \\ \nu' \in \{1,2,\ldots,rd_{\mathbf{x}}\} \\ n' \in \{1,2,\ldots\}}} \frac{|g_{nn'\nu'}(\mathbf{k}', \mathbf{k} - \mathbf{k}')|^2}{N_p} \mathscr{D}_{\substack{0,\nu' \\ \mathbf{k}-\mathbf{k}'}}(\mathrm{i}(\omega_{n_2} - \omega_{n_1})) \left[\mathscr{F}_{n'\mathbf{k}'}(\mathrm{i}\omega_{n_1})\mathscr{G}_{n-\mathbf{k}}(-\mathrm{i}\omega_{n_2}) + \mathscr{F}_{n\mathbf{k}}(\mathrm{i}\omega_{n_2})\mathscr{G}_{n'\mathbf{k}'}(\mathrm{i}\omega_{n_1})\right] \tag{26.95}$$

Proof 26.31

Now we switch to Matsubara-frequencies yielding

$$\text{l.h.s.} = \frac{1}{\hbar\beta} \sum_{\omega_{n_1} \in \Omega_{+1}} \left(-\hbar \mathscr{G}_{\substack{0,n \\ \text{Gorkov}}}(\mathrm{i}\omega_{n_1}, \mathbf{k})\right)^{-1} \mathscr{G}_{\substack{n \\ \text{Gorkov}}}(\mathrm{i}\omega_{n_1}, \mathbf{k}) \mathrm{e}^{-\mathrm{i}\omega_{n_1}\tau} \tag{26.96}$$

Correction note. On the left-hand side the second factor has to be $\mathscr{F}_n(\mathrm{i}\omega_{n_1}, \mathbf{k})$ (the equation of motion is the one for $\mathscr{F}_n$), not $\mathscr{G}_{\substack{n \\ \text{Gorkov}}}(\mathrm{i}\omega_{n_1}, \mathbf{k})$. It uses that $\mathscr{F}_n$ is anti-periodic (Fact after the Definition of the Gorkov-Green-function) and $(-\mathrm{i}\omega + (\epsilon_n(\mathbf{k}) - \mu)/\hbar) = (-\hbar \mathscr{G}_{\substack{0,n \\ \text{Gorkov}}}(\mathrm{i}\omega, \mathbf{k}))^{-1}$. When comparing coefficients below, the frequency on the left-hand side is called ω_{n_2}.

For the r.h.s. we consider only the temporal components at first...

First Term:

We consider

$$\begin{aligned}
\int_0^{\hbar\beta} \mathrm{d}\tau' \mathscr{D}_0(\tau - \tau')\mathscr{F}(\tau - \tau')\mathscr{G}(-\tau') &= \oint\!\!\!\sum_{\substack{\tau' \in (0,\hbar\beta) \\ \omega_{n_{1,2}} \in \Omega_{-1} \\ \omega_{n_3} \in \Omega_{+1}}} \mathrm{e}^{-\mathrm{i}\omega_{n_3} + \mathrm{i}\omega_{n_1}(\tau' - \tau) - \mathrm{i}\omega_{n_2}\tau'} \mathscr{D}_0(\mathrm{i}\omega_{n_3})\mathscr{F}(\mathrm{i}\omega_{n_1})\mathscr{G}(-\mathrm{i}\omega_{n_2}) \cdot \left(\frac{1}{\hbar\beta}\right)^3 \\
&= \ldots \\
&= \left(\frac{1}{\hbar\beta}\right)^2 \sum_{\omega_{n_{1,2}} \in \Omega_{-1}} \mathrm{e}^{-\mathrm{i}\omega_{n_2}\tau} \mathscr{D}_0(\mathrm{i}(\omega_{n_2} - \omega_{n_1}))\mathscr{F}(\mathrm{i}\omega_{n_1})\mathscr{G}(-\mathrm{i}\omega_{n_2})
\end{aligned} \tag{26.97}$$

Note (filling the "…"). In the exponent the first term is $-\mathrm{i}\omega_{n_3}(\tau-\tau')$. With $\mathscr{G}(-\tau') = \frac{1}{\hbar\beta}\sum_{\omega_{n_2}} \mathscr{G}(-\mathrm{i}\omega_{n_2})\mathrm{e}^{-\mathrm{i}\omega_{n_2}\tau'}$ (relabel $\omega_{n_2} \to -\omega_{n_2}$, $\Omega_{-1} = -\Omega_{-1}$) the τ'-integral is $\int_0^{\hbar\beta} \mathrm{d}\tau'\, \mathrm{e}^{\mathrm{i}\tau'(\omega_{n_3}+\omega_{n_1}-\omega_{n_2})} = \hbar\beta\,\delta_{\omega_{n_3},\omega_{n_2}-\omega_{n_1}}$ (Corollary 1.12; $\omega_{n_3}+\omega_{n_1}-\omega_{n_2}$ is bosonic). The remaining exponential is $\mathrm{e}^{-\mathrm{i}(\omega_{n_3}+\omega_{n_1})\tau} = \mathrm{e}^{-\mathrm{i}\omega_{n_2}\tau}$, which gives the last line. The second term $\int \mathrm{d}\tau' \mathscr{D}_0(\tau-\tau')\mathscr{F}_n(\tau')\mathscr{G}_{n'}(\tau-\tau')$ is computed exactly as in the proof of Theorem 26.25. In the next equation $\mathrm{e}^{-\omega_{n_2}\tau}$ means $\mathrm{e}^{-\mathrm{i}\omega_{n_2}\tau}$, and $\mathscr{F}_{n'\mathbf{k}'} \equiv \mathscr{F}_{n'}(\cdot,\mathbf{k}')$, $\mathscr{G}_{n-\mathbf{k}} \equiv \mathscr{G}_{\substack{n\\ \text{Gorkov}}}(\cdot,-\mathbf{k})$.

this gives therefore for both components on the r.h.s.

$$\left(\frac{1}{\hbar\beta}\right)^2 \sum_{\substack{\omega_{n_{1,2}}\in\Omega_{-1}\\ \mathbf{k}'\in Q\\ \nu'\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ n'\in\{1,2,\dots\}}} \frac{|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{N_p} \mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\mathrm{i}(\omega_{n_2}-\omega_{n_1}))\mathrm{e}^{-\omega_{n_2}\tau}\left[\mathscr{F}_{n'\mathbf{k}'}(\mathrm{i}\omega_{n_1})\mathscr{G}_{n-\mathbf{k}}(-\mathrm{i}\omega_{n_2}) + \mathscr{F}_{n\mathbf{k}}(\mathrm{i}\omega_{n_2})\mathscr{G}_{n'\mathbf{k}'}(\mathrm{i}\omega_{n_1})\right] \tag{26.98}$$

Comparing coefficients yields thous

$$\left(\mathscr{G}_{\substack{0,n\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_2},\mathbf{k})\right)^{-1}\mathscr{F}_n(\mathrm{i}\omega_{n_2},\mathbf{k}) = \frac{-1}{\beta}\sum_{\substack{\omega_{n_1}\in\Omega_{-1}\\ \mathbf{k}'\in Q\\ \nu'\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ n'\in\{1,2,\dots\}}} \frac{|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{N_p} \mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\mathrm{i}(\omega_{n_2}-\omega_{n_1}))\left[\mathscr{F}_{n'\mathbf{k}'}(\mathrm{i}\omega_{n_1})\mathscr{G}_{n-\mathbf{k}}(-\mathrm{i}\omega_{n_2}) + \mathscr{F}_{n\mathbf{k}}(\mathrm{i}\omega_{n_2})\mathscr{G}_{n'\mathbf{k}'}(\mathrm{i}\omega_{n_1})\right] \tag{26.99}$$

or (equivalently)

$$\mathscr{F}_n(\mathrm{i}\omega_{n_2},\mathbf{k}) = \mathscr{G}_{\substack{0,n\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_2},\mathbf{k})\frac{-1}{\beta}\sum_{\substack{\omega_{n_1}\in\Omega_{-1}\\ \mathbf{k}'\in Q\\ \nu'\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ n'\in\{1,2,\dots\}}} \frac{|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{N_p} \mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\mathrm{i}(\omega_{n_2}-\omega_{n_1}))\left[\mathscr{F}_{n'\mathbf{k}'}(\mathrm{i}\omega_{n_1})\mathscr{G}_{n-\mathbf{k}}(-\mathrm{i}\omega_{n_2}) + \mathscr{F}_{n\mathbf{k}}(\mathrm{i}\omega_{n_2})\mathscr{G}_{n'\mathbf{k}'}(\mathrm{i}\omega_{n_1})\right] \tag{26.100}$$

From here, with Equation (Dyson-Equation in the SC-case) we can read off

$$\underset{n}{\Sigma_{11}}(\mathrm{i}\omega_{n_2},\mathbf{k}) = \sum_{\substack{\mathrm{i}\omega_{n_1}\in\Omega_{-1}\\ \mathbf{k}'\in Q\\ n'\in\{1,2,3,\dots\}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}}} \frac{-|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{\beta N_p} \mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}\left(\mathrm{i}(\omega_{n_2}-\omega_{n_1})\right)\mathscr{G}_{n'}(\mathrm{i}\omega_{n_1},\mathbf{k}') \tag{26.101}$$

and

$$\underset{n}{\Sigma_{12}}(\mathrm{i}\omega_{n_2},\mathbf{k}) = \sum_{\substack{\mathrm{i}\omega_{n_1}\in\Omega_{-1}\\ \mathbf{k}'\in Q\\ n'\in\{1,2,3,\dots\}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}}} \frac{+|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{\beta N_p} \mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}\left(\mathrm{i}(\omega_{n_2}-\omega_{n_1})\right)\mathscr{F}_{n'}(\mathrm{i}\omega_{n_1},\mathbf{k}') \tag{26.102}$$

notice the poorly exchanged roles of ω_{n_1} and ω_{n_2} w.r.t. the equations at the beginning of the section...

But it is ok, since this is the first time latexing this stuff.

(Checked: both expressions are correct and agree with the Corollary at the beginning of the subsection after relabeling $\omega_{n_1} \leftrightarrow \omega_{n_2}$; the summation index is ν'. Strictly speaking, the two scalar equations for $\mathscr{G}$ and $\mathscr{F}$ (the first row of the Dyson-equation) determine Σ_{11} and Σ_{12} uniquely, because $(\Sigma_{11}, \Sigma_{12})\widehat{\mathscr{G}} = \mathscr{G}_0^{-1}(\mathscr{G} - \mathscr{G}_0, \mathscr{F})$ and $\widehat{\mathscr{G}}$ is invertible; cf. the proof of that Corollary.)

Preparation 3/4 and 4/4: Equations of Motion for the normal, spin-down Green-Function and the first anomalous Green-Function

We look at the remaining equation of motions. First let's recall

$$-\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(-\tau, -\mathbf{k}) = -\frac{1}{\hbar}\left\langle \mathrm{T}_\tau\, c^\dagger_{n,\downarrow}(\tau, -\mathbf{k}) c_{n,\downarrow}(0, -\mathbf{k})\right\rangle \tag{26.103}$$

and analogously for $\mathscr{F}^\dagger_n$.

Definition 26.32 We introduce the function

$$\widetilde{\mathscr{G}}_{\substack{n\\ X}}(\tau, \mathbf{k}) = -\frac{1}{\hbar}\left\langle \mathrm{T}_\tau\, c^\dagger_{n,\downarrow}(\tau, -\mathbf{k}) X(0)\right\rangle \tag{26.104}$$

Remark 26.32.1 Notice that this implies

$$-\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(-\tau, -\mathbf{k}) = \widetilde{\mathscr{G}}_{\substack{n\\ X=c_{n,\downarrow}(-\mathbf{k})}}(\tau, \mathbf{k}) \quad \text{and} \quad \mathscr{F}^\dagger_n = \widetilde{\mathscr{G}}_{\substack{n\\ X=c^\dagger_{n,\uparrow}(+\mathbf{k})}}(\tau, \mathbf{k}) \tag{26.105}$$

Lemma 26.33 We obtain the derivative

$$\begin{aligned}
\partial_\tau \widetilde{\mathscr{G}}_{\substack{n\\ X}}(\tau, \mathbf{k}) &= -\frac{1}{\hbar^2}\left(\epsilon_n(\mathbf{k}) - \mu\right)\left\langle \mathrm{T}_\tau\, c^\dagger_{n,\downarrow}(\tau, -\mathbf{k}) X(0)\right\rangle \\
&\quad - \frac{1}{\hbar^2}\sum_{\substack{\mathbf{k}' \in \mathrm{Q}\\ \nu' \in \{1,2,\dots,rd_{\mathrm{x}}\}\\ n' \in \{1,2,\dots\}}} \frac{g^*_{nn'\nu'}(-\mathbf{k}', \mathbf{k}' - \mathbf{k})}{\hbar\sqrt{N_p}}\left\langle (b_{\nu'}(\tau, \mathbf{k} - \mathbf{k}') + b^\dagger_{\nu'}(\tau, \mathbf{k}' - \mathbf{k})) c^\dagger_{n',\downarrow}(\tau, -\mathbf{k}') X(0)\right\rangle + \begin{cases} \frac{1}{\hbar}\delta(\tau), & X = c_{n,\downarrow}(-\mathbf{k}) \\ 0, & X = c^\dagger_{n,\uparrow}(+\mathbf{k}) \end{cases} \\
&\equiv \begin{cases} \partial_\tau \mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau, -\mathbf{k}), & X = c_{n,\downarrow}(-\mathbf{k}) \\ \partial_\tau \mathscr{F}^\dagger_n(\tau, \mathbf{k}), & X = c^\dagger_{n,\uparrow}(+\mathbf{k}) \end{cases}
\end{aligned} \tag{26.106}$$

Correction note. Three errors:

1. The sign of the δ-term is wrong. Differentiating the time-ordering gives $-\frac{1}{\hbar}\delta(\tau)\{c^\dagger_{n\downarrow}(-\mathbf{k}), X\}$, i.e. $-\frac{1}{\hbar}\delta(\tau)$ for $X = c_{n\downarrow}(-\mathbf{k})$ (second line of the proof). The sign is lost in the third line of the proof. Check: the free solution must be $(\widehat{\mathscr{G}}_0)_{22}(\mathrm{i}\omega, \mathbf{k}) = 1/(\mathrm{i}\hbar\omega + \epsilon_n(\mathbf{k}) - \mu)$ (Lemma 26.13), which requires $(\partial_\tau - \frac{\epsilon_n(\mathbf{k})-\mu}{\hbar})(\widehat{\mathscr{G}}_0)_{22}(\tau, \mathbf{k}) = -\frac{1}{\hbar}\delta(\tau)$.
2. The prefactor of the second line is $-\frac{1}{\hbar}$, not $-\frac{1}{\hbar^2}$: $\partial_\tau \widetilde{\mathscr{G}} = \ldots + \frac{1}{\hbar}\langle \mathrm{T}_\tau[c^\dagger, \frac{H-\mu N}{\hbar}]_{\mathrm{H}} X\rangle$, and the commutator already contains $g^*/(\hbar\sqrt{N_p})$. In total, the coupling enters as $g^*/(\hbar^2\sqrt{N_p})$.

3. For $X = c_{n\downarrow}(-\mathbf{k})$ one has $\widetilde{\mathscr{G}} = (\widehat{\mathscr{G}}_n)_{22}(\tau,\mathbf{k}) = -\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau,-\mathbf{k})$, hence $\partial_\tau\widetilde{\mathscr{G}} = -\partial_\tau[\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau,-\mathbf{k})]$ (minus sign missing in the last line).

With $\widetilde{\mathscr{G}}$ on the left-hand side, the corrected Lemma reads

$$\left(\partial_\tau - \frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\right)\widetilde{\mathscr{G}}^{n}_{X}(\tau,\mathbf{k}) = -\frac{\delta_{X,c_{n\downarrow}(-\mathbf{k})}}{\hbar}\delta(\tau) - \sum_{\substack{\mathbf{k}'\in\mathrm{Q}\\ \nu'\in\{1,\ldots,rd_{\mathbf{x}}\}\\ n'\in\{1,2,\ldots\}}} \frac{g^*_{nn'\nu'}(-\mathbf{k}',\mathbf{k}'-\mathbf{k})}{\hbar^2\sqrt{N_p}}\left\langle \mathrm{T}_\tau\left(b_{\nu'}(\tau,\mathbf{k}-\mathbf{k}')+b^\dagger_{\nu'}(\tau,\mathbf{k}'-\mathbf{k})\right)c^\dagger_{n',\downarrow}(\tau,-\mathbf{k}')X(0)\right\rangle_{\mathrm{SC}}, \tag{26.107}$$

where $\delta_{X,c_{n\downarrow}(-\mathbf{k})} = 1$ for $X = c_{n\downarrow}(-\mathbf{k})$ and $= 0$ for $X = c^\dagger_{n\uparrow}(\mathbf{k})$.

Proof 26.33 Therefore we now consider the derivative

$$\begin{aligned}
\partial_\tau\widetilde{\mathscr{G}}^{n}_{X}(\tau,\mathbf{k}) &\overset{\text{for } X\in\{c,c^\dagger\}}{=} -\frac{\partial_\tau}{\hbar}\left(\theta(\tau)\left\langle c^\dagger_{n,\downarrow}(\tau,-\mathbf{k})X(0)\right\rangle + \theta(-\tau)\zeta\left\langle X(0)c^\dagger_{n,\downarrow}(\tau,-\mathbf{k})\right\rangle\right)\\
&\overset{\text{cf. Def. 8.12 or so}}{=} -\frac{1}{\hbar}\left(\delta(\tau)\left[c^\dagger_{n,\downarrow}(0,-\mathbf{k}),X(0)\right]_\zeta\right) + \frac{1}{\hbar}\left\langle \mathrm{T}_\tau\left[c^\dagger_{n,\downarrow}(-\mathbf{k}),\frac{H-\mu N}{\hbar}\right]_{\mathrm{H}}(\tau)X(0)\right\rangle\\
&= \frac{1}{\hbar}\left\langle \mathrm{T}_\tau\left[c^\dagger_{n,\downarrow}(-\mathbf{k}),\frac{H-\mu N}{\hbar}\right]_{\mathrm{H}}(\tau)X(0)\right\rangle + \begin{cases}\frac{1}{\hbar}\delta(\tau), & X = c_{n,\downarrow}(-\mathbf{k})\\ 0, & X = c^\dagger_{n,\uparrow}(+\mathbf{k})\end{cases}
\end{aligned} \tag{26.108}$$

Correction note. In the second line $[\cdot,\cdot]_\zeta$ with $\zeta = -1$ is the anti-commutator, $\{c^\dagger_{n\downarrow}(-\mathbf{k}),c_{n\downarrow}(-\mathbf{k})\} = 1$ and $\{c^\dagger_{n\downarrow}(-\mathbf{k}),c^\dagger_{n\uparrow}(\mathbf{k})\} = 0$. Hence the third line has $-\frac{1}{\hbar}\delta(\tau)$ (not $+\frac{1}{\hbar}\delta(\tau)$) for $X = c_{n\downarrow}(-\mathbf{k})$. The second term uses $\partial_\tau c^\dagger_{\mathrm{H}}(\tau) = -\frac{1}{\hbar}[c^\dagger, H-\mu N]_{\mathrm{H}}(\tau)$ (corrected Lemma 26.18).

Therefore we need to compute the commutator[12] whereas we use in the second equation sign the results from earlier calculations and in the third equation sign we make the replacement $\mathbf{k}^\dagger \mapsto -\mathbf{k}'$ and we also use the symmetry of ϵ w.r.t. inversion symmetry such that we obtain

$$\begin{aligned}
\left[c^\dagger_{n,\downarrow}(-\mathbf{k}),\frac{H-\mu N}{\hbar}\right] &= \left[\frac{H-\mu N}{\hbar},c_{n,\downarrow}(-\mathbf{k})\right]^\dagger\\
&= \left(-\frac{\epsilon_n(-\mathbf{k})-\mu}{\hbar}c_{n,\downarrow}(-\mathbf{k}) - \sum_{\substack{\mathbf{k}'\in\mathrm{Q}\\ \nu'\in\{1,2,\ldots rd_{\mathbf{x}}\}\\ n'\in\{1,2,\ldots,\}}}\frac{g_{nn'\nu'}(-\mathbf{k}',-\mathbf{k}-\mathbf{k}')}{\hbar\sqrt{N_p}}(b_{\nu'}(-\mathbf{k}-\mathbf{k}')+b^\dagger_{\nu'}(+\mathbf{k}+\mathbf{k}'))c_{n',\downarrow}(\mathbf{k}')\right)^\dagger\\
&= -\frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}c^\dagger_{n,\downarrow}(-\mathbf{k}) - \sum_{\substack{\mathbf{k}'\in\mathrm{Q}\\ \nu'\in\{1,2,\ldots rd_{\mathbf{x}}\}\\ n'\in\{1,2,\ldots,\}}}\frac{g^*_{nn'\nu'}(-\mathbf{k}',\mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}}(b_{\nu'}(\mathbf{k}-\mathbf{k}')+b^\dagger_{\nu'}(+\mathbf{k}'-\mathbf{k}))c^\dagger_{n',\downarrow}(-\mathbf{k}')
\end{aligned} \tag{26.110}$$

[12] Notice (as a Lemma) that one has on the one hand

$$[A,B] = AB-BA \;\Rightarrow\; [A,B]^\dagger = (AB-BA)^\dagger = B^\dagger A^\dagger - A^\dagger B^\dagger = -[A^\dagger,B^\dagger] = [B^\dagger,A^\dagger] \tag{26.109}$$

This gives us (depending on the choice of X) two equations of motion

$$\begin{aligned}\partial_\tau \widetilde{\mathscr{G}}_{n\atop X}(\tau,\mathbf{k}) &= -\frac{1}{\hbar^2}\left(\epsilon_n(\mathbf{k})-\mu\right)\left\langle \mathrm{T}_\tau\, c^\dagger_{n,\downarrow}(\tau,-\mathbf{k})X(0)\right\rangle \\ &\quad -\frac{1}{\hbar^2}\sum_{\substack{\mathbf{k}'\in \mathrm{Q}\\ \nu'\in\{1,2,\dots,rd_{\mathrm{x}}\}\\ n'\in\{1,2,\dots\}}} \frac{g^*_{nn'\nu'}(-\mathbf{k}',\mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}}\left\langle (b_{\nu'}(\tau,\mathbf{k}-\mathbf{k}')+b^\dagger_{\nu'}(\tau,\mathbf{k}'-\mathbf{k}))c^\dagger_{n',\downarrow}(\tau,-\mathbf{k}')X(0)\right\rangle + \begin{cases}\frac{1}{\hbar}\delta(\tau), & X=c_{n,\downarrow}(-\mathbf{k})\\ 0, & X=c^\dagger_{n,\uparrow}(+\mathbf{k})\end{cases} \\ &\equiv \begin{cases}\partial_\tau \mathscr{G}_{n\atop \text{Gorkov}}(-\tau,-\mathbf{k}), & X=c_{n,\downarrow}(-\mathbf{k})\\ \partial_\tau \mathscr{F}^\dagger_n(\tau,\mathbf{k}), & X=c^\dagger_{n,\uparrow}(+\mathbf{k})\end{cases}\end{aligned} \tag{26.111}$$

Note. The commutator computation above is correct (with $\mathbf{k}^\dagger \mapsto -\mathbf{k}'$ read as $\mathbf{k}' \mapsto -\mathbf{k}'$, and with $(b_\nu(\mathbf{q}) + b^\dagger_\nu(-\mathbf{q}))^\dagger = b_\nu(-\mathbf{q}) + b^\dagger_\nu(\mathbf{q})$). The last equation repeats the statement of the Lemma and contains the same three errors; the corrected version is Equation (26.107).

Definition 26.34 Now we introduce the auxiliary-Green-function: For $\tau,\tau' \in (0,\hbar\beta)$ we have

$$\widetilde{\mathscr{G}_{\text{aux}}}_{\substack{\nu'\nu n'\\ X}}(\tau,\tau',\mathbf{k},\mathbf{k}') = -\frac{1}{\hbar}\left\langle \left(b_{\nu'}(\mathbf{k}-\mathbf{k}')+b^\dagger_{\nu'}(\mathbf{k}'-\mathbf{k})\right)c^\dagger_{n'\downarrow}(\tau',-\mathbf{k}')X(0)\right\rangle \tag{26.112}$$

Correction note. As in Equation (26.40), the phonon operators carry the time τ and the expectation value is time-ordered, $\widetilde{\mathscr{G}}_{\text{aux}}(\tau,\tau',\mathbf{k},\mathbf{k}') = -\frac{1}{\hbar}\langle \mathrm{T}_\tau(b_{\nu'}(\tau,\mathbf{k}-\mathbf{k}')+b^\dagger_{\nu'}(\tau,\mathbf{k}'-\mathbf{k}))c^\dagger_{n'\downarrow}(\tau',-\mathbf{k}')X(0)\rangle_{\mathrm{SC}}$. The index ν in the subscript is not used; it means $\nu'n'$.

Remark 26.34.1 Notice that this allows us to rewrite the equations of motion as

$$\partial_\tau \widetilde{\mathscr{G}}_{X}(\tau,\mathbf{k}) = \frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\widetilde{\mathscr{G}}_{X}(\tau,\mathbf{k}) + \sum_{\substack{\mathbf{k}'\in \mathrm{Q}\\ \nu'\in\{1,2,3,\dots,rd_{\mathrm{x}}\}\\ n'\in\{1,2,\dots\}}} \frac{g_{nn'\nu'}(-\mathbf{k}',\mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}}\widetilde{\mathscr{G}_{\text{aux}}}_{\substack{\nu'\nu n'\\ X}}(\tau,\tau',\mathbf{k},\mathbf{k}') + \begin{cases}\frac{1}{\hbar}\delta(\tau), & X=c_{n,\downarrow}(-\mathbf{k})\\ 0, & X=c^\dagger_{n,\uparrow}(+\mathbf{k})\end{cases} \tag{26.113}$$

Correction note. From Equation (26.107) and $\langle \mathrm{T}_\tau(b+b^\dagger)c^\dagger X\rangle_{\mathrm{SC}} = -\hbar\widetilde{\mathscr{G}}_{\text{aux}}(\tau,\tau,\dots)$ the correct equation is

$$\partial_\tau \widetilde{\mathscr{G}}_{X}(\tau,\mathbf{k}) = \tfrac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\widetilde{\mathscr{G}}_{X}(\tau,\mathbf{k}) + \sum_{\mathbf{k}',\nu',n'} \frac{g^*_{nn'\nu'}(-\mathbf{k}',\mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}}\widetilde{\mathscr{G}}_{\text{aux}\atop \nu'n'\ X}(\tau,\tau,\mathbf{k},\mathbf{k}') - \frac{\delta_{X,c_{n\downarrow}(-\mathbf{k})}}{\hbar}\delta(\tau),$$

i.e. (a) g^* instead of g, (b) equal times (τ,τ) in $\widetilde{\mathscr{G}}_{\text{aux}}$, (c) $-\frac{1}{\hbar}\delta(\tau)$.

Lemma 26.35 We obtain the τ-derivative of $\widetilde{\mathscr{G}_{\text{aux}}}_{\substack{\nu'\nu n'\\ X}}$ as

$$\begin{aligned}&\left(\partial_\tau^2-\omega^2_{\nu'}(\mathbf{k}-\mathbf{k}')\right)\widetilde{\mathscr{G}_{\text{aux}}}_{\substack{\nu'\nu n'\\ X}}(\tau,\tau',\mathbf{k},\mathbf{k}') \\ &= -\frac{2\omega_{\nu'}(\mathbf{k}-\mathbf{k}')}{\hbar}\sum_{\substack{\mathbf{q}\in \mathrm{Q}\\ m,m'\in\{1,2,\dots\}\\ \sigma\in\{\downarrow,\uparrow\}}} \frac{g_{mm'\nu'(\mathbf{q},\mathbf{k}'-\mathbf{k})}}{\hbar\sqrt{N_p}}\left\langle \mathrm{T}_\tau\, c^\dagger_{m,\sigma}(\tau,\mathbf{q}+\mathbf{k}'-\mathbf{k})c_{m'\sigma}(\tau,\mathbf{q})c^\dagger_{n',\downarrow}(-\mathbf{k}',\tau')X(0)\right\rangle\end{aligned} \tag{26.114}$$

Proof 26.35 Completely analogous to the previous Lemma TBReferenced giving

(Lemma 26.22 resp. Lemma 26.28: the phonon operators enter through the same combination $b_{\nu'}(\tau, \mathbf{k}-\mathbf{k}') + b^\dagger_{\nu'}(\tau, \mathbf{k}'-\mathbf{k})$, and only the fermionic spectators $c^\dagger_{n'\downarrow}(\tau', -\mathbf{k}')$, $X(0)$ are different. In the last operator the arguments are $(\tau', -\mathbf{k}')$; the expectation value is $\langle \ldots \rangle_{\mathrm{SC}}$. The Lemma is correct.)

Corollary 26.36 This gives the equation

$$\widetilde{\mathscr{G}^{\mathrm{aux}}_{\substack{\nu' \nu n' \\ X}}}(\tau, \tau', \mathbf{k}, \mathbf{k}') = \sum\!\!\!\!\!\!\int_{\substack{\mathbf{q}\in \mathrm{Q} \\ \tau' \in (0,\hbar\beta) \\ m,m' \in \{1,2,\ldots\} \\ \sigma \in \{\downarrow,\uparrow\}}} (-1) \mathscr{D}_{\substack{0,\nu' \\ \mathbf{k}-\mathbf{k}'}}(\tau - \tau') \frac{g_{mm'\nu'}(\mathbf{q}, \mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}} \left\langle \mathrm{T}_\tau \, c^\dagger_{m,\sigma}(\tau, \mathbf{q}+\mathbf{k}'-\mathbf{k}) c_{m'\sigma}(\tau, \mathbf{q}) c^\dagger_{n',\downarrow}(-\mathbf{k}', \tau') X(0) \right\rangle \tag{26.115}$$

Proof 26.36 Analogous to Corollary TBReferenced.

(Corollary 26.23.) *Correction note.* As in Corollary 26.23, one exchanges the roles of τ and τ', multiplies with $\mathscr{D}_0(\tau - \tau')$ and integrates over the phonon time τ'. Therefore the left-hand side is the equal-time function $\widetilde{\mathscr{G}}_{\mathrm{aux}}(\tau, \tau, \mathbf{k}, \mathbf{k}')$. On the right-hand side the electron-pair carries the integration time τ', and $c^\dagger_{n'\downarrow}$ carries the time τ:

$$\widetilde{\mathscr{G}^{\mathrm{aux}}_{\substack{\nu' n' \\ X}}}(\tau, \tau, \mathbf{k}, \mathbf{k}') = -\sum\!\!\!\!\!\!\int_{\mathbf{q},\tau',m,m',\sigma} \mathscr{D}_{\substack{0,\nu' \\ \mathbf{k}-\mathbf{k}'}}(\tau - \tau') \frac{g_{mm'\nu'}(\mathbf{q}, \mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}} \left\langle \mathrm{T}_\tau \, c^\dagger_{m,\sigma}(\tau', \mathbf{q}+\mathbf{k}'-\mathbf{k}) c_{m'\sigma}(\tau', \mathbf{q}) c^\dagger_{n',\downarrow}(\tau, -\mathbf{k}') X(0) \right\rangle_{\mathrm{SC}}.$$

Inserting this into the corrected Remark above gives, with $\widetilde{\mathrm{CORR}}$ from the following Notation (with these times),

$$\left(\partial_\tau - \tfrac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\right) \widetilde{\mathscr{G}^n_X}(\tau, \mathbf{k}) = -\tfrac{\delta_{X, c_{n\downarrow}(-\mathbf{k})}}{\hbar}\delta(\tau) - \sum\!\!\!\!\!\!\int_{\substack{\mathbf{q},\mathbf{k}',\tau',\nu' \\ m,m',n'}} \frac{g^*_{nn'\nu'}(-\mathbf{k}', \mathbf{k}'-\mathbf{k}) g_{mm'\nu'}(\mathbf{q}, \mathbf{k}'-\mathbf{k})}{\hbar^2 N_p} \mathscr{D}_{\substack{0,\nu' \\ \mathbf{k}-\mathbf{k}'}}(\tau - \tau') \sum_{\sigma\in\{\downarrow,\uparrow\}} \widetilde{\mathrm{CORR}}(\sigma, X). \tag{26.116}$$

Notation 26.37 Now we simplify this again, using the Nambu-formalism. Therefore we rewrite (analogous to page twohundred-fifty-something)

$$c_{n'\downarrow}(\tau, -\mathbf{k}') = \eta_{n',2}(\tau, \mathbf{k}') \tag{26.117}$$

and obtain, with

$$\widetilde{\mathrm{CORR}}(\sigma, X) = \left\langle \mathrm{T}_\tau \, c^\dagger_{m,\sigma}(\tau, \mathbf{q}+\mathbf{k}'-\mathbf{k}) c_{m'\sigma}(\tau, \mathbf{q}) c^\dagger_{n',\downarrow}(-\mathbf{k}', \tau') X(0) \right\rangle \tag{26.118}$$

the different cases

$$\{\widetilde{\mathrm{CORR}}(\sigma, X)\}_{\substack{\sigma\in\{\downarrow,\uparrow\} \\ X\in\{c_{n,\downarrow}(-\mathbf{k}), c^\dagger_{n,\uparrow}(\mathbf{k})\}}} \tag{26.119}$$

i.e. four terms in total.

Correction note. The first equation has to read $c^\dagger_{n'\downarrow}(\tau,-\mathbf{k}') = \eta_{n',2}(\tau,\mathbf{k}')$ (with a dagger, cf. the Notation in Preparation 2/4). In $\widetilde{\mathrm{CORR}}$ the times are $c^\dagger_{m\sigma}(\tau',\ldots)c_{m'\sigma}(\tau',\ldots)c^\dagger_{n'\downarrow}(\tau,-\mathbf{k}')X(0)$ (as used in the proofs below), and $\langle\ldots\rangle = \langle\ldots\rangle_{\mathrm{SC}}$. Moreover $X = c_{n\downarrow}(-\mathbf{k}) = \overline{\eta}_{n,2}(0,\mathbf{k})$ and $X = c^\dagger_{n\uparrow}(\mathbf{k}) = \overline{\eta}_{n,1}(0,\mathbf{k})$, i.e. $X = \overline{\eta}_{n,j}(0,\mathbf{k})$ with $j = 2$ resp. $j = 1$, and $\widetilde{\mathscr{G}}_X = (\widehat{\mathscr{G}}_n)_{2j}$.

Lemma 26.38 For $X = c_{n,\downarrow}(-\mathbf{k})$ we obtain

$$\sum_{\sigma\in\{\downarrow,\uparrow\}} \widetilde{\mathrm{CORR}}(\sigma,X) = \delta_{n,n'}\delta_{m,m'}\delta_{\mathbf{k},\mathbf{k}'}\mathscr{G}^{\ n}_{\mathrm{Gorkov}}(-\tau,-\mathbf{k})\mathscr{G}^{\ m}_{\mathrm{Gorkov}}(0,\mathbf{q}) - \delta_{n',m'}\delta_{n,m}\delta_{-\mathbf{q},\mathbf{k}'}\mathscr{G}^{\ n'}_{\mathrm{Gorkov}}(\tau'-\tau,-\mathbf{k}')\mathscr{G}^{\ n}_{\mathrm{Gorkov}}(-\tau',-\mathbf{k}')$$
$$+ \quad \delta_{n,m'}\delta_{n',m}\delta_{\mathbf{q},\mathbf{k}}\mathscr{F}_n(\tau',\mathbf{k})\mathscr{F}^\dagger_{n'}(\tau-\tau',\mathbf{k}') - \delta_{m,m'}\delta_{n,n'}\delta_{\mathbf{k},\mathbf{k}'}\mathscr{G}^{\ m}_{\mathrm{Gorkov}}(0,\mathbf{q})(-1)\mathscr{G}^{\ n}_{\mathrm{Gorkov}}(-\tau,-\mathbf{k}) \tag{26.120}$$

Correction note. (i) The whole right-hand side has to be multiplied by $\hbar^2$: the decoupling gives $\langle \mathrm{T}_\tau \eta\eta\overline{\eta}\overline{\eta}\rangle_{\mathrm{SC}} \approx \hbar^2[\widehat{\mathscr{G}}\widehat{\mathscr{G}} - \widehat{\mathscr{G}}\widehat{\mathscr{G}}]$ (as in Preparation 1/4 and 2/4; the $\hbar^2$ is missing from the fourth line of the proof onwards). (ii) In the second term the last factor is $\mathscr{G}^{\ n}_{\mathrm{Gorkov}}(-\tau',-\mathbf{k})$, i.e. the green prime has to be removed: $\widehat{\mathscr{G}}(i_2|i_1') = (\widehat{\mathscr{G}}_n)_{22}(\tau',\mathbf{k}) = -\mathscr{G}^{\ n}_{\mathrm{Gorkov}}(-\tau',-\mathbf{k})$. In the equal-time factors $\mathscr{G}^{\ m}_{\mathrm{Gorkov}}(0,\mathbf{q})$, the "0" means 0^-. Otherwise the Lemma is correct.

Proof 26.38 We find with $c_{n,\downarrow}(-\mathbf{k}) = \overline{\eta}_{n,2}(\mathbf{k})$ for the correlators

(In the first two lines the third operator is $c^\dagger_{n'\downarrow}(\tau,-\mathbf{k}') = \eta_{n'2}(\tau,\mathbf{k}')$, with a dagger; from the line with $\widehat{\mathscr{G}}(i_1,i_2|i_1',i_2')$ onwards a factor $\hbar^2$ is missing. Apart from this, all index assignments and Kronecker-deltas below are correct.)

$$\begin{aligned}
&\sum_{\sigma\in\{\downarrow,\uparrow\}} \left\langle \mathrm{T}_\tau\, c^\dagger_{m,\sigma}(\tau',\mathbf{q}+\mathbf{k}'-\mathbf{k})c_{m'\sigma}(\tau',\mathbf{q})c_{n'\downarrow}(\tau,-\mathbf{k}')c_{n,\downarrow}(0,-\mathbf{k})\right\rangle \\
&= \left\langle \mathrm{T}_\tau\, c^\dagger_{m,\downarrow}(\tau',\mathbf{q}+\mathbf{k}'-\mathbf{k})c_{m'\downarrow}(\tau',\mathbf{q})c_{n'\downarrow}(\tau,-\mathbf{k}')c_{n,\downarrow}(0,-\mathbf{k})\right\rangle + \left\langle \mathrm{T}_\tau\, c^\dagger_{m,\uparrow}(\tau',\mathbf{q}+\mathbf{k}'-\mathbf{k})c_{m'\uparrow}(\tau',\mathbf{q})c_{n'\downarrow}(\tau,-\mathbf{k}')c_{n,\downarrow}(0,-\mathbf{k})\right\rangle \\
&= \left\langle \mathrm{T}_\tau\, \eta_{m,2}(\tau',-\mathbf{q}-\mathbf{k}'+\mathbf{k})\overline{\eta}_{m'2}(\tau',-\mathbf{q})\eta_{n'2}(\tau,+\mathbf{k}')\overline{\eta}_{n,2}(0,\mathbf{k})\right\rangle + \left\langle \mathrm{T}_\tau\, \overline{\eta}_{m,1}(\tau',\mathbf{q}+\mathbf{k}'-\mathbf{k})\eta_{m'1}(\tau',\mathbf{q})\eta_{n'2}(\tau,\mathbf{k}')\overline{\eta}_{n,2}(0,\mathbf{k})\right\rangle \\
&= \left\langle \mathrm{T}_\tau\, \eta_{n'2}(\tau,+\mathbf{k}')\eta_{m,2}(\tau',-\mathbf{q}-\mathbf{k}'+\mathbf{k})\overline{\eta}_{m'2}(\tau',-\mathbf{q})\overline{\eta}_{n,2}(0,\mathbf{k})\right\rangle + \left\langle \mathrm{T}_\tau\, \eta_{m'1}(\tau',\mathbf{q})\eta_{n'2}(\tau,\mathbf{k}')\overline{\eta}_{m,1}(\tau',\mathbf{q}+\mathbf{k}'-\mathbf{k})\overline{\eta}_{n,2}(0,\mathbf{k})\right\rangle \\
&= \widehat{\mathscr{G}}\left(i_1\equiv[n',2,\tau,\mathbf{k}'], i_2\equiv[m,2,\tau',-\mathbf{q}-\mathbf{k}'+\mathbf{k}] \,|\, i_1'\equiv[n,2,0,\mathbf{k}], i_2'\equiv[m',2,\tau',-\mathbf{q}]\right) \\
&+ \widehat{\mathscr{G}}\left(i_1\equiv[m',1,\tau',\mathbf{q}], i_2\equiv[n',2,\tau,\mathbf{k}'] \,|\, i_1'\equiv[n,2,0,\mathbf{k}], i_2'\equiv[m,1,\tau',\mathbf{q}+\mathbf{k}'-\mathbf{k}]\right) \\
&= \underset{\mathbf{k}',\mathbf{k}}{\widehat{\mathscr{G}}^{\ 2,2}_{n',n}}(\tau-0)\underset{-\mathbf{q}-\mathbf{k}'+\mathbf{k},-\mathbf{q}}{\widehat{\mathscr{G}}^{\ 2,2}_{m,m'}}(0) - \underset{\mathbf{k}',-\mathbf{q}}{\widehat{\mathscr{G}}^{\ 2,2}_{n',m'}}(\tau-\tau')\underset{-\mathbf{q}-\mathbf{k}'+\mathbf{k},\mathbf{k}}{\widehat{\mathscr{G}}^{\ 2,2}_{m,n}}(\tau'-0) \quad + \quad \underset{\mathbf{q},\mathbf{k}}{\widehat{\mathscr{G}}^{\ 1,2}_{m',n}}(\tau'-0)\underset{\mathbf{k}',\mathbf{q}+\mathbf{k}'-\mathbf{k}}{\widehat{\mathscr{G}}^{\ 2,1}_{n',m}}(\tau-\tau') - \underset{\mathbf{q},\mathbf{q}+\mathbf{k}'-\mathbf{k}}{\widehat{\mathscr{G}}^{\ 1,1}_{m',m}}(0)\underset{\mathbf{k}',\mathbf{k}}{\widehat{\mathscr{G}}^{\ 2,2}_{n',n}}(\tau-0) \\
&= \delta_{n,n'}\delta_{m,m'}\delta_{\mathbf{k},\mathbf{k}'}\underset{2,2}{\widehat{\mathscr{G}}_{n,\mathbf{k}}}(\tau-0)\underset{2,2}{\widehat{\mathscr{G}}_{m,-\mathbf{q}}}(0) - \delta_{n',m'}\delta_{n,m}\delta_{-\mathbf{q},\mathbf{k}'}\underset{2,2}{\widehat{\mathscr{G}}_{n',\mathbf{k}'}}(\tau-\tau')\underset{2,2}{\widehat{\mathscr{G}}_{n,\mathbf{k}}}(\tau') \quad + \quad \delta_{n,m'}\delta_{n',m}\delta_{\mathbf{q},\mathbf{k}}\underset{1,2}{\widehat{\mathscr{G}}_{n,\mathbf{k}}}(\tau')\underset{2,1}{\widehat{\mathscr{G}}_{n',\mathbf{k}'}}(\tau-\tau') - \delta_{m,m'}\delta_{n,n'}\delta_{\mathbf{k},\mathbf{k}'}\underset{1,1}{\widehat{\mathscr{G}}_{m,\mathbf{q}}}(0)\underset{2,2}{\widehat{\mathscr{G}}_{n,\mathbf{k}}}(\tau) \\
&= \delta_{n,n'}\delta_{m,m'}\delta_{\mathbf{k},\mathbf{k}'}\mathscr{G}^{\ n}_{\mathrm{Gorkov}}(-\tau,-\mathbf{k})\mathscr{G}^{\ m}_{\mathrm{Gorkov}}(0,\mathbf{q}) - \delta_{n',m'}\delta_{n,m}\delta_{-\mathbf{q},\mathbf{k}'}\mathscr{G}^{\ n'}_{\mathrm{Gorkov}}(\tau'-\tau,-\mathbf{k}')\mathscr{G}^{\ n}_{\mathrm{Gorkov}}(-\tau',-\mathbf{k}') \\
&\quad + \quad \delta_{n,m'}\delta_{n',m}\delta_{\mathbf{q},\mathbf{k}}\mathscr{F}_n(\tau',\mathbf{k})\mathscr{F}^\dagger_{n'}(\tau-\tau',\mathbf{k}') - \delta_{m,m'}\delta_{n,n'}\delta_{\mathbf{k},\mathbf{k}'}\mathscr{G}^{\ m}_{\mathrm{Gorkov}}(0,\mathbf{q})(-1)\mathscr{G}^{\ n}_{\mathrm{Gorkov}}(-\tau,-\mathbf{k})
\end{aligned} \tag{26.121}$$

implying that we managed to simplify the complicated correlator.

Lemma 26.39 For $X = c_{n,\uparrow}(+\mathbf{k})$ we obtain

$$\sum_{\sigma\in\{\downarrow,\uparrow\}} \widetilde{\mathrm{CORR}}(\sigma,X) = \delta_{n,n'}\delta_{m,m'}\delta_{\mathbf{k},\mathbf{k}'}\mathscr{F}_n^\dagger(\tau,\mathbf{k})(-1)\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(0,\mathbf{q}) - \delta_{n',m'}\delta_{n,m}\delta_{-\mathbf{q},\mathbf{k}'}(-1)\mathscr{G}_{\substack{n'\\ \text{Gorkov}}}(\tau'-\tau,-\mathbf{k}')\mathscr{F}_n(\tau',\mathbf{k}')$$
$$+ \quad \delta_{n,m'}\delta_{n',m}\delta_{\mathbf{q},\mathbf{k}}\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(\tau',\mathbf{k})\mathscr{F}_{n'}^\dagger(\tau-\tau',\mathbf{k}') - \delta_{m,m'}\delta_{n,n'}\delta_{\mathbf{k},\mathbf{k}'}\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(0,\mathbf{q})\mathscr{F}_n^\dagger(\tau,\mathbf{k}) \tag{26.122}$$

Correction note. (i) $X = c_{n\uparrow}^\dagger(+\mathbf{k})$ (dagger missing in the statement). (ii) As in the previous Lemma, the right-hand side has to be multiplied by $\hbar^2$. (iii) The second term is wrong. From $\widehat{\mathscr{G}}(i_1|i_2')\widehat{\mathscr{G}}(i_2|i_1') = (\widehat{\mathscr{G}}_{n'})_{22}(\tau-\tau',\mathbf{k}')(\widehat{\mathscr{G}}_n)_{21}(\tau',\mathbf{k})$ (cf. the proof) it reads

$$-\delta_{n',m'}\delta_{n,m}\delta_{-\mathbf{q},\mathbf{k}'}(-1)\mathscr{G}_{\substack{n'\\ \text{Gorkov}}}(\tau'-\tau,-\mathbf{k}')\mathscr{F}_n^\dagger(\tau',\mathbf{k}),$$

i.e. $\mathscr{F}_n^\dagger(\tau',\mathbf{k})$ instead of $\mathscr{F}_n(\tau',\mathbf{k}')$. The first, third and fourth term are correct.

Proof 26.39 Then we find with $c_{n,\uparrow}^\dagger(+\mathbf{k}) = \overline{\eta}_{n,1}(\mathbf{k})$ for the correlators

(In the first line the third operator is $c_{n'\downarrow}^\dagger(\tau,-\mathbf{k}')$ and the fourth is $c_{n\uparrow}^\dagger(0,+\mathbf{k})$; a factor $\hbar^2$ is missing from the line with $\widehat{\mathscr{G}}(i_1,i_2|i_1',i_2')$ onwards; in the last line the second term has to be $(-1)\mathscr{G}_{\substack{n'\\ \text{Gorkov}}}(\tau'-\tau,-\mathbf{k}')\mathscr{F}_n^\dagger(\tau',\mathbf{k})$, because the line before correctly contains $(\widehat{\mathscr{G}}_n)_{21}(\tau',\mathbf{k}) = \mathscr{F}_n^\dagger(\tau',\mathbf{k})$.)

$$\begin{aligned}
&\sum_{\sigma\in\{\downarrow,\uparrow\}} \left\langle \mathrm{T}_\tau\, c_{m,\sigma}^\dagger(\tau',\mathbf{q}+\mathbf{k}'-\mathbf{k})c_{m'\sigma}(\tau',\mathbf{q})c_{n'\downarrow}(\tau,-\mathbf{k}')c_{n,\uparrow}^\dagger(0,-\mathbf{k})\right\rangle \\
&= \ldots \text{ (analogous to above)} \\
&= \left\langle \mathrm{T}_\tau\, \eta_{n'2}(\tau,+\mathbf{k}')\eta_{m,2}(\tau',-\mathbf{q}-\mathbf{k}'+\mathbf{k})\overline{\eta}_{m'2}(\tau',-\mathbf{q})\overline{\eta}_{n,1}(0,\mathbf{k})\right\rangle + \left\langle \mathrm{T}_\tau\, \eta_{m'1}(\tau',\mathbf{q})\eta_{n'2}(\tau,\mathbf{k}')\overline{\eta}_{m,1}(\tau',\mathbf{q}+\mathbf{k}'-\mathbf{k})\overline{\eta}_{n,1}(0,\mathbf{k})\right\rangle \\
&= \widehat{\mathscr{G}}\left(i_1\equiv[n',2,\tau,\mathbf{k}'],i_2\equiv[m,2,\tau',-\mathbf{q}-\mathbf{k}'+\mathbf{k}]\,|\,i_1'\equiv[n,1,0,\mathbf{k}],i_2'\equiv[m',2,\tau',-\mathbf{q}]\right) \\
&+ \widehat{\mathscr{G}}\left(i_1\equiv[m',1,\tau',\mathbf{q}],i_2\equiv[n',2,\tau,\mathbf{k}']\,|\,i_1'\equiv[n,1,0,\mathbf{k}],i_2'\equiv[m,1,\tau',\mathbf{q}+\mathbf{k}'-\mathbf{k}]\right) \\
&= \widehat{\mathscr{G}}_{\substack{n',n\\ 2,1\\ \mathbf{k}',\mathbf{k}}}(\tau)\widehat{\mathscr{G}}_{\substack{m,m'\\ 2,2\\ -\mathbf{q}-\mathbf{k}'+\mathbf{k},-\mathbf{q}}}(0) - \widehat{\mathscr{G}}_{\substack{n',m'\\ 2,2\\ \mathbf{k}',-\mathbf{q}}}(\tau-\tau')\widehat{\mathscr{G}}_{\substack{m,n\\ 2,1\\ -\mathbf{q}-\mathbf{k}'+\mathbf{k},\mathbf{k}}}(\tau') + \widehat{\mathscr{G}}_{\substack{m',n\\ 1,1\\ \mathbf{q},\mathbf{k}}}(\tau')\widehat{\mathscr{G}}_{\substack{n',m\\ 2,1\\ \mathbf{k}',\mathbf{q}+\mathbf{k}'-\mathbf{k}}}(\tau-\tau') - \widehat{\mathscr{G}}_{\substack{m',m\\ 1,1\\ \mathbf{q},\mathbf{q}+\mathbf{k}'-\mathbf{k}}}(0)\widehat{\mathscr{G}}_{\substack{n',n\\ 2,1\\ \mathbf{k}',\mathbf{k}}}(\tau) \\
&= \delta_{n,n'}\delta_{m,m'}\delta_{\mathbf{k},\mathbf{k}'}\widehat{\mathscr{G}}_{\substack{n,\mathbf{k}\\ 2,1}}(\tau)\widehat{\mathscr{G}}_{\substack{m,-\mathbf{q}\\ 2,2}}(0) - \delta_{n',m'}\delta_{n,m}\delta_{-\mathbf{q},\mathbf{k}'}\widehat{\mathscr{G}}_{\substack{n',\mathbf{k}'\\ 2,2}}(\tau-\tau')\widehat{\mathscr{G}}_{\substack{n,\mathbf{k}\\ 2,1}}(\tau') + \delta_{n,m'}\delta_{n',m}\delta_{\mathbf{q},\mathbf{k}}\widehat{\mathscr{G}}_{\substack{n,\mathbf{k}\\ 1,1}}(\tau')\widehat{\mathscr{G}}_{\substack{n',\mathbf{k}'\\ 2,1}}(\tau-\tau') - \delta_{m,m'}\delta_{n,n'}\delta_{\mathbf{k},\mathbf{k}'}\widehat{\mathscr{G}}_{\substack{m,\mathbf{q}\\ 1,1}}(0)\widehat{\mathscr{G}}_{\substack{n,\mathbf{k}\\ 2,1}}(\tau) \\
&= \delta_{n,n'}\delta_{m,m'}\delta_{\mathbf{k},\mathbf{k}'}\mathscr{F}_n^\dagger(\tau,\mathbf{k})(-1)\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(0,\mathbf{q}) - \delta_{n',m'}\delta_{n,m}\delta_{-\mathbf{q},\mathbf{k}'}(-1)\mathscr{G}_{\substack{n'\\ \text{Gorkov}}}(\tau'-\tau,-\mathbf{k}')\mathscr{F}_n(\tau',\mathbf{k}') \\
&\quad + \quad \delta_{n,m'}\delta_{n',m}\delta_{\mathbf{q},\mathbf{k}}\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(\tau',\mathbf{k})\mathscr{F}_{n'}^\dagger(\tau-\tau',\mathbf{k}') - \delta_{m,m'}\delta_{n,n'}\delta_{\mathbf{k},\mathbf{k}'}\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(0,\mathbf{q})\mathscr{F}_n^\dagger(\tau,\mathbf{k})
\end{aligned} \tag{26.123}$$

implying that we managed to simplify the complicated correlator. Now we can write down the equation of motion for the Gorkov-Green-function in imaginary time.

Remark 26.39.1 Notice that we obtain for $X = c_{n,\downarrow}(-\mathbf{k})$ the equation we obtain

$$
\begin{aligned}
&-\partial_\tau \mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau,-\mathbf{k})\\
&=+\frac{1}{\hbar}\delta(\tau)+\frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau,-\mathbf{k})\\
&+\sum\!\!\!\!\!\!\int_{\substack{\mathbf{q},\mathbf{k}'\in Q\\ \nu'\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ m,m',n'\in\{1,2,3,\dots\}\\ \tau'\in(0,\hbar\beta)}} \frac{g^*_{nn'\nu'}(-\mathbf{k}',\mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}}(-1)\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\frac{g_{mm'\nu'}(\mathbf{q},\mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}}
\Big[\delta_{n,n'}\delta_{m,m'}\delta_{\mathbf{k},\mathbf{k}'}\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau,-\mathbf{k})\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(0,\mathbf{q})\\
&\qquad -\delta_{n',m'}\delta_{n,m}\delta_{-\mathbf{q},\mathbf{k}'}\mathscr{G}_{\substack{n'\\ \text{Gorkov}}}(\tau'-\tau,-\mathbf{k}')\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau',-\mathbf{k}')\\
&\qquad +\delta_{n,m'}\delta_{n',m}\delta_{\mathbf{q},\mathbf{k}}\mathscr{F}_n(\tau',\mathbf{k})\mathscr{F}^\dagger_{n'}(\tau-\tau',\mathbf{k}')\\
&\qquad -\delta_{m,m'}\delta_{n,n'}\delta_{\mathbf{k},\mathbf{k}'}\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(0,\mathbf{q})(-1)\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau,-\mathbf{k})\Big]
\end{aligned}
\tag{26.124}
$$

Correction note. With the corrected Equation (26.116) and $\widetilde{\mathscr{G}} = -\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau,-\mathbf{k})$ (so that the left-hand side $-\partial_\tau[\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau,-\mathbf{k})]$ is correct) the first line of the right-hand side has to read

$$
-\frac{1}{\hbar}\delta(\tau)-\frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau,-\mathbf{k}),
$$

i.e. both signs are wrong. In the second line, the prefactor $\frac{g^*}{\hbar\sqrt{N_p}}(-1)\mathscr{D}_0\frac{g}{\hbar\sqrt{N_p}}$ multiplies $\sum_\sigma \widetilde{\text{CORR}} = \hbar^2[\dots]$ (the bracket of the first Lemma, which lacks the $\hbar^2$). Hence the bracket $[\dots]$ as written has to be multiplied by $(-1)\frac{g^*g}{N_p}\mathscr{D}_0$. Finally, in the second line of the bracket, $-\mathbf{k}'$ has to be replaced by $-\mathbf{k}$ (green prime).

Theorem 26.40 For $X = c_{n,\downarrow}(-\mathbf{k})$ this can be used to conclude (...)

Completion of the statement. Neglecting vertex-corrections and the zero-phonon-momentum (Hartree-)terms (terms 1 and 4 in the proof) one has for $(\widehat{\mathscr{G}_n})_{22}(\tau,\mathbf{k}) = -\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau,-\mathbf{k})$

$$
\begin{aligned}
\left(-\partial_\tau+\frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\right)\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau,-\mathbf{k}) &= -\frac{1}{\hbar}\delta(\tau)+\sum\!\!\!\!\!\!\int_{\substack{\tau'\in(0,\hbar\beta)\\ \mathbf{k}'\in Q\\ n'\in\{1,\dots,\infty\}\\ \nu'\in\{1,\dots,rd_{\mathbf{x}}\}}} \frac{|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{N_p}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\\
&\quad\cdot\left[\mathscr{G}_{\substack{n'\\ \text{Gorkov}}}(\tau'-\tau,-\mathbf{k}')\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau',-\mathbf{k})-\mathscr{F}^\dagger_{n'}(\tau-\tau',\mathbf{k}')\mathscr{F}_n(\tau',\mathbf{k})\right],
\end{aligned}
\tag{26.125}
$$

and in Matsubara-space this is Equation (26.28).

Proof 26.40 We obtain

$$
\begin{aligned}
&-\partial_\tau \mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau,-\mathbf{k}) \\
&= +\frac{1}{\hbar}\delta(\tau) + \frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau,-\mathbf{k}) \\
&+ \sum\!\!\!\!\!\!\int_{\substack{\mathbf{q},\mathbf{k}'\in \mathrm{Q}\\ \nu'\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ m,m',n'\in\{1,2,3,\dots\}\\ \tau'\in(0,\hbar\beta)}} \frac{g^*_{nn'\nu'}(-\mathbf{k}',\mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}}(-1)\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\frac{g_{mm'\nu'}(\mathbf{q},\mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}} \quad \Big[\delta_{n,n'}\delta_{m,m'}\delta_{\mathbf{k},\mathbf{k}'}\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau,-\mathbf{k})\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(0,\mathbf{q}) \\
&\qquad\qquad - \delta_{n',m'}\delta_{n,m}\delta_{-\mathbf{q},\mathbf{k}'}\mathscr{G}_{\substack{n'\\ \text{Gorkov}}}(\tau'-\tau,-\mathbf{k}')\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau',-\mathbf{k}) \\
&\qquad\qquad + \delta_{n,m'}\delta_{n',m}\delta_{\mathbf{q},\mathbf{k}}\mathscr{F}_n(\tau',\mathbf{k})\mathscr{F}^\dagger_{n'}(\tau-\tau',\mathbf{k}') \\
&\qquad\qquad - \delta_{m,m'}\delta_{n,n'}\delta_{\mathbf{k},\mathbf{k}'}\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(0,\mathbf{q})(-1)\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau,-\mathbf{k})\Big]
\end{aligned}
\tag{26.126}
$$

which can (equivalently) be rewritten as

$$
\Big[-\partial_\tau - \frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\Big]\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau,-\mathbf{k}) = +\frac{1}{\hbar}\delta(\tau) + 1 + 2 + 3 + 4 \tag{26.127}
$$

Correction note. Correctly (cf. the note after the Remark): $\big[-\partial_\tau + \frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\big]\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau,-\mathbf{k}) = -\frac{1}{\hbar}\delta(\tau)+1+2+3+4$, where $1,\dots,4$ carry the prefactor $(-1)g^*g/N_p$ (no $\hbar^2$ in the denominator).

Now we will simplify the individual terms as

$$
1 \overset{\text{kill } n',m',\mathbf{k}'}{=} \sum\!\!\!\!\!\!\int_{\substack{\mathbf{q}\in\mathrm{Q}\\ \tau'\in(0,\hbar\beta)\\ \nu'\in\{1,2,3,\dots,rd_{\mathbf{x}}\}\\ m\in\{1,2,3,\dots\}}} (-1)\frac{g^*_{nn\nu'}(-\mathbf{k},0)}{\hbar\sqrt{N_p}}\frac{g_{mm\nu'}(\mathbf{q},0)}{\hbar\sqrt{N_p}}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{0}}}(\tau-\tau')\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau,-\mathbf{k})\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(0,\mathbf{q}) \tag{26.128}
$$

and

$$
\begin{aligned}
2 &\overset{\text{kill } m,m',\mathbf{q}}{=} \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}'\in\mathrm{Q}\\ \tau'\in(0,\hbar\beta)\\ \nu'\in\{1,2,3,\dots,rd_{\mathbf{x}}\}\\ n'\in\{1,2,3,\dots\}}} \frac{g^*_{nn'\nu'}(-\mathbf{k}',\mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}}\frac{g_{nn'\nu'}(-\mathbf{k}',\mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\mathscr{G}_{\substack{n'\\ \text{Gorkov}}}(\tau'-\tau,-\mathbf{k}')\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau',\mathbf{k}) \\
&= \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}'\in\mathrm{Q}\\ \tau'\in(0,\hbar\beta)\\ \nu'\in\{1,2,3,\dots,rd_{\mathbf{x}}\}\\ n'\in\{1,2,3,\dots\}}} \frac{|g_{nn'\nu'}(-\mathbf{k}',\mathbf{k}'-\mathbf{k})|^2}{\hbar^2 N_p}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\mathscr{G}_{\substack{n'\\ \text{Gorkov}}}(\tau'-\tau,-\mathbf{k}')\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau',\mathbf{k})
\end{aligned}
\tag{26.129}
$$

and

$$
\begin{aligned}
3 &\overset{\text{kill } m,m',\mathbf{q}}{=} \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}'\in\mathrm{Q}\\ \tau'\in(0,\hbar\beta)\\ \nu'\in\{1,2,3,\dots,rd_{\mathbf{x}}\}\\ n'\in\{1,2,3,\dots\}}} \frac{g^*_{mn'\nu'}(-\mathbf{k}',\mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}}\frac{g_{nn'\nu'}(-\mathbf{k}',\mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\mathscr{F}_n(\tau',\mathbf{k})\mathscr{F}_{n'}(\tau-\tau',\mathbf{k}') \\
&= \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}'\in\mathrm{Q}\\ \tau'\in(0,\hbar\beta)\\ \nu'\in\{1,2,3,\dots,rd_{\mathbf{x}}\}\\ n'\in\{1,2,3,\dots\}}} \frac{|g_{nn'\nu'}(-\mathbf{k}',\mathbf{k}'-\mathbf{k})|^2}{\hbar^2 N_p}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\mathscr{F}_n(\tau',\mathbf{k})\mathscr{F}_{n'}(\tau-\tau',\mathbf{k}')
\end{aligned}
\tag{26.130}
$$

and

$$4 \overset{\text{kill } n',m',\mathbf{k}'}{=} \oint\!\!\!\!\!\!\sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ \tau'\in(0,\hbar\beta)\\ \nu'\in\{1,2,3,\dots,rd_{\mathbf{x}}\}\\ m\in\{1,2,3,\dots\}}} \frac{g^*_{nn\nu'}(-\mathbf{k},0)}{\hbar\sqrt{N_p}} \frac{g_{mm\nu'}(\mathbf{q},0)}{\hbar\sqrt{N_p}} \mathscr{D}_{\mathbf{0},\nu'}(\tau-\tau')(-1)\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(0,\mathbf{q})\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau,-\mathbf{k}) \tag{26.131}$$

Correction note and completion of the proof. With the $\hbar^2$ of the decoupling, all four terms carry $1/N_p$ instead of $1/(\hbar^2 N_p)$, and terms 1 and 4 carry the prefactor (-1) (term 1 has it, term 4 as written has it through the explicit (-1)). Furthermore:

- Term 2: the last factor is $\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau',-\mathbf{k})$. The sign + is correct: $(-1)\cdot(-1)=+1$.
- Term 3: the correct expression is

$$3 = -\oint\!\!\!\!\!\!\sum_{\mathbf{k}',\tau',\nu',n'} \frac{|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{N_p} \mathscr{D}_{\mathbf{k}-\mathbf{k}',\nu'}(\tau-\tau')\mathscr{F}_n(\tau',\mathbf{k})\mathscr{F}^\dagger_{n'}(\tau-\tau',\mathbf{k}').$$

  Three corrections: the sign ((-1) from the prefactor times + from the bracket), $\mathscr{F}^\dagger_{n'}$ instead of $\mathscr{F}_{n'}$, and the second coupling. After terminating $m=n'$, $m'=n$, $\mathbf{q}=\mathbf{k}$ one has

$$g_{n'n\nu'}(\mathbf{k},\mathbf{k}'-\mathbf{k}) = g^*_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}') \text{ (hermiticity)}, \qquad g^*_{nn'\nu'}(-\mathbf{k}',\mathbf{k}'-\mathbf{k}) = g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}') \text{ (inversion)}.$$

  The product is again $|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2$; in term 2 also $|g_{nn'\nu'}(-\mathbf{k}',\mathbf{k}'-\mathbf{k})|^2 = |g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2$.
- Terms 1 and 4 are the zero-phonon-momentum (Hartree-)terms ($\mathbf{k}'=\mathbf{k}$), which are dropped as in Theorem 26.24.

Keeping terms 2 and 3 gives Equation (26.125). *Matsubara-representation.* The left-hand side of Equation (26.125) is

$$\Big(\partial_\tau - \frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\Big)(\widehat{\mathscr{G}}_n)_{22}(\tau,\mathbf{k}) = \frac{1}{\hbar\beta}\sum_{\omega_{n_1}} \mathrm{e}^{-\mathrm{i}\omega_{n_1}\tau}\Big(-\frac{1}{\hbar}\Big)\big(\mathrm{i}\hbar\omega_{n_1}+\epsilon_n(\mathbf{k})-\mu\big)(\widehat{\mathscr{G}}_n)_{22}(\mathrm{i}\omega_{n_1},\mathbf{k}),$$

and $\mathrm{i}\hbar\omega_{n_1}+\epsilon_n(\mathbf{k})-\mu = [(\widehat{\mathscr{G}}_{0,n})_{22}(\mathrm{i}\omega_{n_1},\mathbf{k})]^{-1}$ (Lemma 26.13). Both terms on the right-hand side are of the form $\int_0^{\hbar\beta}\mathrm{d}\tau'\,\mathscr{D}_0(\tau-\tau')A(\tau-\tau')B(\tau')$ with $A\in\{(\widehat{\mathscr{G}}_{n'})_{22}(\cdot,\mathbf{k}'),\mathscr{F}^\dagger_{n'}(\cdot,\mathbf{k}')\}$ and $B\in\{(\widehat{\mathscr{G}}_n)_{22}(\cdot,\mathbf{k}),\mathscr{F}_n(\cdot,\mathbf{k})\}$, using $\mathscr{G}_{\substack{n'\\ \text{Gorkov}}}(\tau'-\tau,-\mathbf{k}')\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(-\tau',-\mathbf{k}) = (\widehat{\mathscr{G}}_{n'})_{22}(\tau-\tau',\mathbf{k}')(\widehat{\mathscr{G}}_n)_{22}(\tau',\mathbf{k})$. Exactly as in the proof of Theorem 26.25 one finds

$$\int_0^{\hbar\beta}\mathrm{d}\tau'\,\mathscr{D}_0(\tau-\tau')A(\tau-\tau')B(\tau') = \frac{1}{(\hbar\beta)^2}\sum_{\omega_{n_1},\omega_{n_2}\in\Omega_{-1}} \mathrm{e}^{-\mathrm{i}\omega_{n_1}\tau}\mathscr{D}_0(\mathrm{i}(\omega_{n_1}-\omega_{n_2}))A(\mathrm{i}\omega_{n_2})B(\mathrm{i}\omega_{n_1}).$$

Comparing coefficients of $\mathrm{e}^{-\mathrm{i}\omega_{n_1}\tau}$ and multiplying with $-\hbar(\widehat{\mathscr{G}}_{0,n})_{22}$ gives

$$(\widehat{\mathscr{G}}_n)_{22}(\mathrm{i}\omega_{n_1},\mathbf{k}) = (\widehat{\mathscr{G}}_{0,n})_{22}(\mathrm{i}\omega_{n_1},\mathbf{k})\Big[1+\sum_{\omega_{n_2},\mathbf{k}',n',\nu'}\frac{|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{\beta N_p}\mathscr{D}_{\mathbf{k}-\mathbf{k}',\nu'}(\mathrm{i}(\omega_{n_1}-\omega_{n_2}))$$
$$\cdot\big(\mathscr{F}^\dagger_{n'}(\mathrm{i}\omega_{n_2},\mathbf{k}')\mathscr{F}_n(\mathrm{i}\omega_{n_1},\mathbf{k}) - (\widehat{\mathscr{G}}_{n'})_{22}(\mathrm{i}\omega_{n_2},\mathbf{k}')(\widehat{\mathscr{G}}_n)_{22}(\mathrm{i}\omega_{n_1},\mathbf{k})\big)\Big],$$

which is Equation (26.28) because $(\widehat{\mathscr{G}}_n)_{22}(\mathrm{i}\omega,\mathbf{k}) = -\mathscr{G}_{\underset{\text{Gorkov}}{n}}(-\mathrm{i}\omega,-\mathbf{k})$ and $(\widehat{\mathscr{G}}_{0,n})_{22}(\mathrm{i}\omega,\mathbf{k}) = -\mathscr{G}_{\underset{\text{Gorkov}}{0,n}}(-\mathrm{i}\omega,-\mathbf{k})$ (Lemma 26.12).

Theorem 26.41 For $X = c^\dagger_{n,\uparrow}(\mathbf{k})$ we are able to conclude now (...)

Completion of the statement. In the same approximation as in Theorem 26.40,

$$\left(\partial_\tau - \frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\right)\mathscr{F}^\dagger_n(\tau,\mathbf{k}) = -\oint\limits_{\substack{\tau'\in(0,\hbar\beta)\\ \mathbf{k}'\in\mathrm{Q}\\ n'\in\{1,\dots,\infty\}\\ \nu'\in\{1,\dots,rd_{\mathbf{x}}\}}} \frac{|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{N_p}\mathscr{D}_{\underset{\mathbf{k}-\mathbf{k}'}{0,\nu'}}(\tau-\tau') \cdot\Big[\mathscr{G}_{\underset{\text{Gorkov}}{n'}}(\tau'-\tau,-\mathbf{k}')\mathscr{F}^\dagger_n(\tau',\mathbf{k}) + \mathscr{F}^\dagger_{n'}(\tau-\tau',\mathbf{k}')\mathscr{G}_{\underset{\text{Gorkov}}{n}}(\tau',\mathbf{k})\Big], \tag{26.132}$$

and in Matsubara-space this is Equation (26.27).

Proof 26.41 Then we find

$$\partial_\tau\mathscr{F}^\dagger_n(\tau,\mathbf{k}) = \frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\mathscr{F}^\dagger_n(\tau,\mathbf{k}) + \dots \tag{26.133}$$

with

$$\dots = \oint\limits_{\substack{\mathbf{k}',\mathbf{q}\in\mathrm{Q}\\ \nu'\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ m,m',n'\in\{1,2,3,\dots\}\\ \tau'\in(0,\hbar\beta)}} \frac{g^*_{nn'\nu'}(-\mathbf{k}',\mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}}(-1)\frac{g_{mm'\nu'}(\mathbf{q},\mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}}\mathscr{D}_{\underset{\mathbf{k}-\mathbf{k}'}{0,\nu'}}\sum_{i=1}^{4}\boxed{i} \tag{26.134}$$

This can (equivalently) be rewritten as

$$\left(\partial_\tau - \frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\right)\mathscr{F}^\dagger_n(\tau,\mathbf{k}) = \sum_{i=1}^{4} i \tag{26.135}$$

with the individual terms given as

$$\begin{aligned}\sum_{i=1}^{4} i = \oint\limits_{\substack{\mathbf{k}',\mathbf{q}\in\mathrm{Q}\\ \nu'\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ m,m',n'\in\{1,2,3,\dots\}\\ \tau'\in(0,\hbar\beta)}} &\frac{g^*_{nn'\nu'}(-\mathbf{k}',\mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}}(-1)\frac{g_{mm'\nu'}(\mathbf{q},\mathbf{k}'-\mathbf{k})}{\hbar\sqrt{N_p}}\mathscr{D}_{\underset{\mathbf{k}-\mathbf{k}'}{0,\nu'}}\cdot\Big[\delta_{n,n'}\delta_{m,m'}\delta_{\mathbf{k},\mathbf{k}'}\mathscr{F}^\dagger_n(\tau,\mathbf{k})(-1)\mathscr{G}_{\underset{\text{Gorkov}}{n}}(0,\mathbf{q})\\ &+\delta_{n',m'}\delta_{n,m}\delta_{\mathbf{k}',-\mathbf{q}}\mathscr{G}_{\underset{\text{Gorkov}}{n'}}(\tau'-\tau,-\mathbf{k}^\dagger)\mathscr{F}^\dagger_n(\tau^\dagger,\mathbf{k}^\dagger)\\ &+\delta_{n,m'}\delta_{m,n'}\delta_{\mathbf{q},\mathbf{k}}\mathscr{G}_{\underset{\text{Gorkov}}{n}}(\tau',\mathbf{k})\mathscr{F}^\dagger_{n'}(\tau^\dagger-\tau,\mathbf{k}^\dagger)\\ &+\delta_{m,m'}\delta_{n,n'}\delta_{\mathbf{k},\mathbf{k}'}\mathscr{G}_{\underset{\text{Gorkov}}{m}}(0,\mathbf{q})\mathscr{F}^\dagger_n(\tau,\mathbf{k})\Big]\end{aligned} \tag{26.136}$$

Correction note. The prefactor is $\frac{g^*}{\hbar\sqrt{N_p}}(-1)\frac{g}{\hbar\sqrt{N_p}}\mathscr{D}_0(\tau-\tau')\cdot\hbar^2 = -\frac{g^*g}{N_p}\mathscr{D}_0(\tau-\tau')$ (the $\hbar^2$ of the decoupling and the argument $\tau-\tau'$ of $\mathscr{D}_0$ are missing). The bracket has to be the bracket of the (corrected) Lemma for $X = c^\dagger_{n\uparrow}(\mathbf{k})$:

$$\Big[-\delta_{nn'}\delta_{mm'}\delta_{\mathbf{k}\mathbf{k}'}\mathscr{F}^{\dagger}_{n}(\tau,\mathbf{k})\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(0,\mathbf{q}) + \delta_{n'm'}\delta_{nm}\delta_{\mathbf{k}',-\mathbf{q}}\mathscr{G}_{\substack{n'\\ \text{Gorkov}}}(\tau'-\tau,-\mathbf{k}')\mathscr{F}^{\dagger}_{n}(\tau',\mathbf{k})$$
$$+\delta_{nm'}\delta_{mn'}\delta_{\mathbf{q}\mathbf{k}}\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(\tau',\mathbf{k})\mathscr{F}^{\dagger}_{n'}(\tau-\tau',\mathbf{k}') - \delta_{mm'}\delta_{nn'}\delta_{\mathbf{k}\mathbf{k}'}\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(0,\mathbf{q})\mathscr{F}^{\dagger}_{n}(\tau,\mathbf{k})\Big],$$

i.e. in the first line $\mathscr{G}_m$ (not $\mathscr{G}_n$), in the second and third line $\tau', \mathbf{k}', \mathbf{k}$ instead of $\tau^\dagger, \mathbf{k}^\dagger$, the third line has $\mathscr{F}^{\dagger}_{n'}(\tau-\tau',\mathbf{k}')$, and the fourth line has a minus sign.

therefore we obtain the individual contributions

$$1 \overset{\text{kill } n',m',\mathbf{k}'}{=} \sum\!\!\!\!\!\!\int_{\substack{\mathbf{q}\in Q\\ \tau'\in(0,\hbar\beta)\\ \nu'\in\{1,2,3,\ldots,rd_{\mathbf{x}}\}\\ m\in\{1,2,3,\ldots\}}} \frac{g^*_{nn\nu'}(-\mathbf{k},0)g_{mm\nu'}(\mathbf{q},0)}{\hbar^2 N_p}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{0}}}(\tau-\tau')\mathscr{F}^{\dagger}_{n}(\tau,\mathbf{k})\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(0,\mathbf{q}) \tag{26.137}$$

and

$$\begin{aligned} 2 &\overset{\text{kill } m,m',\mathbf{q}}{=} \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}'\in Q\\ \tau'\in(0,\hbar\beta)\\ \nu'\in\{1,2,3,\ldots,rd_{\mathbf{x}}\}\\ n'\in\{1,2,3,\ldots\}}} \frac{-g^*_{nn'\nu'}(-\mathbf{k}',\mathbf{k}'-\mathbf{k})g_{nn'\nu'}(-\mathbf{k}',\mathbf{k}'-\mathbf{k})}{\hbar^2 N_p}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\mathscr{G}_{\substack{n'\\ \text{Gorkov}}}(\tau'-\tau,\mathbf{k}')\mathscr{F}^{\dagger}_{n}(\tau^\dagger,\mathbf{k}^\dagger) \\ &= \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}'\in Q\\ \tau'\in(0,\hbar\beta)\\ \nu'\in\{1,2,3,\ldots,rd_{\mathbf{x}}\}\\ n'\in\{1,2,3,\ldots\}}} \frac{-|g^*_{nn'\nu'}(-\mathbf{k}',\mathbf{k}'-\mathbf{k})|^2}{\hbar^2 N_p}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\mathscr{G}_{\substack{n'\\ \text{Gorkov}}}(\tau'-\tau,\mathbf{k}')\mathscr{F}^{\dagger}_{n}(\tau^\dagger,\mathbf{k}^\dagger) \end{aligned} \tag{26.138}$$

and

$$3 \overset{\text{kill } m,m',\mathbf{q}}{=} \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}'\in Q\\ \tau'\in(0,\hbar\beta)\\ \nu'\in\{1,2,3,\ldots,rd_{\mathbf{x}}\}\\ n'\in\{1,2,3,\ldots\}}} \frac{-g^*_{nn'\nu'}(-\mathbf{k}',\mathbf{k}'-\mathbf{k})g_{n'n\nu'}(\mathbf{k},\mathbf{k}'-\mathbf{k})}{\hbar^2 N_p}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(\tau',\mathbf{k})\mathscr{F}^{\dagger}_{n'}(\tau-\tau^\dagger,\mathbf{k}^\dagger) \tag{26.139}$$

and

$$4 \overset{\text{kill } n',m',\mathbf{k}'}{=} \sum\!\!\!\!\!\!\int_{\substack{\mathbf{q}\in Q\\ \tau'\in(0,\hbar\beta)\\ \nu'\in\{1,2,3,\ldots,rd_{\mathbf{x}}\}\\ m\in\{1,2,3,\ldots\}}} \frac{g^*_{nn\nu'}(-\mathbf{k},0)g_{mm\nu'}(\mathbf{q},0)}{\hbar^2 N_p}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{0}}}(\tau-\tau')\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(0,\mathbf{q})\mathscr{F}^{\dagger}_{n}(\tau,\mathbf{k}) \tag{26.140}$$

Now we do "the usual thing" and neglect the terms in $g(\bullet,\Gamma)$ and take the Matsubara-transformation of these equations. (To-be-continued, but easy!).

Correction note and completion of the proof. With the corrected prefactor $-g^*g/N_p$ (no $\hbar^2$ in the denominator), terms 1 and 4 (zero phonon momentum, $\mathbf{k}'=\mathbf{k}$) are dropped. Terms 2 and 3 are, after using inversion symmetry resp. hermiticity for the couplings as for the $X = c_{n\downarrow}(-\mathbf{k})$ case,

$$2+3 = -\sum\!\!\!\!\!\!\int_{\mathbf{k}',\tau',\nu',n'} \frac{|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{N_p}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\Big[\mathscr{G}_{\substack{n'\\ \text{Gorkov}}}(\tau'-\tau,-\mathbf{k}')\mathscr{F}^{\dagger}_{n}(\tau',\mathbf{k}) + \mathscr{G}_{\substack{n\\ \text{Gorkov}}}(\tau',\mathbf{k})\mathscr{F}^{\dagger}_{n'}(\tau-\tau',\mathbf{k}')\Big].$$

(In term 2 above the momentum of $\mathscr{G}_{n'}$ has to be $-\mathbf{k}'$, and $\tau^\dagger, \mathbf{k}^\dagger$ mean $\tau', \mathbf{k}$ resp. $\tau', \mathbf{k}'$; term 3 is correct up to the $\hbar^2$.) This proves Equation (26.132). *Matsubara-representation.* As in the proof of Theorem 26.40, the left-hand side becomes $\frac{1}{\hbar\beta}\sum_{\omega_{n_1}} \mathrm{e}^{-\mathrm{i}\omega_{n_1}\tau}(-\frac{1}{\hbar})[(\widehat{\mathscr{G}}_{0,n})_{22}(\mathrm{i}\omega_{n_1},\mathbf{k})]^{-1}\mathscr{F}^\dagger_n(\mathrm{i}\omega_{n_1},\mathbf{k})$. On the right-hand side we write $\mathscr{G}_{\substack{n'\\ \text{Gorkov}}}(\tau'-\tau,-\mathbf{k}') = -(\widehat{\mathscr{G}}_{n'})_{22}(\tau-\tau',\mathbf{k}')$ and use the convolution formula from that proof. Comparing coefficients gives

$$\mathscr{F}^\dagger_n(\mathrm{i}\omega_{n_1},\mathbf{k}) = (\widehat{\mathscr{G}}_{0,n})_{22}(\mathrm{i}\omega_{n_1},\mathbf{k}) \sum_{\omega_{n_2},\mathbf{k}',n',\nu'} \frac{|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{\beta N_p} \mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\mathrm{i}(\omega_{n_1}-\omega_{n_2})) \cdot \left[\mathscr{F}^\dagger_{n'}(\mathrm{i}\omega_{n_2},\mathbf{k}')\mathscr{G}_{\substack{n\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_1},\mathbf{k}) - (\widehat{\mathscr{G}}_{n'})_{22}(\mathrm{i}\omega_{n_2},\mathbf{k}')\mathscr{F}^\dagger_n(\mathrm{i}\omega_{n_1},\mathbf{k})\right],$$

which is Equation (26.27) (insert $(\widehat{\mathscr{G}}_{0,n})_{22}(\mathrm{i}\omega,\mathbf{k}) = -\mathscr{G}_{\substack{0,n\\ \text{Gorkov}}}(-\mathrm{i}\omega,-\mathbf{k})$, $(\widehat{\mathscr{G}}_{n'})_{22}(\mathrm{i}\omega,\mathbf{k}') = -\mathscr{G}_{\substack{n'\\ \text{Gorkov}}}(-\mathrm{i}\omega,-\mathbf{k}')$).

Fact 26.42 The equation of motion for the anomalous Green-function in imaginary time reads

$$\partial_\tau \mathscr{F}^\dagger_n(\tau,\mathbf{k}) = \text{See above} \tag{26.141}$$

$= \dfrac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\mathscr{F}^\dagger_n(\tau,\mathbf{k}) + \big(\text{right-hand side of Equation (26.132)}\big)$, cf. Theorem 26.41.

Remark 26.42.1 *Summary of Preparations 1/4 – 4/4.* Theorem 26.24, the Corollary at the end of Preparation 2/4, and Theorems 26.40 and 26.41 are the four entries of one matrix equation. With $\sigma_3\widehat{\mathscr{G}}\sigma_3 = \left(\begin{smallmatrix} \mathscr{G} & -\mathscr{F} \\ -\mathscr{F}^\dagger & (\widehat{\mathscr{G}})_{22}\end{smallmatrix}\right)$ one checks entry by entry that

$$\Big(\sigma_0\partial_\tau + \tfrac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\sigma_3\Big)\widehat{\mathscr{G}}_{\substack{n\\ \text{Gorkov}}}(\tau,\mathbf{k}) = -\tfrac{1}{\hbar}\delta(\tau)\sigma_0 + \oint_{\substack{\tau'\in(0,\hbar\beta)\\ \mathbf{k}'\in\mathrm{Q}\\ n'\in\{1,\dots,\infty\}\\ \nu'\in\{1,\dots,rd_{\mathrm{x}}\}}} \frac{|g_{nn'\nu'}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{N_p}\mathscr{D}_{\substack{0,\nu'\\ \mathbf{k}-\mathbf{k}'}}(\tau-\tau')\,\sigma_3\widehat{\mathscr{G}}_{\substack{n'\\ \text{Gorkov}}}(\tau-\tau',\mathbf{k}')\sigma_3\,\widehat{\mathscr{G}}_{\substack{n\\ \text{Gorkov}}}(\tau',\mathbf{k}). \tag{26.142}$$

(E.g. the 1, 1-entry is $\mathscr{G}_{n'}\mathscr{G}_n - \mathscr{F}_{n'}\mathscr{F}^\dagger_n$, the 2, 1-entry is $-\mathscr{F}^\dagger_{n'}\mathscr{G}_n + (\widehat{\mathscr{G}}_{n'})_{22}\mathscr{F}^\dagger_n$.) In Matsubara-space, with $(\sigma_0\partial_\tau + \frac{\epsilon_n(\mathbf{k})-\mu}{\hbar}\sigma_3) \to -\frac{1}{\hbar}\widehat{\mathscr{G}}^{-1}_{0,n}(\mathrm{i}\omega_{n_1},\mathbf{k})$ (Lemma 26.13) and the convolution formula from the proof of Theorem 26.40, this becomes

$$\widehat{\mathscr{G}}_{\substack{n\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_1},\mathbf{k}) = \widehat{\mathscr{G}}_{\substack{0,n\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_1},\mathbf{k}) + \widehat{\mathscr{G}}_{\substack{0,n\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_1},\mathbf{k})\widehat{\Sigma}_{\substack{n\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_1},\mathbf{k})\widehat{\mathscr{G}}_{\substack{n\\ \text{Gorkov}}}(\mathrm{i}\omega_{n_1},\mathbf{k})$$

with $\widehat{\Sigma}$ from Equation (26.33). This is the compact form of Equations (26.25) – (26.28) and of the Corollary on the self-energy components.

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Everything from here onwards has to be double-checked. Especially Thm 3.13

26.1.6. Derivation of the Eliashberg-Equations

Notation 26.43 For the self-energy we introduce abbreviations as

$$\Sigma_m(\mathrm{i}\omega_n,\mathbf{k}) = \mathrm{i}\hbar\omega_n\Big[1 - Z_m(\mathrm{i}\omega_n,\mathbf{k})\Big]\sigma_0 + \phi_m(\mathrm{i}\omega_n,\mathbf{k})\sigma_1 + \chi_m(\mathrm{i}\omega_n,\mathbf{k})\sigma_3 \overset{\star\star\star}{=} \begin{pmatrix} \Sigma_m(\mathrm{i}\omega_n,\mathbf{k}) & \Xi_m(\mathrm{i}\omega_n,\mathbf{k}) \\ \Xi_m^*(\mathrm{i}\omega_n,\mathbf{k}) & -\Sigma_m(-\mathrm{i}\omega_n,-\mathbf{k}) \end{pmatrix} \tag{26.143}$$

whereas $\star\star\star$ only holds in the case that ϕ is real. (Is this the case???)

Answer / note. (i) Notation clash: in $\star\star\star$, Σ_m on the right denotes the 1, 1-entry Σ_{11}, while Σ_m on the left is the whole matrix $\hat{\Sigma}_m$. (ii) From Equations (26.33), the inversion symmetry $|g_{nn'\nu}(-\mathbf{k}',\mathbf{k}'-\mathbf{k})| = |g_{nn'\nu}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|$ and $\mathscr{D}_0(\mathrm{i}\omega) = \mathscr{D}_0(-\mathrm{i}\omega) \in \mathbb{R}$ one finds exactly $\Sigma_{22}(\mathrm{i}\omega_n,\mathbf{k}) = -\Sigma_{11}(-\mathrm{i}\omega_n,-\mathbf{k})$. Therefore $\chi = \frac{1}{2}[\Sigma_{11}(\mathrm{i}\omega_n,\mathbf{k}) + \Sigma_{11}(-\mathrm{i}\omega_n,-\mathbf{k})]$ and $\mathrm{i}\hbar\omega_n(1-Z) = \frac{1}{2}[\Sigma_{11}(\mathrm{i}\omega_n,\mathbf{k}) - \Sigma_{11}(-\mathrm{i}\omega_n,-\mathbf{k})]$ are well defined, with $Z(\mathrm{i}\omega_n,\mathbf{k}) = Z(-\mathrm{i}\omega_n,-\mathbf{k})$, $\chi(\mathrm{i}\omega_n,\mathbf{k}) = \chi(-\mathrm{i}\omega_n,-\mathbf{k})$. (iii) The off-diagonal part is in general $\phi_1\sigma_1 + \phi_2\sigma_2$, i.e. $\Sigma_{12} = \phi_1 - \mathrm{i}\phi_2$, $\Sigma_{21} = \phi_1 + \mathrm{i}\phi_2$. With $\mathscr{F}^\dagger(\mathrm{i}\omega_n,\mathbf{k}) = [\mathscr{F}(-\mathrm{i}\omega_n,\mathbf{k})]^*$ (Remark after Lemma 26.12) and Equations (26.31) and Σ_{12} one gets $\Sigma_{21}(\mathrm{i}\omega_n,\mathbf{k}) = [\Sigma_{12}(-\mathrm{i}\omega_n,\mathbf{k})]^*$. Hence $\phi_2 = 0$ (the σ_1-ansatz) is equivalent to $\phi(\mathrm{i}\omega_n,\mathbf{k}) = [\phi(-\mathrm{i}\omega_n,\mathbf{k})]^*$. For an even-frequency gap, $\phi(\mathrm{i}\omega_n,\mathbf{k}) = \phi(-\mathrm{i}\omega_n,\mathbf{k})$, this means $\phi \in \mathbb{R}$. In the operator formalism this cannot be proven; it is an *assumption* (choice of the global U(1)-phase plus time-reversal symmetry), consistent with the Gorkov-ansatz: if ϕ is real, the inverse in Corollary 26.44 gives $\mathscr{F} = \mathscr{F}^\dagger = -\phi/\theta$, and the self-consistency closes. Under this assumption $\Xi_m = \Xi_m^* = \phi_m$ in $\star\star\star$.

Corollary 26.44 Combining the Dyson-equation (26.21) with Eq. (26.143) for the self-energy yields for the full Green-function

$$\mathscr{G}_{\underset{\text{Gorkov}}{m}}(\mathrm{i}\omega_n,\mathbf{k}) = \frac{-1}{\theta_m(\mathrm{i}\omega_n,\mathbf{k})}\Big[\hbar\mathrm{i}\omega_n Z_m(\mathrm{i}\omega_n,\mathbf{k})\sigma_0 + \phi_m(\mathrm{i}\omega_n,\mathbf{k})\sigma_1 + \big(\chi_m(\mathrm{i}\omega_n,\mathbf{k}) + (\epsilon_m(\mathbf{k}) - \mu)\big)\,\sigma_3\Big] \tag{26.144}$$

with

$$\theta_m(\mathrm{i}\omega_n,\mathbf{k}) = \hbar^2\omega_n^2 Z_m(\mathbf{k},\mathrm{i}\omega_n)^2 + \Big[\chi_m(\mathbf{k},\mathrm{i}\omega_n) + (\epsilon_m(\mathbf{k}) - \mu)\Big]^2 + \phi_m(\mathrm{i}\omega_n,\mathbf{k})^2 \tag{26.145}$$

Note. Correct (checked). On the left-hand side the whole Gorkov-matrix $\hat{\mathscr{G}}_{\underset{\text{Gorkov}}{m}}(\mathrm{i}\omega_n,\mathbf{k})$ is meant (with a hat), and $Z_m(\mathbf{k},\mathrm{i}\omega_n) \equiv Z_m(\mathrm{i}\omega_n,\mathbf{k})$ etc. In components: $\mathscr{G}_{\underset{\text{Gorkov}}{m}} = -(\mathrm{i}\hbar\omega_n Z_m + \epsilon_m(\mathbf{k}) - \mu + \chi_m)/\theta_m$, $\mathscr{F}_m = \mathscr{F}_m^\dagger = -\phi_m/\theta_m$, $(\hat{\mathscr{G}}_m)_{22} = -(\mathrm{i}\hbar\omega_n Z_m - \epsilon_m(\mathbf{k}) + \mu - \chi_m)/\theta_m$.

Proof 26.44

We use the decompositions in Equation (26.143) for self-energy and Equation (26.19) for the non-interacting Gorkov-Green-Function and insert them into the Dyson-equation (26.21) to obtain

$$\widehat{\mathscr{G}}^{-1}_{\substack{m\\ \text{Gorkov}}}(\mathrm{i}\omega_n,\mathbf{k}) = \hbar\mathrm{i}\omega_n Z_m(\mathrm{i}\omega_n,\mathbf{k})\sigma_0 - \phi_m(\mathrm{i}\omega_n,\mathbf{k})\sigma_1 - \left(\chi_m(\mathrm{i}\omega_n,\mathbf{k}) + (\epsilon_m(\mathbf{k})-\mu)\right)\sigma_3 \tag{26.146}$$

which can be inverted with the inversion-formula for 2x2-matrices[13] to

$$\widehat{\mathscr{G}}_{\substack{m\\ \text{Gorkov}}}(\mathrm{i}\omega_n,\mathbf{k}) = \frac{\hbar\mathrm{i}\omega_n Z_m(\mathrm{i}\omega_n,\mathbf{k})\sigma_0 + \phi_m(\mathrm{i}\omega_n,\mathbf{k})\sigma_1 + \left(\chi_m(\mathrm{i}\omega_n,\mathbf{k}) + (\epsilon_m(\mathbf{k})-\mu)\right)\sigma_3}{\operatorname{Det}\widehat{\mathscr{G}}^{-1}_{\substack{m\\ \text{Gorkov}}}(\mathrm{i}\omega_n,\mathbf{k})} \tag{26.147}$$

Noticing

$$\begin{aligned}\operatorname{Det}\widehat{\mathscr{G}}^{-1}_{\substack{m\\ \text{Gorkov}}}(\mathrm{i}\omega_n,\mathbf{k}) &= -\hbar^2\omega_n^2 Z_m(\mathbf{k},\mathrm{i}\omega_n)^2 - \left(\chi_m(\mathbf{k},\mathrm{i}\omega_n) + (\epsilon_m(\mathbf{k})-\mu)\right)^2 - \left(\phi_m(\mathbf{k},\mathrm{i}\omega_n)\right)^2\\ &= -\left(\hbar^2\omega_n^2 Z_m(\mathbf{k},\mathrm{i}\omega_n)^2 + \left(\chi_m(\mathbf{k},\mathrm{i}\omega_n) + (\epsilon_m(\mathbf{k})-\mu)\right)^2 + \phi_m(\mathbf{k},\mathrm{i}\omega_n)^2\right)\\ &\equiv -\theta_m(\mathrm{i}\omega_n,\mathbf{k})\end{aligned}$$

Inserting this above yields the desired result

$$\widehat{\mathscr{G}}_{\substack{m\\ \text{Gorkov}}}(\mathrm{i}\omega_n,\mathbf{k}) = -\frac{\hbar\mathrm{i}\omega_n Z_m(\mathrm{i}\omega_n,\mathbf{k})\sigma_0 + \phi_m(\mathrm{i}\omega_n,\mathbf{k})\sigma_1 + \left(\chi_m(\mathrm{i}\omega_n,\mathbf{k}) + (\epsilon_m(\mathbf{k})-\mu)\right)\sigma_3}{\theta_m(\mathrm{i}\omega_n,\mathbf{k})} \tag{26.148}$$

Theorem 26.45 The self-energies for electron-phonon- and electron-electron-interactions are in first (non-vanishing) order perturbation theory given by

$$\Sigma_{\substack{n\\ \text{Gorkov}}}(\mathrm{i}\omega_n,\mathbf{k}) = \Sigma^{\text{ep}}_n(\mathrm{i}\omega_n,\mathbf{k}) + \Sigma^{\text{c}}_n(\mathrm{i}\omega_n,\mathbf{k}) \tag{26.149}$$

with *electron-phonon* and *Coulomb self energies*

$$\Sigma^{\text{ep}}_n(\mathrm{i}\omega_n,\mathbf{k}) = -T\sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ \omega_{n'}\in\Omega_{-1}\\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}\\ m\in\{1,\dots,\infty\}}} \sigma_3\mathscr{G}_{\substack{m\\ \text{Gorkov}}}(\mathrm{i}\omega_{n'},\mathbf{q}+\mathbf{k})\sigma_3|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2\mathscr{D}_\nu(\mathrm{i}\omega_n-\mathrm{i}\omega_{n'},\mathbf{q}) \tag{26.150}$$

$$\Sigma^{\text{c}}_n(\mathrm{i}\omega_n,\mathbf{k}) = -T\sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ \omega_{n'}\in\Omega_{-1}\\ m\in\{1,\dots,\infty\}}} \sigma_3\mathscr{G}^{\text{od}}_{\substack{m\\ \text{Gorkov}}}(\mathrm{i}\omega_{n'},\mathbf{q})\sigma_3 V_{n,m}(\mathbf{k},\mathbf{k}+\mathbf{q},\mathrm{i}\omega_n-\mathrm{i}\omega_{n'}) \tag{26.151}$$

Correction note. (i) What was derived in Section 26.1.5 is Equation (26.33). Substituting $\mathbf{k}'=\mathbf{k}+\mathbf{q}$ (a bijection of Q), using $|g_{nm\nu}(\mathbf{k}+\mathbf{q},-\mathbf{q})|^2 = |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2$ (Lemma 8.37) and $\mathscr{D}_{\substack{0,\nu\\ -\mathbf{q}}} = \mathscr{D}_{\substack{0,\nu\\ \mathbf{q}}}$, it reads

$$\widehat{\Sigma}^{\text{ep}}_n(\mathrm{i}\omega_n,\mathbf{k}) = -\frac{1}{\beta N_p}\sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ \omega_{n'}\in\Omega_{-1}\\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}\\ m\in\{1,\dots,\infty\}}} \sigma_3\widehat{\mathscr{G}}_{\substack{m\\ \text{Gorkov}}}(\mathrm{i}\omega_{n'},\mathbf{k}+\mathbf{q})\sigma_3|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2\mathscr{D}_{0,\nu}(\mathrm{i}\omega_n-\mathrm{i}\omega_{n'},\mathbf{q}). \tag{26.152}$$

[13] Cf. Waste-Folder 1 Topic 22: For $A = a_0\sigma_0 + \mathbf{a}\cdot\boldsymbol{\sigma}$

Compared with the Theorem: the factor $1/N_p$ is missing there; T has to be read as $k_B T = 1/\beta$; $\mathscr{D}_\nu$ is the *bare* propagator $\mathscr{D}_{0,\nu}$ (no phonon self-energy has been included); $\mathscr{G}$ is the Gorkov-matrix $\widehat{\mathscr{G}}$. (ii) The result is not first-order perturbation theory. It is the self-consistent Migdal-approximation: vertex-corrections and zero-phonon-momentum terms are neglected, with the full $\widehat{\mathscr{G}}$ inside. (iii) The Hamiltonian (26.1) contains no electron-electron interaction. Hence $\Sigma_c \equiv 0$ in this chapter, and the Coulomb part is *not* proven here. It has to be added by hand (e.g. as a μ^*-term) or derived from a Hamiltonian with Coulomb interaction.

Proof 26.45 These equations will be proven in section 26.1.5.

Lemma 26.46 Writing out these equations gives for the electron-phonon self-energy

$$\Sigma_{\mathrm{ep}\,m}(\mathrm{i}\omega_n, \mathbf{k}) = -T \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ \omega_{n'}\in\Omega_{-1} \\ \nu\in\{1,\dots,rd_{\mathbf{x}}\} \\ n\in\{1,\dots,\infty\}}} \begin{pmatrix} \mathscr{G}_{\mathrm{Gorkov}\;n}(\bullet) & -\mathscr{F}_n(\bullet) \\ -\mathscr{F}_n^*(\bullet) & -\mathscr{G}_{\mathrm{Gorkov}\;n}(-\bullet) \end{pmatrix}_{\bullet=(\mathrm{i}\omega_{n'},\mathbf{q}+\mathbf{k})} |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 \mathscr{D}_\nu(\mathrm{i}\omega_n - \mathrm{i}\omega_{n'}, \mathbf{q}) \tag{26.153}$$

Correction note. The lower left entry is $-\mathscr{F}_n^\dagger(\bullet)$, not $-\mathscr{F}_n^*(\bullet)$ (in the Matsubara-representation $\mathscr{F}^\dagger(\mathrm{i}\omega,\mathbf{k}) = [\mathscr{F}(-\mathrm{i}\omega,\mathbf{k})]^* \neq [\mathscr{F}(\mathrm{i}\omega,\mathbf{k})]^*$). Here the roles of m and n are exchanged w.r.t. the Theorem, and with the corrections of the Theorem the prefactor is $-1/(\beta N_p)$ and $\mathscr{D}_\nu \equiv \mathscr{D}_{0,\nu}$. The proof of this Lemma was referenced as the proof of the previous Corollary (bew: Beweis_3_2); the correct proof is the one below.

Proof 26.46 We need to compute

$$\sigma_3 \widehat{\mathscr{G}}_{\mathrm{Gorkov}\;m}(\mathrm{i}\omega_{n'}, \mathbf{q}+\mathbf{k})\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \mathscr{G}_{\mathrm{Gorkov}\;m}(\bullet) & \mathscr{F}_m(\bullet) \\ \mathscr{F}_m^*(\bullet) & -\mathscr{G}_{\mathrm{Gorkov}\;m}(-\bullet) \end{pmatrix}_{\bullet=(\mathrm{i}\omega_{n'},\mathbf{q}+\mathbf{k})} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{26.154}$$

$$= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \mathscr{G}_{\mathrm{Gorkov}\;m}(\bullet) & -\mathscr{F}_m(\bullet) \\ \mathscr{F}_m^*(\bullet) & \mathscr{G}_{\mathrm{Gorkov}\;m}(-\bullet) \end{pmatrix}_{\bullet=(\mathrm{i}\omega_{n'},\mathbf{q}+\mathbf{k})} \tag{26.155}$$

$$= \begin{pmatrix} \mathscr{G}_{\mathrm{Gorkov}\;m}(\bullet) & -\mathscr{F}_m(\bullet) \\ -\mathscr{F}_m^*(\bullet) & -\mathscr{G}_{\mathrm{Gorkov}\;m}(-\bullet) \end{pmatrix}_{\bullet=(\mathrm{i}\omega_{n'},\mathbf{q}+\mathbf{k})} \tag{26.156}$$

Note. The matrix algebra is correct; again $\mathscr{F}_m^*$ has to be read as $\mathscr{F}_m^\dagger$. In general $\sigma_3 \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right) \sigma_3 = \left(\begin{smallmatrix} a & -b \\ -c & d \end{smallmatrix}\right)$.

Definition 26.47 We introduce the *density of states per spin at the Fermi-level* as

$$N_{\mathrm{F}} = \boxed{\text{TBD.}} \tag{26.157}$$

Completion. The standard choice, per spin, per unit cell and per energy, is

$$N_{\mathrm{F}} = \frac{1}{N_p} \sum_{\substack{\mathbf{k}\in\mathrm{Q} \\ m\in\{1,\dots,\infty\}}} \delta\big(\epsilon_m(\mathbf{k}) - \mu\big), \tag{26.158}$$

so that N_F has the unit 1/Energy. The Eliashberg-equations below depend only on λ/N_F. Therefore the choice of N_F only matters for the interpretation of λ.

Definition 26.48 We introduce[14] the *anisotropic electron-phonon coupling strength*

$$\begin{aligned}\lambda^{n,m}_{\mathbf{k},\mathbf{k}+\mathbf{q}}(\omega_n) &= \frac{N_F}{\hbar}\oint_{\substack{\omega\in(0,\infty)\\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} \frac{2\omega}{\omega_n^2+\omega^2}|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2\delta\left(\omega-\omega_\nu(\mathbf{q})\right)\\ &= \frac{N_F}{\hbar}\sum_{\nu\in\{1,\dots,rd_{\mathbf{x}}\}} \frac{2\omega_\nu(\mathbf{q})}{\omega_n^2+\omega_\nu^2(\mathbf{q})}|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2\\ &= -N_F\sum_{\nu\in\{1,\dots,rd_{\mathbf{x}}\}} \mathscr{D}_{0,\nu}(i\omega_n,\mathbf{q})|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2\end{aligned} \tag{26.159}$$

Remark 26.48.1 Notice that the electron-phonon coupling strength has the unit of an energy.

Correction note. λ is dimensionless: $[N_F] = 1/\text{Energy}$, $[1/\hbar] = 1/(\text{Energy}\times\text{Time})$, $[2\omega/(\omega_n^2+\omega^2)] = \text{Time}$, $[|g|^2] = \text{Energy}^2$. The last equation sign of the Definition is correct: $\mathscr{D}_{0,\nu}(i\omega_n,\mathbf{q}) = -\frac{1}{\hbar}\frac{2\omega_\nu(\mathbf{q})}{\omega_n^2+\omega_\nu^2(\mathbf{q})}$ (Theorem 13.10); here ω_n is a bosonic Matsubara-frequency.

Corollary 26.49 This definition allows us to rewrite the electron-phonon self-energy as

$$\Sigma^{\text{ep}}_n(i\omega_n,\mathbf{k}) = \frac{T}{\hbar N_F}\sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ \omega_{n'}\in\Omega_{-1}\\ m\in\{1,\dots,\infty\}}} \sigma_3\mathscr{G}^{\,m}_{\text{Gorkov}}(i\omega_{n'},\mathbf{q}+\mathbf{k})\sigma_3\lambda^{n,m}_{\mathbf{k},\mathbf{k}+\mathbf{q}}(\omega_n-\omega_{n'}) \tag{26.160}$$

This expression has the incorrect unit.

Correction note. The factor $1/\hbar$ is wrong and the factor $1/N_p$ is missing; the correct expression is

$$\hat{\Sigma}^{\text{ep}}_n(i\omega_n,\mathbf{k}) = \frac{1}{\beta N_p N_F}\sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ \omega_{n'}\in\Omega_{-1}\\ m\in\{1,\dots,\infty\}}} \sigma_3\hat{\mathscr{G}}^{\,m}_{\text{Gorkov}}(i\omega_{n'},\mathbf{k}+\mathbf{q})\sigma_3\lambda^{n,m}_{\mathbf{k},\mathbf{k}+\mathbf{q}}(\omega_n-\omega_{n'}). \tag{26.161}$$

Unit check: $[1/\beta] = [1/N_F] = \text{Energy}$, $[\hat{\mathscr{G}}(i\omega)] = 1/\text{Energy}$, λ dimensionless, hence $[\hat{\Sigma}] = \text{Energy}$, as it must be ($\hat{\Sigma} = \hat{\mathscr{G}}_0^{-1} - \hat{\mathscr{G}}^{-1}$).

Proof 26.49 Follows from TBD.

Equation (26.152) and the last line of the Definition of λ, which gives $\sum_\nu |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2\mathscr{D}_{0,\nu}(i(\omega_n-\omega_{n'}),\mathbf{q}) = -\lambda^{n,m}_{\mathbf{k},\mathbf{k}+\mathbf{q}}(\omega_n-\omega_{n'})/N_F$. The two minus signs cancel.

Theorem 26.50 Assuming all expressions are exact, lets us conclude *the Eliashberg-equations*

[14] Cf. [06 Superhydrides] in "Success of Eliashberg".

$$Z_n(\mathrm{i}\omega_n,\mathbf{k}) = 1 + \frac{T}{\omega_n} \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ \omega_{n'}\in\Omega_{-1} \\ m\in\{1,\ldots,\infty\}}} \frac{Z_m(\mathrm{i}\omega_{n'},\mathbf{k}+\mathbf{q})}{\theta_m(\mathrm{i}\omega_{n'},\mathbf{k}+\mathbf{q})} \frac{\lambda_{n,m}(\mathrm{i}\omega_n - \mathrm{i}\omega_{n'};\mathbf{k},\mathbf{k}+\mathbf{q})}{N_\mathrm{F}} \tag{26.162}$$

$$\chi_n(\mathrm{i}\omega_n,\mathbf{k}) = -T \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ \omega_{n'}\in\Omega_{-1} \\ m\in\{1,\ldots,\infty\}}} \frac{\epsilon_m(\mathbf{k}+\mathbf{q}) - \mu + \chi_m(\mathrm{i}\omega_{n'},\mathbf{k}+\mathbf{q})}{\theta_m(\mathrm{i}\omega_{n'},\mathbf{k}+\mathbf{q})} \frac{\lambda_{n,m}(\mathrm{i}\omega_n - \mathrm{i}\omega_{n'};\mathbf{k},\mathbf{k}+\mathbf{q})}{N_\mathrm{F}} \tag{26.163}$$

$$\phi_n(\mathrm{i}\omega_n,\mathbf{k}) = T \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ \omega_{n'}\in\Omega_{-1} \\ m\in\{1,\ldots,\infty\}}} \frac{\phi_m(\mathrm{i}\omega_{n'},\mathbf{k}+\mathbf{q})}{\theta_m(\mathrm{i}\omega_{n'},\mathbf{k}+\mathbf{q})} \left[\frac{\lambda_{n,m}(\mathrm{i}\omega_n - \mathrm{i}\omega_{n'};\mathbf{k},\mathbf{k}+\mathbf{q})}{N_\mathrm{F}} + V_{n,m}(\mathrm{i}\omega_n - \mathrm{i}\omega_{n'};\mathbf{k},\mathbf{k}+\mathbf{q})\right] \tag{26.164}$$

Correction note. (i) In the equation for Z_n the factor $\omega_{n'}$ is missing in the numerator (without it the right-hand side has the unit of a time). (ii) In all three equations T has to be read as $k_\mathrm{B}T = 1/\beta$, and the factor $1/N_p$ of the $\mathbf{q}$-sum is missing. (iii) With the Hamiltonian (26.1) the Coulomb term $V_{n,m}$ is absent (cf. the note after Theorem 26.45). It is the term one adds by hand. (iv) The λ in the Theorem is $\lambda^{\,n,m}_{\mathbf{k},\mathbf{k}+\mathbf{q}}(\omega_n - \omega_{n'})$ from the Definition. The corrected Eliashberg-equations for the self-consistent Migdal-approximation of the Hamiltonian (26.1) read, with θ_m from Corollary 26.44 and all functions with index m evaluated at $(\mathrm{i}\omega_{n'},\mathbf{k}+\mathbf{q})$,

$$Z_n(\mathrm{i}\omega_n,\mathbf{k}) = 1 + \frac{1}{\omega_n \beta N_p N_\mathrm{F}} \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ \omega_{n'}\in\Omega_{-1} \\ m\in\{1,\ldots,\infty\}}} \lambda^{\,n,m}_{\mathbf{k},\mathbf{k}+\mathbf{q}}(\omega_n - \omega_{n'}) \frac{\omega_{n'} Z_m}{\theta_m} \tag{26.165}$$

$$\chi_n(\mathrm{i}\omega_n,\mathbf{k}) = -\frac{1}{\beta N_p N_\mathrm{F}} \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ \omega_{n'}\in\Omega_{-1} \\ m\in\{1,\ldots,\infty\}}} \lambda^{\,n,m}_{\mathbf{k},\mathbf{k}+\mathbf{q}}(\omega_n - \omega_{n'}) \frac{\epsilon_m(\mathbf{k}+\mathbf{q}) - \mu + \chi_m}{\theta_m} \tag{26.166}$$

$$\phi_n(\mathrm{i}\omega_n,\mathbf{k}) = \frac{1}{\beta N_p N_\mathrm{F}} \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ \omega_{n'}\in\Omega_{-1} \\ m\in\{1,\ldots,\infty\}}} \lambda^{\,n,m}_{\mathbf{k},\mathbf{k}+\mathbf{q}}(\omega_n - \omega_{n'}) \frac{\phi_m}{\theta_m}, \tag{26.167}$$

under the assumption that ϕ is real (cf. the note after the Notation). Together with Equation (26.158) for N_F and the number equation below, these form a closed system for Z, χ, ϕ, μ.

Proof 26.50

Inserting Equation (26.144) for the Green-function into Equation (26.150) for the self-energy, and comparing coefficients with Equation (26.143) for the self-energy, we obtain the Eliashberg-equations

$$\begin{aligned}\hat{\Sigma}^{\text{ep}}_{n,m}(\mathrm{i}\omega_n,\mathbf{k}) &= T\sum_{\substack{\mathbf{k}'\in Q\\ \omega_{n'}\in\Omega_{-1}}} \hbar\mathrm{i}\omega_{n'}\frac{Z_m(\mathrm{i}\omega_{n'},\mathbf{k}')}{\theta_m(\mathrm{i}\omega_{n'},\mathbf{k}')}\sigma_3\sigma_0\sigma_3\sum_\nu |g_{mn\nu}(\mathbf{k},\mathbf{k}')|^2\mathscr{D}_\nu(\mathrm{i}\omega_n-\mathrm{i}\omega_{n'},\mathbf{k}-\mathbf{k}')\\ &\quad - T\sum_{\substack{\mathbf{k}'\in Q\\ \omega_{n'}\in\Omega_{-1}}} \frac{\phi_m(\mathrm{i}\omega_{n'},\mathbf{k}')}{\theta_m(\mathrm{i}\omega_{n'},\mathbf{k}')}\sigma_1\sum_\nu |g_{mn\nu}(\mathbf{k},\mathbf{k}')|^2\mathscr{D}_\nu(\mathrm{i}\omega_n-\mathrm{i}\omega_{n'},\mathbf{k}-\mathbf{k}')\\ &\quad + T\sum_{\substack{\mathbf{k}'\in Q\\ \omega_{n'}\in\Omega_{-1}}} \frac{\chi_m(\mathrm{i}\omega_{n'},\mathbf{k}')+(\epsilon_m(\mathbf{k})-\mu)}{\theta_m(\mathrm{i}\omega_{n'},\mathbf{k}')}\sigma_3\sum_\nu |g_{mn\nu}(\mathbf{k},\mathbf{k}')|^2\mathscr{D}_\nu(\mathrm{i}\omega_n-\mathrm{i}\omega_{n'},\mathbf{k}-\mathbf{k}')\\ &\overset{!!!}{=} \mathrm{i}\omega_n\left(1-Z_m(\mathrm{i}\omega_n,\mathbf{k})\right)\sigma_0+\phi_m(\mathrm{i}\omega_n,\mathbf{k})\sigma_1+\chi_m(\mathrm{i}\omega_n,\mathbf{k})\sigma_3\end{aligned}$$

In this equation, all of the momentum-indices are messed up!

Notice further, that we used the following identities for the Pauli-matrices ToBeWrittenDown.

Note on the calculation above. The signs $+,-,+$ of the three lines are correct, when written with $|g|^2\mathscr{D}_\nu$. But $|g_{mn\nu}(\mathbf{k},\mathbf{k}')|^2$ has to be $|g_{mn\nu}(\mathbf{k},\mathbf{k}'-\mathbf{k})|^2$, $\epsilon_m(\mathbf{k})$ has to be $\epsilon_m(\mathbf{k}')$, a factor $1/N_p$ and the sum over m are missing, and on the right-hand side $\mathrm{i}\hbar\omega_n$ instead of $\mathrm{i}\omega_n$. A clean version of the proof reads as follows.

Step 1 (Pauli-matrices). From $\sigma_3^2=\sigma_0$ and $\sigma_1\sigma_3=-\sigma_3\sigma_1$ we get

$$\sigma_3\sigma_0\sigma_3=\sigma_0,\qquad \sigma_3\sigma_1\sigma_3=-\sigma_1,\qquad \sigma_3\sigma_3\sigma_3=\sigma_3.$$

Step 2. With Corollary 26.44, abbreviating $Z'_m\equiv Z_m(\mathrm{i}\omega_{n'},\mathbf{k}+\mathbf{q})$ etc. and $\xi'_m\equiv\epsilon_m(\mathbf{k}+\mathbf{q})-\mu$,

$$\sigma_3\hat{\mathscr{G}}^{\,m}_{\text{Gorkov}}(\mathrm{i}\omega_{n'},\mathbf{k}+\mathbf{q})\sigma_3=-\frac{1}{\theta'_m}\left[\mathrm{i}\hbar\omega_{n'}Z'_m\sigma_0-\phi'_m\sigma_1+(\xi'_m+\chi'_m)\sigma_3\right].$$

Step 3. Inserting this into Equation (26.161) gives, with $\lambda\equiv\lambda^{\,n,m}_{\mathbf{k},\mathbf{k}+\mathbf{q}}(\omega_n-\omega_{n'})$,

$$\hat{\Sigma}_n(\mathrm{i}\omega_n,\mathbf{k})=-\frac{1}{\beta N_p N_{\mathrm{F}}}\sum_{\mathbf{q},\omega_{n'},m}\frac{\lambda}{\theta'_m}\left[\mathrm{i}\hbar\omega_{n'}Z'_m\sigma_0-\phi'_m\sigma_1+(\xi'_m+\chi'_m)\sigma_3\right].$$

Step 4. The left-hand side is $\mathrm{i}\hbar\omega_n(1-Z_n)\sigma_0+\phi_n\sigma_1+\chi_n\sigma_3$ (Notation, Equation (26.143)). Since $\sigma_0,\sigma_1,\sigma_3$ are linearly independent, the coefficients agree:

$$\begin{aligned}\mathrm{i}\hbar\omega_n(1-Z_n) &= -\frac{1}{\beta N_p N_{\mathrm{F}}}\sum\lambda\frac{\mathrm{i}\hbar\omega_{n'}Z'_m}{\theta'_m},\\ \phi_n &= +\frac{1}{\beta N_p N_{\mathrm{F}}}\sum\lambda\frac{\phi'_m}{\theta'_m},\\ \chi_n &= -\frac{1}{\beta N_p N_{\mathrm{F}}}\sum\lambda\frac{\xi'_m+\chi'_m}{\theta'_m}.\end{aligned}$$

Dividing the first equation by $-\mathrm{i}\hbar\omega_n$ ($\omega_n\neq 0$ for fermionic Matsubara-frequencies) gives Equations (26.165) – (26.167). The right-hand side contains no σ_2-component, so the real-ϕ ansatz is self-consistent. ■

Lemma 26.51 Fixing the number of particles n by demanding charge-neutrality yields the additional equation

$$n = 1 - 2T \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ \omega_{n'}\in\Omega_{-1} \\ m\in\{1,\dots,\infty\}}} \frac{\epsilon_m(\mathbf{k}+\mathbf{q}) - \mu + \chi_m(\mathrm{i}\omega_{n'}\mathbf{k}+\mathbf{q})}{\theta_m(\mathrm{i}\omega_{n'},\mathbf{k}+\mathbf{q})} \tag{26.168}$$

Correction note. As written, the right-hand side still depends on the free variable $\mathbf{k}$, the "1" is not summed over bands and wavevectors, the normalization $1/N_p$ is missing, and T means $1/\beta$. The correct statement for the number n of electrons per unit cell (both spins, in the bands m taken into account) is

$$n = \frac{1}{N_p} \sum_{\substack{\mathbf{k}\in \mathrm{Q} \\ m\in\{1,\dots,\infty\}}} \Big[1 - \frac{2}{\beta} \sum_{\omega_{n'}\in\Omega_{-1}} \frac{\epsilon_m(\mathbf{k}) - \mu + \chi_m(\mathrm{i}\omega_{n'},\mathbf{k})}{\theta_m(\mathrm{i}\omega_{n'},\mathbf{k})}\Big]. \tag{26.169}$$

(Shifting $\mathbf{k}\mapsto\mathbf{k}+\mathbf{q}$ under the sum shows that this is the formula of the Lemma with $\sum_{\mathbf{q}}$, once the "1" is put inside the sum and $1/N_p$ is added.)

Proof 26.51 Cf. 06 Superhydrides Success of Eliashberg. ToBeDone. -

Proof of Equation (26.169). We assume, as in the Notation, that Z_m, χ_m, ϕ_m are even in $\omega_{n'}$ (true for an inversion-symmetric solution, since $Z(\mathrm{i}\omega,\mathbf{k}) = Z(-\mathrm{i}\omega,-\mathbf{k})$, $\chi(\mathrm{i}\omega,\mathbf{k}) = \chi(-\mathrm{i}\omega,-\mathbf{k})$), and that $Z_m\to 1$, $\chi_m,\phi_m\to 0$ for $|\omega_{n'}|\to\infty$.

Step 1. Since $\mathscr{G}^{\ m}_{\mathrm{Gorkov}}(0^-,\mathbf{k}) = -\frac{1}{\hbar}\langle \mathrm{T}_\tau\, c_{m\uparrow}(0^-,\mathbf{k}) c^\dagger_{m\uparrow}(0,\mathbf{k})\rangle_{\mathrm{SC}} = +\frac{1}{\hbar}\langle c^\dagger_{m\uparrow}(\mathbf{k}) c_{m\uparrow}(\mathbf{k})\rangle_{\mathrm{SC}}$, spin-degeneracy and Lemma 1.11 give

$$n = \frac{1}{N_p}\sum_{\mathbf{k},m,\sigma}\langle c^\dagger_{m\sigma}(\mathbf{k}) c_{m\sigma}(\mathbf{k})\rangle_{\mathrm{SC}} = \frac{2}{N_p}\sum_{\mathbf{k},m}\frac{1}{\beta}\sum_{\omega_{n'}\in\Omega_{-1}} \mathrm{e}^{\mathrm{i}\omega_{n'}0^+}\mathscr{G}^{\ m}_{\mathrm{Gorkov}}(\mathrm{i}\omega_{n'},\mathbf{k}).$$

Step 2. By Corollary 26.44, $\mathscr{G}^{\ m}_{\mathrm{Gorkov}} = -\mathrm{i}\hbar\omega_{n'} Z_m/\theta_m - (\epsilon_m(\mathbf{k}) - \mu + \chi_m)/\theta_m$. The second part decays like $\omega_{n'}^{-2}$; the convergence factor can be dropped there. The first part is odd in $\omega_{n'}$ and decays only like $1/(\mathrm{i}\hbar\omega_{n'})$. We write it as $\frac{1}{\mathrm{i}\hbar\omega_{n'}} + R(\omega_{n'})$ with an odd remainder $R = o(1/\omega_{n'})$, whose symmetric Matsubara-sum vanishes. With $\frac{1}{\beta}\sum_{\omega_{n'}} \mathrm{e}^{\mathrm{i}\omega_{n'}0^+}\frac{1}{\mathrm{i}\hbar\omega_{n'}} = \frac{1}{2}$ (the Fermi-function at zero energy, cf. Theorem 13.6) we get

$$\frac{1}{\beta}\sum_{\omega_{n'}} \mathrm{e}^{\mathrm{i}\omega_{n'}0^+}\mathscr{G}^{\ m}_{\mathrm{Gorkov}}(\mathrm{i}\omega_{n'},\mathbf{k}) = \frac{1}{2} - \frac{1}{\beta}\sum_{\omega_{n'}}\frac{\epsilon_m(\mathbf{k}) - \mu + \chi_m(\mathrm{i}\omega_{n'},\mathbf{k})}{\theta_m(\mathrm{i}\omega_{n'},\mathbf{k})}.$$

Inserting this into Step 1 gives Equation (26.169). As a check: for $Z=1$, $\chi=\phi=0$ one gets $\frac{1}{2} - \frac{1}{\beta}\sum_\omega \frac{\xi}{\hbar^2\omega^2+\xi^2} = \frac{1}{2} - \frac{1}{2}\tanh\frac{\beta\xi}{2} = \frac{1}{\mathrm{e}^{\beta\xi}+1}$. ■

From here onwards everything should be fine again.

==========

26.1.7. Simplified Equations

For reasons that will be clear in the subsequent chapters, we consider the following limiting case.

Corollary 26.52 In the limiting case $Z \equiv 1$, $\chi \equiv 0$ we obtain, changing the notation $\phi \equiv \delta$, the system of gap equations

$$\overline{\delta}_n(k') = \sum_{\substack{k \in \mathrm{i}\Omega_{-1} \times \mathrm{Q} \\ \nu \in \{1,\ldots,rd_{\mathbf{x}}\} \\ m \in \{1,2,3,\ldots,\infty\}}} \frac{\overline{\delta}_m(k)}{\omega_k^2 + \frac{\left(\epsilon_m(\mathbf{k}) - \mu\right)^2}{\hbar^2} + |\delta(k)|^2} \frac{2\omega_\nu(\mathbf{k}-\mathbf{k}')}{\omega_{k-k'}^2 + \omega_\nu^2(\mathbf{k}-\mathbf{k}')} \frac{|g_{mn\nu}(\mathbf{k}', \mathbf{k}-\mathbf{k}')|^2}{\hbar^3 \beta N_p} \tag{26.170}$$

Note (checked against Equation (26.167)). The formula is correct if the change of notation is $\phi \equiv \hbar\delta$ (not $\phi \equiv \delta$): ϕ is an energy, while δ is a frequency, as $\omega_k^2 + \ldots + |\delta|^2$ shows. Moreover $|\delta(k)|^2$ means $|\delta_m(k)|^2$, ω_k and $\omega_{k-k'}$ are the (fermionic resp. bosonic) Matsubara-frequencies of k and $k-k'$, and the bar ($\overline{\delta}$) can be dropped because the kernel is real. Since ϕ was assumed real, $|\delta_m|^2 = \delta_m^2$. With $Z \equiv 1$, $\chi \equiv 0$ one has $\theta_m = \hbar^2(\omega_k^2 + (\epsilon_m(\mathbf{k}) - \mu)^2/\hbar^2 + \delta_m^2)$, and $\lambda/N_\mathrm{F} = \frac{1}{\hbar}\sum_\nu \frac{2\omega_\nu}{\omega^2+\omega_\nu^2}|g|^2$ gives the factor $1/\hbar^3$ after dividing by $\hbar$ on both sides. The limit $Z \equiv 1$, $\chi \equiv 0$ is not a solution of Equations (26.165) and (26.166). It is an additional approximation, which neglects mass-renormalization and band-shift.

Proof 26.52

The Eliashberg-Equations from 03-EPW reads for ϕ:

$$\overline{\phi}_n(\mathrm{i}\omega_j, \mathbf{k}) = \frac{T}{N_\mathrm{F}} \sum_{\substack{\mathbf{q} \in \mathrm{Q} \\ \omega_{j'} \in \Omega_{-1} \\ m \in \{1,\ldots,\infty\}}} \frac{\overline{\phi}_m(\mathrm{i}\omega_{j'}, \mathbf{k}+\mathbf{q})}{\theta_m(\mathrm{i}\omega_{j'}, \mathbf{k}+\mathbf{q})} \lambda_{n,m}(\mathrm{i}\omega_j - \mathrm{i}\omega_{j'}; \mathbf{k}, \mathbf{k}+\mathbf{q}) \tag{26.171}$$

with

$$\theta_m(\mathrm{i}\omega_n, \mathbf{k}) = \hbar^2\omega_n^2 Z_m(\mathbf{k}, \mathrm{i}\omega_n)^2 + \left(\chi_m(\mathbf{k}, \mathrm{i}\omega_n) + (\epsilon_m(\mathbf{k}) - \mu)\right)^2 + \phi_m(\mathrm{i}\omega_n, \mathbf{k})^2 \tag{26.172}$$

and

$$\lambda^{n,m}_{\mathbf{k},\mathbf{k}+\mathbf{q}}(\omega_n) = N_\mathrm{F} \sum\!\!\!\!\!\!\int_{\substack{\omega \in (0,\infty) \\ \nu \in \{1,\ldots,rd_{\mathbf{x}}\}}} \frac{2\omega}{\omega_n^2 + \omega^2} |g_{mn\nu}(\mathbf{k}, \mathbf{q})|^2 \delta\left(\omega - \omega_\nu(\mathbf{q})\right) \tag{26.173}$$

Considering now the limiting case $Z \equiv 1$, $\chi \equiv 0$ we obtain

$$\begin{aligned}
\overline{\phi}_n(\mathrm{i}\omega_j,\mathbf{k}) &= \sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ \omega_{j'}\in\Omega_{-1}\\ m\in\{1,\dots,\infty\}}} \frac{\overline{\phi}_m(\mathrm{i}\omega_{j'},\mathbf{k}+\mathbf{q})}{\hbar^2\omega_{j'}^2+\left(\epsilon_m(\mathbf{k}+\mathbf{q})-\mu\right)^2+|\phi_m(\mathrm{i}\omega_{j'},\mathbf{k}+\mathbf{q})|^2}|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2\frac{2\omega_\nu(\mathbf{q})}{\left(\omega_j-\omega_{j'}\right)^2+\omega_\nu(\mathbf{q})^2}\frac{1}{\hbar\beta}\\
&\overset{\mathbf{q}\mapsto\mathbf{q}-\mathbf{k}}{=} \sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ \omega_{j'}\in\Omega_{-1}\\ m\in\{1,\dots,\infty\}}} \frac{\overline{\phi}_m(\mathrm{i}\omega_{j'},\mathbf{q})}{\hbar^2\omega_{j'}^2+\left(\epsilon_m(\mathbf{q})-\mu\right)^2+|\phi_m(\mathrm{i}\omega_{j'},\mathbf{q})|^2}|g_{mn\nu}(\mathbf{k},\mathbf{q}-\mathbf{k})|^2\frac{2\omega_\nu(\mathbf{q}-\mathbf{k})}{\left(\omega_j-\omega_{j'}\right)^2+\omega_\nu(\mathbf{q}-\mathbf{k})^2}\frac{1}{\hbar\beta}\\
&\overset{q\equiv(\mathbf{q},\mathrm{i}\omega_{j'}),k\equiv(\mathbf{k},\mathrm{i}\omega_j)}{=} \sum_{\substack{q\in\mathrm{Q}\times\Omega_{-1}\\ m\in\{1,\dots,\infty\}}} \frac{\overline{\phi}_m(q)}{\hbar^2\omega_q^2+\left(\epsilon_m(q)-\mu\right)^2+|\phi_m(q)|^2}|g_{mn\nu}(\mathbf{k},\mathbf{q}-\mathbf{k})|^2\frac{2\omega_\nu(\mathbf{q}-\mathbf{k})}{\omega_{q-k}^2+\omega_\nu(\mathbf{q}-\mathbf{k})^2}\frac{1}{\hbar\beta}
\end{aligned}$$

which can be summarized as

$$\overline{\phi}_n(k) = \sum_{\substack{q\in\mathrm{Q}\times\Omega_{-1}\\ m\in\{1,\dots,\infty\}}} \frac{\overline{\phi}_m(q)}{\hbar^2\omega_q^2+\left(\epsilon_m(q)-\mu\right)^2+|\phi_m(q)|^2}|g_{mn\nu}(\mathbf{k},\mathbf{q}-\mathbf{k})|^2\frac{2\omega_\nu(\mathbf{q}-\mathbf{k})}{\omega_{q-k}^2+\omega_\nu(\mathbf{q}-\mathbf{k})^2}\frac{1}{\hbar\beta}$$

Note: The template for this was 03-EPW.

Correction note. (i) The λ quoted at the beginning lacks the factor $1/\hbar$ of the Definition of λ; with the Definition (as used from the second equation on, where the $1/(\hbar\beta)$ appears) everything is consistent. (ii) A factor $1/N_p$ (from the $\mathbf{q}$-sum, cf. Equation (26.167)) and the sum over ν are missing from the second equation on. (iii) To arrive at the Corollary one still has to insert $\phi = \hbar\delta$ and divide by $\hbar$, which gives the $1/\hbar^3$ there. In the last two lines $\epsilon_m(q)$ means $\epsilon_m(\mathbf{q})$.

Remark 26.52.1 Notice that this can be rewritten, using $\hbar\delta \equiv \Delta$ and $\xi_m(\mathbf{k}) \equiv \epsilon_m(\mathbf{k}) - \mu$ in energy-units as

$$\overline{\Delta}_n(k') = \frac{1}{N_x N_y N_z}\frac{1}{\beta}\sum_{\substack{k\in\mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}\\ m\in\{1,2,3,\dots,\infty\}}} \frac{\overline{\Delta}_m(k)}{\Omega_k^2+\xi_m^2(\mathbf{k})+|\Delta_m(k)|^2}\frac{2\,\Omega_\nu(\mathbf{k}-\mathbf{k}')}{\Omega_{k-k'}^2+\Omega_\nu^2(\mathbf{k}-\mathbf{k}')}|g_{mn\nu}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2 \tag{26.174}$$

Remark 26.52.2 This is a convolution of discrete functions! Can one now use smart convolution-theorems? [15]

Remark 26.52.3 Notice that we can get an upper bound for gap-function by introducing the maximal value

$$|\delta_{\max}| = \max\left\{|\delta_m(k)| \quad | \quad k \in \Omega_{-1}\times\mathrm{Q} \wedge m \in \{1,2,3,\dots,\infty\}\right\} \tag{26.175}$$

which allows us to estimate

[15] For example the derivative of the temperature!!!

$$
\begin{aligned}
0 \leq |\delta_m(k)| \leq & \sum_{\substack{k \in \mathrm{i}\Omega_{-1} \times \mathbb{Q} \\ \nu \in \{1,\ldots,rd_{\mathbf{x}}\} \\ m \in \{1,2,3,\ldots,\infty\}}} \frac{|\delta_m(k)|}{\omega_k^2 + \frac{\left(\epsilon_m(\mathbf{k}) - \mu\right)^2}{\hbar^2} + |\delta_m(k)|^2} \frac{2\omega_\nu(\mathbf{k}-\mathbf{k}')}{\omega_{k-k'}^2 + \omega_\nu^2(\mathbf{k}-\mathbf{k}')} \frac{|g_{mn\nu}(\mathbf{k}', \mathbf{k}-\mathbf{k}')|^2}{\hbar^3 \beta N_p} \\
\leq & |\delta_{\max}| \sum_{\substack{k \in \mathrm{i}\Omega_{-1} \times \mathbb{Q} \\ \nu \in \{1,\ldots,rd_{\mathbf{x}}\} \\ m \in \{1,2,3,\ldots,\infty\}}} \frac{1}{\omega_k^2 + \frac{\left(\epsilon_m(\mathbf{k}) - \mu\right)^2}{\hbar^2}} \frac{2\omega_\nu(\mathbf{k}-\mathbf{k}')}{\omega_{k-k'}^2 + \omega_\nu^2(\mathbf{k}-\mathbf{k}')} \frac{|g_{mn\nu}(\mathbf{k}', \mathbf{k}-\mathbf{k}')|^2}{\hbar^3 \beta N_p}
\end{aligned}
\tag{26.176}
$$

which can be evaluated further with the Residue-theorem TBDone.

26.2. Eliashberg-Theory in the Field Integral Formalism

We divide the whole procedure into several steps. All this time we will have a mean-field-theory for the bosonic field in mind (in analogy to Altlands description of superconductivity). The second quantized Hamiltonian of the underlying system is as in section 26.1.4.

26.2.1. The Electron-Electron-Interactions originating from the Phonons

Theorem 26.53 The effective electron-electron interaction can be decomposed into so-called *Spin-Singlet*-contributions („↓↑“) and two *Spin-Triplet*-contributions („↓↓“, „↑↑“) as

$$
\begin{aligned}
S_{\text{el-el-int}}[\psi, \overline{\psi}] = & \sum_{\alpha_1,\ldots,\alpha_4 \in \Xi} \overline{\psi}_{\alpha_1} \overline{\psi}_{\alpha_2} V_{\alpha_1,\alpha_2;\alpha_3,\alpha_4} \psi_{\alpha_4} \psi_{\alpha_3} \\
= & \sum_{\substack{q,k,k' \in \mathbb{Q} \times \Omega_{-1} \\ m_{\alpha_1},\ldots,m_{\alpha_4} \in \{1,2,3,\ldots\}}} \overline{\psi}_{m_{\alpha_1}\uparrow}(q+k) \overline{\psi}_{m_{\alpha_2}\downarrow}(-k) V^{\downarrow\uparrow}_{m_{\alpha_1},m_{\alpha_2};m_{\alpha_3},m_{\alpha_4}}(q,k,k') \psi_{m_{\alpha_3}\downarrow}(q-k') \psi_{m_{\alpha_4}\uparrow}(k') \\
& + \sum_{\substack{q,k,k' \in \mathbb{Q} \times \Omega_{-1} \\ m_{\alpha_1},\ldots,m_{\alpha_4} \in \{1,2,3,\ldots\}}} \overline{\psi}_{m_{\alpha_1}\uparrow}(q+k) \overline{\psi}_{m_{\alpha_2}\uparrow}(-k) V^{\uparrow\uparrow}_{m_{\alpha_1},m_{\alpha_2};m_{\alpha_3},m_{\alpha_4}}(q,k,k') \psi_{m_{\alpha_3}\uparrow}(q-k') \psi_{m_{\alpha_4}\uparrow}(k') \\
& + \sum_{\substack{q,k,k' \in \mathbb{Q} \times \Omega_{-1} \\ m_{\alpha_1},\ldots,m_{\alpha_4} \in \{1,2,3,\ldots\}}} \overline{\psi}_{m_{\alpha_1}\downarrow}(q+k) \overline{\psi}_{m_{\alpha_2}\downarrow}(-k) V^{\downarrow\downarrow}_{m_{\alpha_1},m_{\alpha_2};m_{\alpha_3},m_{\alpha_4}}(q,k,k') \psi_{m_{\alpha_3}\downarrow}(q-k') \psi_{m_{\alpha_4}\downarrow}(k') \\
= & S_{\downarrow\uparrow}[\psi, \overline{\psi}] + S_{\uparrow\uparrow}[\psi, \overline{\psi}] + S_{\downarrow\downarrow}[\psi, \overline{\psi}]
\end{aligned}
$$

with spin-triplet vertices as above and spin-singlet matrix-elements (after adding up and collecting the individual contributions) given as

$$
\begin{aligned}
&2V^{\sigma\sigma}_{m_{\alpha_1},m_{\alpha_2};m_{\alpha_3},m_{\alpha_4}}(q,k,k') \\
&= V^{\downarrow\uparrow}_{m_{\alpha_1},m_{\alpha_2};m_{\alpha_3},m_{\alpha_4}}(q,k,k') \\
&= \frac{-1}{\hbar\beta N_p}\sum_{\nu\in\{1,\dots,rd_{\mathbf{x}}\}}\frac{2\omega_\nu(\mathbf{k}+\mathbf{q}-\mathbf{k}')}{\omega^2_{k+q-k'}+\omega^2_\nu(\mathbf{k}+\mathbf{q}-\mathbf{k}')}\frac{g_{m_{\alpha_1}m_{\alpha_4}\nu}(\mathbf{k}',\mathbf{k}+\mathbf{q}-\mathbf{k}')g^*_{m_{\alpha_3}m_{\alpha_2}\nu}(-\mathbf{k},\mathbf{k}+\mathbf{q}-\mathbf{k}')}{\hbar^2} \\
&= \frac{-1}{\hbar\beta N_p}\sum_{\nu\in\{1,\dots,rd_{\mathbf{x}}\}}\frac{2\omega_\nu(\mathbf{k}+\mathbf{q}-\mathbf{k}')}{\omega^2_{k+q-k'}+\omega^2_\nu(\mathbf{k}+\mathbf{q}-\mathbf{k}')}\frac{g_{m_{\alpha_1}m_{\alpha_4}\nu}(\mathbf{k}',\mathbf{k}+\mathbf{q}-\mathbf{k}')g_{m_{\alpha_2}m_{\alpha_3}\nu}(\mathbf{q}-\mathbf{k}',-(\mathbf{k}+\mathbf{q}-\mathbf{k}'))}{\hbar^2}
\end{aligned}
\tag{26.177}
$$

Proof 26.53 See Appendix, Proofs, page 627.

Lemma 26.54 The vertices in Equation (26.177) are lesser than zero iff

- either $\mathbf{k}=-\mathbf{k}'$ AND $m_{\alpha_1}=m_{\alpha_3}$ AND $m_{\alpha_4}=m_{\alpha_2}$ (upper equation - „[N]on-[E]liashberg-[T]heory“ cases),
- or $\mathbf{q}=0$ AND $m_{\alpha_1}=m_{\alpha_2}$ AND $m_{\alpha_4}=m_{\alpha_3}$ (lower equation - „[E]liashberg-[T]heory“ cases).

Proof 26.54 Referring to Equations (8.44), (8.45) proves the theorem.

Remark 26.54.1 Notice that the BCS-action in Equation (30.4) turns out to be a special case of the spin-singlet contributions in the limit of constant vertices.

Theorem 26.55 We decompose the spin-singlet contributions as

$$
S[\psi,\overline{\psi}] \equiv S^{\mathrm{ET}}[\psi,\overline{\psi}] + S^{\mathrm{NET}}[\psi,\overline{\psi}] + S^{\mathrm{RPC}}[\psi,\overline{\psi}] \tag{26.178}
$$

whereas for the ([N]on-)[E]liashberg-[T]heory contribution

$$
\begin{aligned}
S^{\mathrm{ET}}[\psi,\overline{\psi}] = &\sum_{\substack{k,k'\in\Omega_{-1}\times\mathrm{Q}\\ m,n\in\{1,2,3\dots\}}}\overline{\psi}_{m\uparrow}(k)\overline{\psi}_{m\downarrow}(-k)V^{\mathrm{ET}}_{\downarrow\uparrow\,m,n}(k,k')\psi_{n\downarrow}(-k')\psi_{n\uparrow}(k') \\
&+\sum_{\substack{\sigma\in\{\downarrow,\uparrow\}\\ k,k'\in\Omega_{-1}\times\mathrm{Q}\\ m,n\in\{1,2,3\dots\}}}\overline{\psi}_{m\sigma}(k)\overline{\psi}_{m\sigma}(-k)V^{\mathrm{ET}}_{\sigma\sigma\,m,n}(k,k')\psi_{n\sigma}(-k')\psi_{n\sigma}(k')
\end{aligned}
$$

whereas the first term produces the off-diagonal contributions to the Gorkov-Green-functions.

$$\begin{aligned} S^{\mathrm{NET}}_{\downarrow\uparrow}[\psi,\overline{\psi}] = & \sum_{\substack{q,k\in \mathrm{i}\Omega_{-1}\times\mathbb{Q}\\ m,n\in\{1,2,3\ldots\}}} \overline{\psi}_{m\uparrow}(q)\psi_{m\downarrow}(q)V^{\mathrm{NET}}_{\substack{\downarrow\uparrow\\ m,n}}(q+k,-k)\psi_{n\uparrow}(k)\overline{\psi}_{n\downarrow}(k) \\ & + \sum_{\substack{\sigma\in\{\downarrow,\uparrow\}\\ q,k\in \mathrm{i}\Omega_{-1}\times\mathbb{Q}\\ m,n\in\{1,2,3\ldots\}}} \overline{\psi}_{m\sigma}(q)\psi_{m\sigma}(q)V^{\mathrm{NET}}_{\substack{\sigma\sigma\\ m,n}}(q-k,k)\psi_{n\sigma}(-k)\overline{\psi}_{n\sigma}(-k) \end{aligned} \tag{26.179}$$

whereas the terms in the second line should be able to produce the diagonal contributions to the Gorkov-Green-functions. The remaining terms are the [R]andom [P]hase [C]ancellations. (We assume them to be random phases that don't contribute to the physical observables.) Then we have, when we take the double contributions into account, the vertices

$$2V^{\mathrm{ET}}_{\substack{\sigma\sigma\\ m,n}}(k,k') = V^{\mathrm{ET}}_{\substack{\downarrow\uparrow\\ m,n}}(k,k') = \frac{-2}{\hbar\beta N_p}\sum_{\nu\in\{1,\ldots,rd_{\mathbf{x}}\}} \frac{\omega_\nu(\mathbf{k}-\mathbf{k}')}{\omega^2_{k-k'}+\omega^2_\nu(\mathbf{k}-\mathbf{k}')}\frac{|g_{mn\nu}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{\hbar^2} \tag{26.180}$$

$$2V^{\mathrm{NET}}_{\substack{\sigma\sigma\\ m,n}}(q+k,-k) = V^{\mathrm{NET}}_{\substack{\downarrow\uparrow\\ m,n}}(q+k,-k) = \frac{-2}{\hbar\beta N_p}\sum_{\nu\in\{1,\ldots,rd_{\mathbf{x}}\}} \frac{\omega_\nu(-\mathbf{k}+\mathbf{q})}{\omega^2_{-k+q}+\omega^2_\nu(-\mathbf{k}+\mathbf{q})}\frac{|g_{mn\nu}(+\mathbf{k},-\mathbf{k}+\mathbf{q})|^2}{\hbar^2} \tag{26.181}$$

Proof 26.55 See Appendix, Proofs, page 630.

26.2.2. Electron-Electron-Interactions for Spin-Singlet Eliashberg-Theory

In order to prove the validity of our approach, we derive the [E]liashberg-[T]heory-equations from a limiting case of our theory.

Approximation 26.56 We approximate the interactions by focusing on the ET-↓↑-contributions and neglecting the other terms as

$$S_{\text{el-el-int}}[\psi,\overline{\psi}] = S^{\mathrm{ET}}_{\downarrow\uparrow}[\psi,\overline{\psi}] + S_{\Delta V}[\psi,\overline{\psi}] \approx S^{\mathrm{ET}}_{\downarrow\uparrow}[\psi,\overline{\psi}]$$

with the Eliashberg contribution

$$S^{\mathrm{ET}}_{\downarrow\uparrow}[\psi,\overline{\psi}] = \sum_{\substack{k,k'\in \mathrm{i}\Omega_{-1}\times\mathbb{Q}\\ m,n\in\{1,2,3\ldots\}}} \overline{\psi}_{m\uparrow}(k)\overline{\psi}_{m\downarrow}(-k)V^{\mathrm{ET}}_{\substack{\downarrow\uparrow\\ m,n}}(k,k')\psi_{n\downarrow}(-k')\psi_{n\uparrow}(k')$$

and the vertex

$$V^{\mathrm{ET}}_{\substack{\downarrow\uparrow\\ m,n}}(k,k') = \frac{-2}{\hbar\beta N_p}\sum_{\nu\in\{1,\ldots,rd\}} \frac{\omega_\nu(\mathbf{k}-\mathbf{k}')}{\omega^2_{k-k'}+\omega^2_\nu(\mathbf{k}-\mathbf{k}')}\frac{|g_{mn\nu}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{\hbar^2} \tag{26.182}$$

Fact 26.57 The key observation is now to see that this interaction term falls exactly into Theorem 17.10, with the second equation in Equation (17.6) being applicable, whereas

$$\overline{\mathrm{Q}}^{\mathsf{T}} \equiv \overline{\mathrm{Q}}_m^{\mathsf{T}}(\mathbf{k}) \equiv \overline{\psi}_{m\uparrow}(k)\overline{\psi}_{m\downarrow}(-k), \qquad P \equiv P_n(\mathbf{k}') \equiv \psi_{n\downarrow}(-k')\psi_{n\uparrow}(k') \tag{26.183}$$

Notation 26.58 We condense the notation even further, by introducing the multi-index

$$A \equiv (k, m, \downarrow, \uparrow) \in \Pi, \quad B \equiv (k', n; \downarrow, \uparrow) \in \Pi \quad \text{with} \quad \Pi \equiv \mathrm{i}\Omega_{-1} \times \mathrm{Q} \times \{1, 2, 3, \ldots\} \times \{\downarrow\} \times \{\uparrow\} \tag{26.184}$$

and density-like terms

$$\overline{\rho}(A) \equiv \overline{\psi}_{m\uparrow}(k)\overline{\psi}_{m\downarrow}(-k), \qquad \rho(B) \equiv \psi_{n\downarrow}(-k')\psi_{n\uparrow}(k') \tag{26.185}$$

with $\rho(A) = \psi_{m\downarrow}(-k)\psi_{m\uparrow}(k)$.

Remark 26.58.1 Notice that with this, we can rewrite the Eliashberg-interaction term as a bilinear

$$S^{\mathrm{ET}}_{\downarrow\uparrow}[\psi, \overline{\psi}] = \sum_{A,B \in \Pi} \overline{\rho}(A) V^{\mathrm{ET}}_{\downarrow\uparrow}(A, B) \rho(B) \tag{26.186}$$

26.2.3. Hubbard-Stratanovich-Transformation

We now exchange the quartic interaction for a quadratic-part through the Cooper-channel. We therefore have to find the inverse of $V^{\mathrm{ET}}_{\downarrow\uparrow}$.

Hypothesis 26.59 We assume, the existence of another generalised matrix $\left(V^{\mathrm{ET}}_{\downarrow\uparrow}\right)^{-1} \equiv \Lambda^{\mathrm{ET}}_{\downarrow\uparrow}$ such that the inverse relation holds

$$\left(V^{\mathrm{ET}}_{\downarrow\uparrow} \cdot \Lambda^{\mathrm{ET}}_{\downarrow\uparrow}\right)(A, A') = \sum_B V^{\mathrm{ET}}_{\downarrow\uparrow}(A, B)\Lambda^{\mathrm{ET}}_{\downarrow\uparrow}(B, A') = \delta(A, A'). \tag{26.187}$$

Remark 26.59.1 For the moment, we will not bother with the concrete shape of this inverse matrix. We simply assume its existence and give it a name to perform further mathematical operations.

Lemma 26.60 Performing a Hubbard-Stratanovich-transformation of the Eliashberg-interaction term through the Cooper-channel yields

$$\begin{aligned}\exp\, -S^{\mathrm{ET}}_{\downarrow\uparrow}[\psi,\overline{\psi}] &= \exp\, -\sum_{A,B\in\Pi^2}\overline{\rho}(A)V^{\mathrm{ET}}_{\downarrow\uparrow}(A,B)\rho(B)\\ &= \int \mathscr{D}(\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow})\exp+\left[\sum_{A,B\in\Pi^2}\overline{\delta}(A)\Lambda^{\mathrm{ET}}_{\downarrow\uparrow}(A,B)\delta(B)-\sum_{A\in\Pi}\left(\overline{\delta}(A)\rho(A)+\overline{\rho}(A)\delta(A)\right)\right]\\ &= \int \mathscr{D}(\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow})\exp-\left[S_{\mathrm{aux.}}[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]+S_{\mathrm{int}}[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow},\psi,\overline{\psi}]\right].\end{aligned}$$

Proof 26.60 Shifting variables according to

$$\delta(A)\mapsto\delta(A)+\sum_{B\in\Pi}V^{\mathrm{ET}}_{\downarrow\uparrow}(A,B)\rho(B),\qquad \overline{\delta}(A)\mapsto\overline{\delta}(A)+\sum_{B\in\Pi}\overline{\rho}(B)V^{\mathrm{ET}}_{\downarrow\uparrow}(B,A)\tag{26.188}$$

proves the Lemma.

Fact 26.61 The full action, in absense of external sources, now reads

$$S_{\mathrm{tot}}[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow},\psi,\overline{\psi}]=S_{\mathrm{el}}[\psi,\overline{\psi}]+S_{\mathrm{aux}}[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]+S_{\mathrm{int}}[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow},\psi,\overline{\psi}]\tag{26.189}$$

with

- $S_{\mathrm{el}}[\psi,\overline{\psi}]\equiv\sum_{\substack{\sigma\in\{\downarrow,\uparrow\}\\ k\in\mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ m\in\{1,2,3,\dots\}}}\overline{\psi}_{m\sigma}(k)\left(-\frac{1}{\hbar}\mathscr{G}^{-\mathrm{F}}_{0\,m,\sigma}(k)\right)\psi_{m\sigma}(k)$
- $S_{\mathrm{aux}}[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]=-\sum_{A,B\in\Pi^2}\overline{\delta}(A)\Lambda^{\mathrm{ET}}_{\downarrow\uparrow}(A,B)\delta(B)$
- $S_{\mathrm{int}}[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow},\psi,\overline{\psi}]=\sum_{\substack{k\in\mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ m\in\{1,2,3,\dots\}}}\overline{\delta}_{m\downarrow\uparrow}(k)\psi_{m\downarrow}(-k)\psi_{m\uparrow}(k)+\overline{\psi}_{m\uparrow}(k)\overline{\psi}_{m\downarrow}(-k)\delta_{m\downarrow\uparrow}(k)$

Definition 26.62 We now introduce Nambu-spinors as

$$\eta^{\dagger}_{m}(k)=\begin{pmatrix}\overline{\psi}_{m,\uparrow}(k) & \psi_{m,\downarrow}(-k)\end{pmatrix},\qquad \eta_{m'}(k')=\begin{pmatrix}\psi_{m'\uparrow}(k')\\ \overline{\psi}_{m'\downarrow}(-k')\end{pmatrix}\tag{26.190}$$

Remark 26.62.1 Notice that this allows us to rewrite the electronic contributions as

$$\begin{aligned}S_{\mathrm{el}}[\psi,\overline{\psi}]+S_{\mathrm{int}}[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow},\psi,\overline{\psi}] &= \sum_{\substack{k\in\mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ m\in\{1,2,\dots\}}}\begin{pmatrix}\overline{\psi}_{m,\uparrow}(k)\\ \psi_{m,\downarrow}(-k)\end{pmatrix}^{\mathrm{T}}\begin{pmatrix}-\frac{1}{\hbar}\mathscr{G}^{-\mathrm{F}}_{0\,m\uparrow}(k) & \delta_{m\downarrow\uparrow}(k)\\ \overline{\delta}_{m\downarrow\uparrow}(k) & +\frac{1}{\hbar}\mathscr{G}^{-\mathrm{F}}_{0\,m\downarrow}(-k)\end{pmatrix}\begin{pmatrix}\psi_{m\uparrow}(k)\\ \overline{\psi}_{m\downarrow}(-k)\end{pmatrix}\\ &= \sum_{\substack{k\in\mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ m\in\{1,2,\dots\}}}\overline{\eta}^{\mathrm{T}}_{m}(k)\left[-\frac{1}{\hbar}\mathscr{G}^{-1}{}_{m\;[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]}(k)\right]\eta_{m}(k)\end{aligned}$$

Gorkov

Lemma 26.63 One finds for the imaginary time components of the Nambu-spinors the identity in imaginary time space

$$\overline{\eta}_m^{\mathrm{T}}(\tau,\mathbf{k}) = \begin{pmatrix}\overline{\psi}_{m\uparrow}(\tau,\mathbf{k}) & \psi_{m\downarrow}(\tau,-\mathbf{k})\end{pmatrix} \qquad \eta_m(\tau,\mathbf{k}) = \begin{pmatrix}\psi_{m\uparrow}(\tau,\mathbf{k}) \\ \overline{\psi}_{m\downarrow}(\tau,-\mathbf{k})\end{pmatrix} \tag{26.191}$$

Proof 26.63 See Appendix, Proofs, page 631.

Corollary 26.64 We note the correlators

$$\left\langle \eta_{m1}(\tau,\mathbf{k})\overline{\eta}_{m,1}(\tau',\mathbf{k})\right\rangle = \left\langle \psi_{m\uparrow}(\tau,\mathbf{k})\overline{\psi}_{m,\uparrow}(\tau',\mathbf{k})\right\rangle = -\hbar \underset{\substack{[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov,11}}}{\mathscr{G}_m}(\tau-\tau',\mathbf{k}) = -\hbar \underset{\text{Gorkov}}{\mathscr{G}_{m\uparrow}}(\tau-\tau',\mathbf{k}) \tag{26.192}$$

$$\left\langle \eta_{m1}(\tau,\mathbf{k})\overline{\eta}_{m,2}(\tau',\mathbf{k})\right\rangle = \left\langle \psi_{m\uparrow}(\tau,\mathbf{k})\psi_{m,\uparrow}(\tau',-\mathbf{k})\right\rangle = -\hbar \underset{\substack{[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov,12}}}{\mathscr{G}_m}(\tau-\tau',\mathbf{k}) = -\hbar \mathscr{F}_m(\tau-\tau',\mathbf{k}) \tag{26.193}$$

$$\left\langle \eta_{m2}(\tau,\mathbf{k})\overline{\eta}_{m,1}(\tau',\mathbf{k})\right\rangle = \left\langle \overline{\psi}_{m\downarrow}(\tau,-\mathbf{k})\overline{\psi}_{m,\uparrow}(\tau',\mathbf{k})\right\rangle = -\hbar \underset{\substack{[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov,21}}}{\mathscr{G}_m}(\tau-\tau',\mathbf{k}) = -\hbar \mathscr{F}_m^\dagger(\tau-\tau',\mathbf{k}) \tag{26.194}$$

$$\left\langle \eta_{m2}(\tau,\mathbf{k})\overline{\eta}_{m,2}(\tau',\mathbf{k})\right\rangle = \left\langle \overline{\psi}_{m\downarrow}(\tau,-\mathbf{k})\psi_{m,\downarrow}(\tau',-\mathbf{k})\right\rangle = -\hbar \underset{\substack{[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov,22}}}{\mathscr{G}_m}(\tau-\tau',\mathbf{k}) = -\hbar\left(-\underset{\text{Gorkov}}{\mathscr{G}_{m\downarrow}}(\tau'-\tau,-\mathbf{k})\right) \tag{26.195}$$

Proof 26.64 See Appendix, Proofs, page 631.

Lemma 26.65 Integrating out the fermions gives us an effective bosonic theory

$$S_{\mathrm{tot}}[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}] \quad = \quad S_{\mathrm{aux.}}[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}] \quad - \quad \mathrm{Tr\,Log} -\frac{1}{\hbar}\underset{\substack{[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}{\mathscr{G}^{-1}} \tag{26.196}$$

Proof 26.65 By using standard-identities about Gauss-Berezin-integrals and using the standard-identity Tr Log • = Log Det • gives us the desired identity.

26.2.4. Spontaneous Symmetry Breaking and Gap-Equations

We now break the U(1) symmetry by applying a saddle-point approximation and keeping only one contribution, analogous to section 30.2.5.

Lemma 26.66 We note the identity

$$\frac{\partial}{\partial\delta(\bullet)}\,\mathrm{Tr}\,\mathrm{Log}-\frac{1}{\hbar}\mathscr{G}^{-1}_{\substack{[\delta_{\downarrow\uparrow},\bar{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}=+\,\mathrm{Tr}\,\mathscr{G}_{\substack{[\delta_{\downarrow\uparrow},\bar{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}\frac{\partial}{\partial\delta(\bullet)}\mathscr{G}^{-1}_{\substack{[\delta_{\downarrow\uparrow},\bar{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}} \tag{26.197}$$

Proof 26.66 With Altlands prescription: We define $f(x)=\mathrm{Log}\left(-\frac{1}{\hbar}x\right)$, such that we obtain $f'(x)=\frac{1}{x}$. This yields for a x-dependent matrix $A\equiv A(x)$ the identity

$$\partial_x\,\mathrm{Tr}\,f(A)=\mathrm{Tr}\left(A^{-1}\partial_x A\right). \tag{26.198}$$

Corollary 26.67 The stationary points of the action are determined by the set of coupled equations

$$\bar{\delta}_{n\downarrow\uparrow}(k')=+\sum_{\substack{k\in\mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ \nu\in\{1,\ldots,rd\}\\ m\in\{1,2,3,\ldots\}}}\mathrm{Tr}_{2\times2}\left(\mathscr{G}_{\substack{m\\ [\delta_{\downarrow\uparrow},\bar{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}\frac{\partial}{\partial\delta_{m\downarrow\uparrow}(k)}\mathscr{G}^{-1}_{\substack{m\\ [\delta_{\downarrow\uparrow},\bar{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}\right)\frac{2\omega_\nu(\mathbf{k}-\mathbf{k}')}{\omega^2_{k-k'}+\omega^2_\nu(\mathbf{k}-\mathbf{k}')}\frac{|g_{mn\nu}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{\hbar^3\beta N_p}$$

Proof 26.67 See Appendix, Proofs, page 632.

Lemma 26.68 One has the identities

$$\frac{\partial}{\partial\delta_{m\downarrow\uparrow}(k)}\mathscr{G}^{-1}_{\substack{m\\ [\delta_{\downarrow\uparrow},\bar{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}=\begin{pmatrix}0&-\hbar\\0&0\end{pmatrix} \tag{26.199}$$

and

$$\mathscr{G}_{\substack{m\\ [\delta_{\downarrow\uparrow},\bar{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}(k)=-\frac{1}{\hbar}\frac{\begin{pmatrix}+\mathrm{i}\omega_k+(\epsilon_m(-\mathbf{k})-\mu)/\hbar & +\delta_{m\downarrow\uparrow}(k)\\ +\bar{\delta}_{m\downarrow\uparrow}(k) & +\mathrm{i}\omega_k-(\epsilon_m(\mathbf{k})-\mu)/\hbar\end{pmatrix}}{+\omega_k^2+\frac{\left(\epsilon_m(\mathbf{k})-\mu\right)^2}{\hbar^2}+|\delta_{m\downarrow\uparrow}(k)|^2} \tag{26.200}$$

Proof 26.68 See Appendix, Proofs, page 632.

Notice that we are now in the position to prove

Lemma 26.69 Remark **??** is true, i.e. it holds that

$$\underset{\substack{[\delta_{\downarrow\uparrow},\bar{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}{\mathscr{G}_{m,12}}(A,A')^{\dagger} = \underset{\substack{[\delta_{\downarrow\uparrow},\bar{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}{\mathscr{G}_{m,21}}(A,A') \tag{26.201}$$

Proof 26.69 See Appendix, Proofs, page 633.

Theorem 26.70 The gap equations become

$$\bar{\delta}_{n\downarrow\uparrow}(k') = + \sum_{\substack{k\in i\Omega_{-1}\times Q\\ \nu\in\{1,\dots,rd\}\\ m\in\{1,2,3,\dots\}}} \frac{\bar{\delta}_{m\downarrow\uparrow}(k)}{\omega_k^2 + \frac{\left(\epsilon_m(\mathbf{k})-\mu\right)^2}{\hbar^2} + |\delta_{m\downarrow\uparrow}(k)|^2} \frac{2\omega_\nu(\mathbf{k}-\mathbf{k}')}{\omega_{k-k'}^2+\omega_\nu^2(\mathbf{k}-\mathbf{k}')} \frac{|g_{mn\nu}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{\hbar^3\beta N_p}.$$

Proof 26.70 See Appendix, Proofs, page 634.

Remark 26.70.1 This result coincides perfectly with the limiting equations from the EPW-code in Equation (26.170).

27. Material Analysis with Quantum Espresso & Wannier90 & Wannier-Tools & EPW & GRIT

We consider only stochiometric crystals, i.e. crystals with a fixed number of atoms per unit cell and a fixed number of valence electrons per atom.

Introduction

Fact 27.1 For fixed (averaged) particle-number and volume we describe a crystal as a system of interacting phonons (massless particles) and electrons (massive particles). We work in the grand canonical ensemble with natural variables depending on the nature of the subsystem of interest, meaning that ...

- *for the phononic part of the system*, we are working in the grand canonical ensemble with natural variables (T, V),
- *for the electronic part of the system*, we are working in the grand canonical ensemble with natural variables (μ, T, V).

Fact 27.2 Notice first that ...

- for *spin-unpolarised systems* (i.e. no spin-dependent exchange-interaction or spin-orbit-coupling) one finds the inequality

  $$\text{"number of at least partially occupied bands"} \times 2 \quad \geq \quad \text{"number of electrons per unit cell"}.$$

  whereas spin-degenerate bands are counted once.
- In the more general notation (i.e. counting two degenerate bands as band nr. 1 and band nr. 2) or in the case of *spin-polarised systems*, one finds the inequality

  $$\text{"number of at least partially occupied bands"} \quad \geq \quad \text{"number of electrons per unit cell"}.$$

Fact 27.3 One has to count the number of expected electrons $\langle N \rangle$. For a crystal containing r atoms in the basis and $Z_1, Z_2, \ldots, Z_r$ valence electrons per atom, the number of expected electrons is given by

$$\begin{aligned} \langle N \rangle &= \text{"number of cells"} \quad \times \quad \text{"the total number of valence electrons per unit-cell"} \\ &= N_x N_y N_z \quad \cdot \quad \left(Z_1 + Z_2 + \ldots + Z_r\right) \\ &\equiv N_x N_y N_z \quad \cdot \quad n_{\text{UC}} \end{aligned} \tag{27.1}$$

27.1. Materials for a Specific Heat Analysis

27.1.1. Rb Crystal - Spacegroup Im3m (Rubidium)

Quantum Espresso Inputs

Crystal Structure from CIF-File

We have the following crystal-structure and atomic basis vectors from the cif-file:

```
&SYSTEM
    A           = 5.6568708402
    (...)
/

CELL_PARAMETERS {alat}
    -0.500000000000000   0.500000000000000   0.500000000000000
    0.500000000000000  -0.500000000000000   0.500000000000000
    0.500000000000000   0.500000000000000  -0.500000000000000

ATOMIC_POSITIONS {crystal}
Rb   0.000000000000000   0.000000000000000   0.000000000000000
```

Computational Input-Parameters

Excerpt from the python-code in which all the parameters are defined:

```
TBD
```

Step 0: vc-relax Calculation

We obtain the following final coordinates.

```
Begin final coordinates
        new unit-cell volume =    611.01184 a.u.^3 (    90.54261 Ang^3 )
        density =      1.56747 g/cm^3

CELL_PARAMETERS (alat= 10.55412041)
    -0.506494229   0.506494229   0.506494229
    0.506494229  -0.506494229   0.506494229
    0.506494229   0.506494229  -0.506494229

ATOMIC_POSITIONS (crystal)
Rb            0.0000000000        0.0000000000        0.0000000000
End final coordinates
```

such that the new input-file for the subsequent calculations reads

```
&SYSTEM
  A           = 5.6575405376
  (...)
```

```
/

CELL_PARAMETERS {alat}
 -0.500000000000000   0.500000000000000   0.500000000000000
  0.500000000000000  -0.500000000000000   0.500000000000000
  0.500000000000000   0.500000000000000  -0.500000000000000

ATOMIC_POSITIONS {crystal}
Rb    0.000000000000000    0.000000000000000    0.000000000000000
```

Step 1: SCF, Band-Structure and (Partial) Density of States

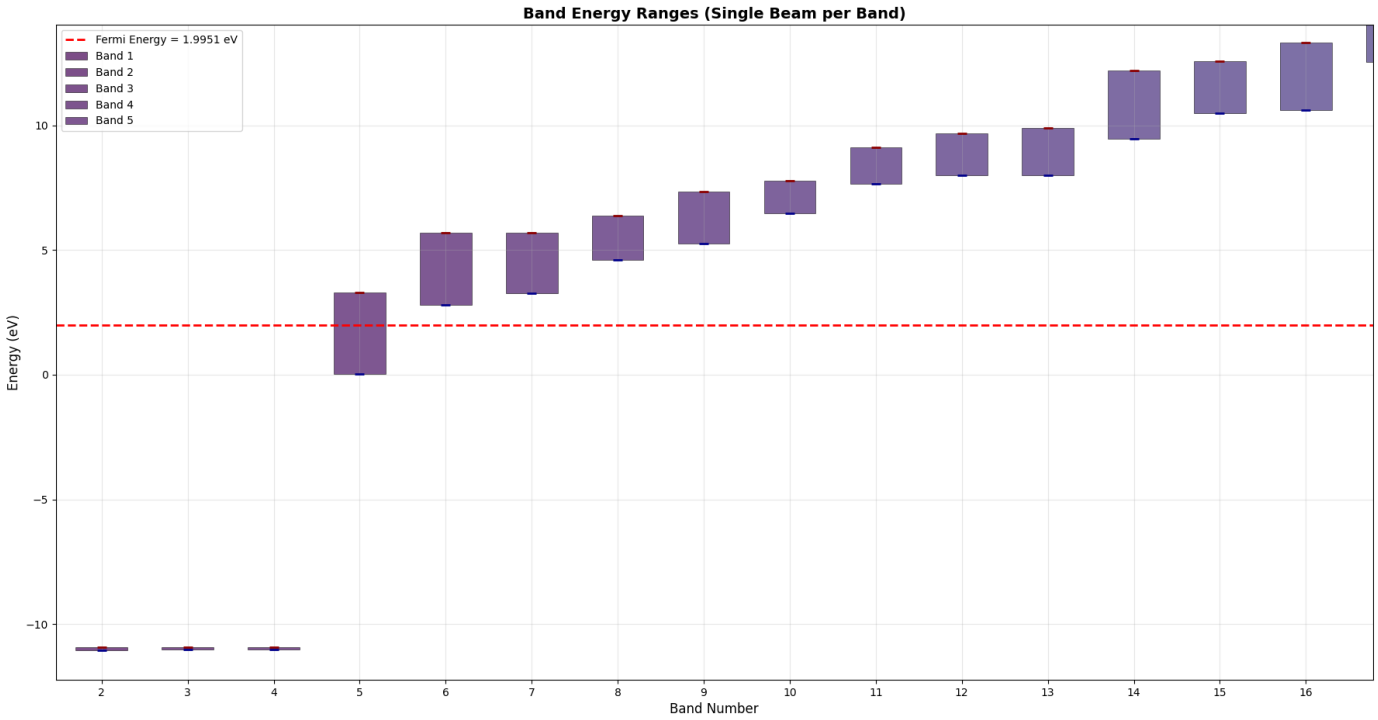


Figure 27.1.: Band-ranges and Band-indices.

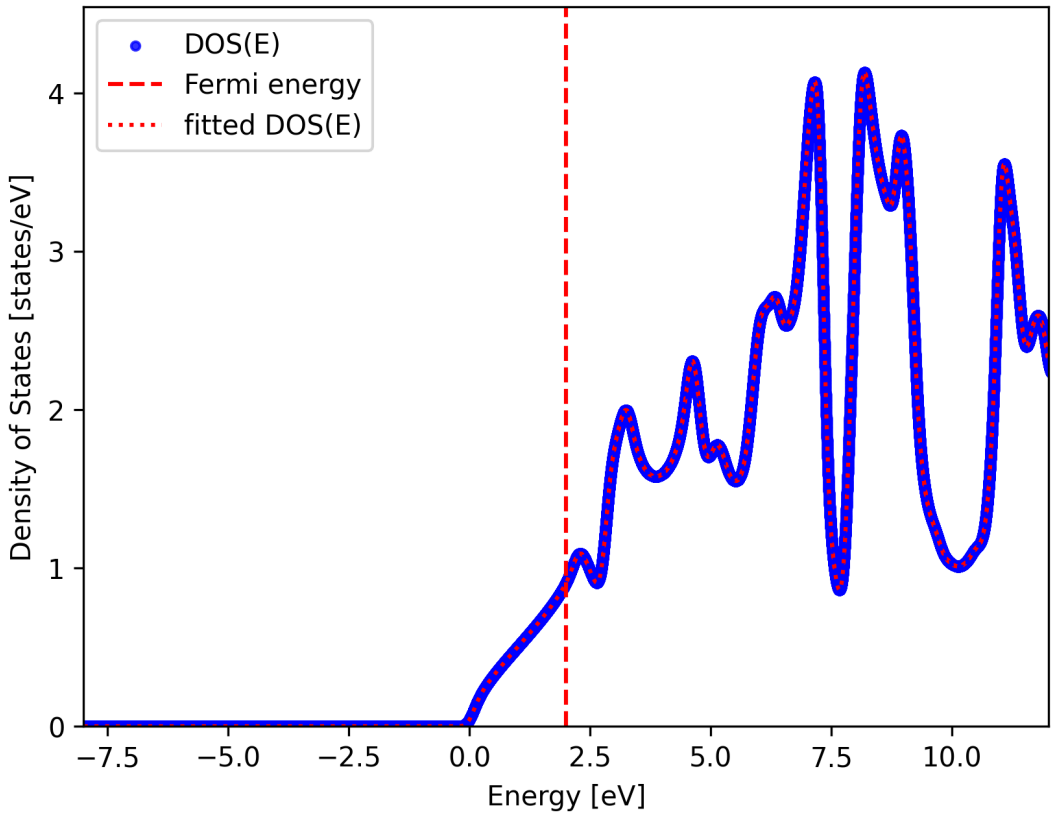


Figure 27.2.: Density of States in the LDA-Approximation.

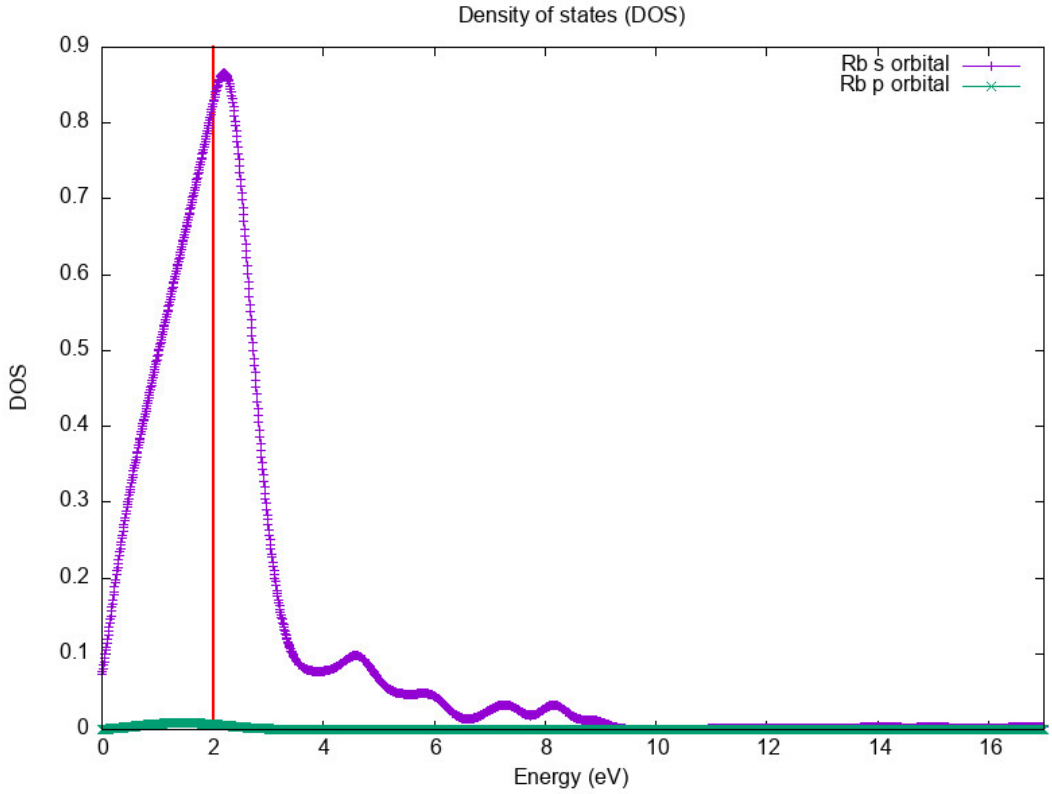


Figure 27.3.: Partial Density of States in the LDA-Approximation.

Notice that the projections give zero overlap for some highest energy, and that we don't see any d-states which is a consequence from the fact that we are using a pseudopotential.

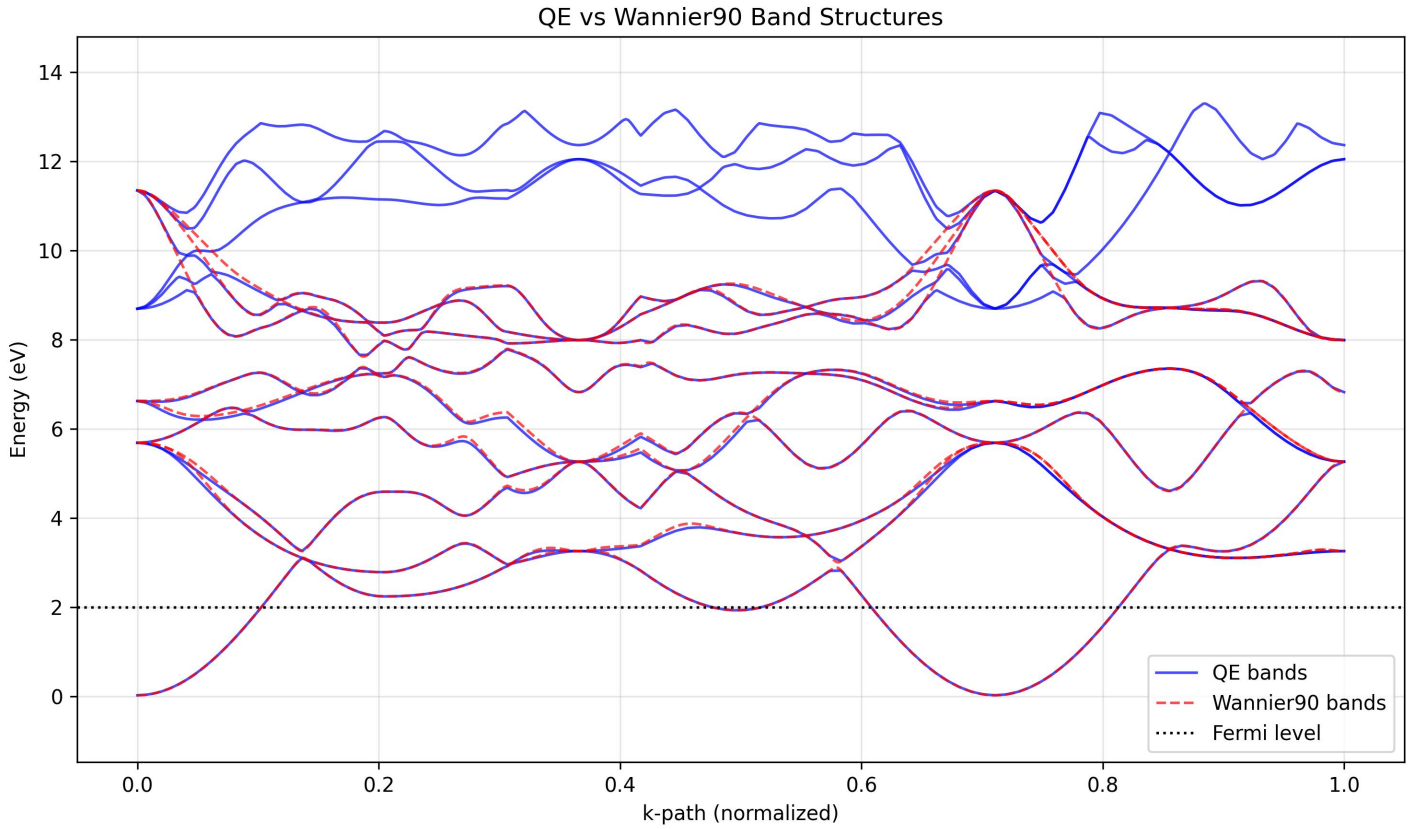


Figure 27.4.: Quantum Espresso vs. Wannier90 Bands.

TBContinued.

27.1.2. Au Crystal - Spacegroup Fm3m (Gold)

27.1.3. Ag Crystal - Spacegroup Fm3m (Silver)

27.1.4. K Crystal - Spacegroup Im3m (Potassium)

27.1.5. Cs Crystal - Spacegroup Im3m (Caesium)

27.1.6. Cu Crystal - Spacegroup Fm3m (Copper)

27.1.7. Si Crystal - Spacegroup Fd3m (Silicon)

27.1.8. C Crystal - Spacegroup Fd3m (Diamond)

27.1.9. KCl Crystal - Spacegroup Fm3m (Potassium Chloride)

27.2. Materials for a Superconductivity Analysis

27.2.1. TaC Crystal - Spacegroup Fm3m (Tantalum Carbide)

27.2.2. CaC6 Crystal - Spacegroup R-3m (Calcium Graphite Intercalation)

27.2.3. Nb Crystal - Spacegroup Im3m (Niobium)

27.2.4. V3 Crystal - Spacegroup ??? (Vanadium Phase)

27.2.5. Nb3Al Crystal - Spacegroup Pm3n (Niobium Aluminide)

27.2.6. Nb3Sn Crystal - Spacegroup Pm3n (Niobium-Tin)

27.2.7. Nb3Ga Crystal - Spacegroup Pm3n (Niobium Gallide)

27.2.8. Nb3Ge Crystal - Spacegroup Pm3n (Niobium Germanide)

27.2.9. MgB2 Crystal - Spacegroup P6/mmm (Magnesium Diboride)

27.2.10. H2S Crystal - Spacegroup ??? (Hydrogen Sulfide)

27.2.11. YH6 Crystal - Spacegroup ??? (Yttrium Hexahydride)

27.2.12. LaH10 Crystal - Spacegroup ??? (Lanthanum Decahydride)

Part V.

Appendices

28. Appendix - Derivation of Self-Energies and Polarizations

28.1. Self Energy of a Diagonalized Gas with Single-Particle-Interactions

Proof 28.1 of Theorem 21.1

Computing the electronic Self-Energy

Preparations

We consider the system

$$\begin{aligned}\left(S_0 + S_{\text{int}}\right)[\psi, \overline{\psi}] &\equiv \sum_{\substack{\omega_n \in \Omega_\zeta \\ \alpha,\alpha' \in \mathscr{A}}} \overline{\psi}_\alpha(\mathrm{i}\omega_n) \left[\left(-\mathrm{i}\omega_n + \frac{\epsilon_\alpha - \mu}{\hbar} \right) \delta_{\alpha,\alpha'} + \frac{V_{\alpha\alpha'}}{\hbar} \right] \psi_{\alpha'}(\mathrm{i}\omega_n) \\ &\equiv \sum_{\substack{\omega_n \in \Omega_\zeta \\ \alpha,\alpha' \in \mathscr{A}}} \overline{\psi}_\alpha(\mathrm{i}\omega_n) \left(-\frac{1}{\hbar} \mathscr{G}^{-1}_{\alpha,\alpha'}(\mathrm{i}\omega_n) \right) \psi_{\alpha'}(\mathrm{i}\omega_n)\end{aligned}$$

and compute the self-energy using the standard-trick. We will use the following trick: Inverting the Dyson-equation with the von Neumann series on the one hand, and re-expressing the imaginary-time-Green-function with help of the field integral on the other hand, gives the two equations

$$\mathscr{G}_{\alpha,\alpha'}(\mathrm{i}\omega_n) = \sum_{n=0}^{\infty} \left[\left(\mathscr{G}_0 \cdot \Sigma \right)^n (\mathrm{i}\omega_n) \cdot \mathscr{G}_0(\mathrm{i}\omega_n) \right]_{\alpha,\alpha'} \tag{28.1}$$

$$\mathscr{G}_{\alpha,\alpha'}(\mathrm{i}\omega_n) = \frac{-1}{\hbar} \left\langle \psi_\alpha(\mathrm{i}\omega_n) \overline{\psi}_{\alpha'}(\mathrm{i}\omega_n) \right\rangle \tag{28.2}$$

The self-energy of the electronic Green-function is known to be given as the sum of all the connected irreducible diagrams of the interaction vertex

$$\Sigma(\mathrm{i}\omega_n) \equiv \sum_{j=1}^{\infty} \Sigma^{(j)}(\mathrm{i}\omega_n) = \Sigma^{(1)}(\mathrm{i}\omega_n) + \Sigma^{(2)}(\mathrm{i}\omega_n) + \dots . \tag{28.3}$$

Inserting this in the upper-equation above and keeping the first non-vanishing terms yields the sets of equations

$$\mathscr{G}_{\alpha,\alpha'}(\mathrm{i}\omega_n) = \mathscr{G}_{\substack{0\\ \alpha,\alpha'}}(\mathrm{i}\omega_n) + \left(\mathscr{G}_0 \cdot \Sigma^{(1)} \cdot \mathscr{G}_0\right)_{\alpha,\alpha'}(\mathrm{i}\omega_n) + \left(\mathscr{G}_0 \cdot \Sigma^{(2)} \cdot \mathscr{G}_0\right)_{\alpha,\alpha'}(\mathrm{i}\omega_n) + \dots \tag{28.4}$$

$$\mathscr{G}_{\alpha,\alpha'}(\mathrm{i}\omega_n) = \frac{-1}{\hbar}\left\langle \psi_\alpha(\mathrm{i}\omega_n)\overline{\psi}_{\alpha'}(\mathrm{i}\omega_n)\right\rangle \tag{28.5}$$

The lower equation can be calculated explicitly with help of the Wick-theorem, linked-cluster-theorem, and the residue-theorem, and then, by comparing the first non-vanishing coefficients with the upper-equation, we can conclude what $\Sigma^{(2)}(\mathrm{i}\omega_n)$ must be.

Fact 1: The action, corresponding to this system, is given by the equation above.

Fact 2: The electronic Green-function is written in second order perturbation-theory as

$$\mathscr{G}_{\alpha\alpha'}(\mathrm{i}\omega_n) = \mathscr{G}^{(0)}_{\alpha\alpha'}(\mathrm{i}\omega_n) + \mathscr{G}^{(1)}_{\alpha\alpha'}(\mathrm{i}\omega_n) + \mathscr{G}^{(2)}_{\alpha\alpha'}(\mathrm{i}\omega_n) + \dots$$

The First Non-Vanishing Order

We therefore calculate

$$\mathscr{G}^{(1)}_{\alpha\alpha'}(\mathrm{i}\omega_n) = \frac{-1}{\hbar}\sum_{\substack{\beta,\beta'\in\mathscr{A}\\ \omega_m\in\Omega_\zeta}} \frac{-V_{\beta\beta'}}{\hbar}\left\langle \psi_\alpha(\mathrm{i}\omega_n)\overline{\psi}_{\alpha'}(\mathrm{i}\omega_n)\overline{\psi}_{\beta}(\mathrm{i}\omega_m)\psi_{\beta'}(\mathrm{i}\omega_m)\right\rangle_0^{\mathrm{CD}} \tag{28.6}$$

where the last expectation-value contains only [C]onnected [D]iagrams (linked-cluster-theorem). We can therefore simply calculate the free correlator and discard the contributions from unconnected diagrams.

We therefore consider the correlator

$$\begin{aligned}
\left\langle \psi_\alpha(\mathrm{i}\omega_n)\overline{\psi}_{\alpha'}(\mathrm{i}\omega_n)\overline{\psi}_{\beta}(\mathrm{i}\omega_m)\psi_{\beta'}(\mathrm{i}\omega_m)\right\rangle_0 &= \left\langle \psi_\alpha(\mathrm{i}\omega_n)\psi_{\beta'}(\mathrm{i}\omega_m)\overline{\psi}_{\alpha'}(\mathrm{i}\omega_n)\overline{\psi}_{\beta}(\mathrm{i}\omega_m)\right\rangle_0 \\
&= \left\langle \psi(A_1)\psi(A_2)\overline{\psi}(B_1)\overline{\psi}(B_2)\right\rangle_0 \\
&= -\left\langle \psi(A_1)\psi(A_2)\overline{\psi}(B_2)\overline{\psi}(B_1)\right\rangle_0 \\
&= -\sum_{\pi\in \mathrm{S}_2}\mathrm{sign}(\pi)^{1-\theta(\zeta)}\prod_{l=1}^{2}\left\langle \psi(A_l)\overline{\psi}(B_{\pi(l)})\right\rangle_0 \\
&= -\hbar^2\sum_{\pi\in \mathrm{S}_2}\mathrm{sign}(\pi)^{1-\theta(\zeta)}\prod_{l=1}^{2}\mathscr{G}_0(A_l, B_{\pi(l)})
\end{aligned}$$

The electronic correlator can now be evaluated with the Wick-theorem. In order to so, we will enumerate all the permutations of the group S_3.

$$\mathrm{S}_2 = \left\{\pi_1, \pi_2\right\} = \left\{\begin{pmatrix}1 & 2\\ 1 & 2\end{pmatrix}, \begin{pmatrix}1 & 2\\ 2 & 1\end{pmatrix}\right\} \quad \text{with signatures} \quad \mathrm{sgn}(\pi_1,\pi_2) = (+1,-1). \tag{28.7}$$

The first contribution is a vacuum diagram and does not contribute to the series expansion (linked cluster theorem). We therefore focus on the second term. We note that

$$A_1 = (\alpha, \mathrm{i}\omega_n), \qquad A_2 = (\beta, \mathrm{i}\omega_m) \tag{28.8}$$

$$B_1 = (\alpha', \mathrm{i}\omega_n), \qquad B_2 = (\beta, \mathrm{i}\omega_m) \tag{28.9}$$

and therefore we obtain for the non-vacuum contribution to the Green-function

$$\mathscr{G}^{(1)}_{\alpha\alpha'}(\mathrm{i}\omega_n) = + \sum_{\beta,\beta' \in \mathscr{A}} \mathscr{G}_{0\ \alpha,\beta}(\mathrm{i}\omega_n)\, V_{\beta,\beta'}\, \mathscr{G}_{0\ \beta'\alpha'}(\mathrm{i}\omega_n)$$

comparison of coefficients gives the first-order correction to the self-energy

$$\Sigma^{(1)}_{\beta\beta'}(\mathrm{i}\omega_n) = +V_{\beta,\beta'} = \text{ „frequency-independent“} \tag{28.10}$$

28.2. Self Energy of a Diagonalized Gas with Quartic Interactions

Proof 28.2 of Theorem 21.2

Computing the electronic Self-Energy

Preparations

We consider the system

$$\begin{aligned}\left(S_0 + S_{\text{int}}\right)[\psi, \overline{\psi}] \equiv & \sum_{\substack{\omega_n \in \Omega_\zeta \\ \alpha,\alpha' \in \mathscr{A}}} \overline{\psi}_\alpha(\mathrm{i}\omega_n) \left[\left(-\mathrm{i}\omega_n + \frac{\epsilon_\alpha - \mu}{\hbar} \right) \delta_{\alpha,\alpha'} \right] \psi_{\alpha'}(\mathrm{i}\omega_n) \\ & + \frac{1}{2} \sum_{\substack{\alpha_1,\alpha_2,\alpha_3,\alpha_4 \in \mathscr{A} \\ \omega_{n_1},\omega_{n_2},\omega_{n_3},\omega_{n_4} \in \Omega_\zeta}} \frac{-V_{\alpha_1\alpha_2\alpha_3\alpha_4} \delta_{\omega_1+\omega_2,\omega_3+\omega_4}}{\hbar^2 \beta} \overline{\psi}_{\alpha_1}(\mathrm{i}\omega_1) \overline{\psi}_{\alpha_2}(\mathrm{i}\omega_2) \psi_{\alpha_3}(\mathrm{i}\omega_3) \psi_{\alpha_4}(\mathrm{i}\omega_4)\end{aligned}$$

and compute the self-energy using the standard-trick. We will use the following trick: Inverting the Dyson-equation with the von Neumann series on the one hand, and re-expressing the imaginary-time-Green-function with help of the field integral on the other hand, gives the two equations

$$\mathscr{G}_{\alpha,\alpha'}(\mathrm{i}\omega_n) = \sum_{n=0}^{\infty} \left[\left(\mathscr{G}_0 \cdot \Sigma \right)^n (\mathrm{i}\omega_n) \cdot \mathscr{G}_0(\mathrm{i}\omega_n) \right]_{\alpha,\alpha'} \tag{28.11}$$

$$\mathscr{G}_{\alpha,\alpha'}(\mathrm{i}\omega_n) = \frac{-1}{\hbar} \left\langle \psi_\alpha(\mathrm{i}\omega_n) \overline{\psi}_{\alpha'}(\mathrm{i}\omega_n) \right\rangle \tag{28.12}$$

The self-energy of the electronic Green-function is known to be given as the sum of all the connected irreducible diagrams of the interaction vertex

$$\Sigma(\mathrm{i}\omega_n) \equiv \sum_{j=1}^{\infty} \Sigma^{(j)}(\mathrm{i}\omega_n) = \Sigma^{(1)}(\mathrm{i}\omega_n) + \Sigma^{(2)}(\mathrm{i}\omega_n) + \dots . \tag{28.13}$$

Inserting this in the upper-equation above and keeping the first non-vanishing terms yields the sets of equations

$$\mathscr{G}_{\alpha,\alpha'}(\mathrm{i}\omega_n) = \mathscr{G}_{0\,\alpha,\alpha'}(\mathrm{i}\omega_n) + \left(\mathscr{G}_0 \cdot \Sigma^{(1)} \cdot \mathscr{G}_0 \right)_{\alpha,\alpha'} (\mathrm{i}\omega_n) + \left(\mathscr{G}_0 \cdot \Sigma^{(2)} \cdot \mathscr{G}_0 \right)_{\alpha,\alpha'} (\mathrm{i}\omega_n) + \dots \tag{28.14}$$

$$\mathscr{G}_{\alpha,\alpha'}(\mathrm{i}\omega_n) = \frac{-1}{\hbar} \left\langle \psi_\alpha(\mathrm{i}\omega_n) \overline{\psi}_{\alpha'}(\mathrm{i}\omega_n) \right\rangle \tag{28.15}$$

The lower equation can be calculated explicitly with help of the Wick-theorem, linked-cluster-theorem, and the residue-theorem, and then, by comparing the first non-vanishing coefficients with the upper-equation, we can conclude what $\Sigma^{(2)}(\mathrm{i}\omega_n)$ must be.

Fact 1: The action, corresponding to this system, is given by the equation above.

Fact 2: The electronic Green-function is written in second order perturbation-theory as

$$\mathscr{G}_{\alpha\alpha'}(\mathrm{i}\omega_n) = \mathscr{G}^{(0)}_{\alpha\alpha'}(\mathrm{i}\omega_n) + \mathscr{G}^{(1)}_{\alpha\alpha'}(\mathrm{i}\omega_n) + \mathscr{G}^{(2)}_{\alpha\alpha'}(\mathrm{i}\omega_n) + \dots$$

The First Non-Vanishing Order

We therefore calculate

$$\mathscr{G}^{(1)}_{\alpha\alpha'}(\mathrm{i}\omega_n) = \frac{-1}{\hbar}\frac{1}{2} \sum_{\substack{\alpha_1,\alpha_2,\alpha_3,\alpha_4 \in \mathscr{A} \\ \omega_{n_1},\omega_{n_2},\omega_{n_3},\omega_{n_4} \in \Omega_\zeta}} \frac{+V_{\alpha_1\alpha_2\alpha_3\alpha_4}\delta_{\omega_{n_1}+\omega_{n_2},\omega_{n_3}+\omega_{n_4}}}{\hbar^2\beta} \left\langle \psi_\alpha(\mathrm{i}\omega_n)\overline{\psi}_{\alpha'}(\mathrm{i}\omega_n)\overline{\psi}_{\alpha_1}(\mathrm{i}\omega_{n_1})\overline{\psi}_{\alpha_2}(\mathrm{i}\omega_{n_2})\psi_{\alpha_3}(\mathrm{i}\omega_{n_3})\psi_{\alpha_4}(\mathrm{i}\omega_{n_4})\right\rangle_0 \tag{28.16}$$

We now focus on the correlator

$$\begin{aligned}
\left\langle \psi_\alpha(\mathrm{i}\omega_n)\overline{\psi}_{\alpha'}(\mathrm{i}\omega_n)\overline{\psi}_{\alpha_1}(\mathrm{i}\omega_1)\overline{\psi}_{\alpha_2}(\mathrm{i}\omega_2)\psi_{\alpha_3}(\mathrm{i}\omega_3)\psi_{\alpha_4}(\mathrm{i}\omega_4)\right\rangle_0 &= \left\langle \psi_\alpha(\mathrm{i}\omega_n)\psi_{\alpha_3}(\mathrm{i}\omega_3)\psi_{\alpha_4}(\mathrm{i}\omega_4)\overline{\psi}_{\alpha'}(\mathrm{i}\omega_n)\overline{\psi}_{\alpha_1}(\mathrm{i}\omega_1)\overline{\psi}_{\alpha_2}(\mathrm{i}\omega_2)\right\rangle_0 \\
&= \left\langle \psi(A_1)\psi(A_2)\psi(A_3)\overline{\psi}(B_1)\overline{\psi}(B_2)\overline{\psi}(B_3)\right\rangle_0 \\
&= -\left\langle \psi(A_1)\psi(A_2)\psi(A_3)\overline{\psi}(B_3)\overline{\psi}(B_2)\overline{\psi}(B_1)\right\rangle_0 \\
&= -\sum_{\pi\in \mathrm{S}_3} \mathrm{sign}(\pi)^{1-\theta(\zeta)} \prod_{l=1}^{3} \left\langle \psi(A_l)\overline{\psi}(B_{\pi(l)})\right\rangle_0 \\
&= +\hbar^3 \sum_{\pi\in \mathrm{S}_3} \mathrm{sign}(\pi)^{1-\theta(\zeta)} \prod_{l=1}^{3} \mathscr{G}_0(A_l, B_{\pi(l)})
\end{aligned}$$

The electronic correlator can now be evaluated with the Wick-theorem. In order to so, we will enumerate all the permutations of the group S_3.

$$\begin{aligned}
\mathrm{S}_3 &= \left\{\pi_1,\pi_2,\pi_3,\pi_4,\pi_5,\pi_6\right\} \\
&= \left\{ \begin{pmatrix}1&2&3\\1&2&3\end{pmatrix}, \begin{pmatrix}1&2&3\\1&3&2\end{pmatrix}, \begin{pmatrix}1&2&3\\2&1&3\end{pmatrix}, \begin{pmatrix}1&2&3\\2&3&1\end{pmatrix}, \begin{pmatrix}1&2&3\\3&1&2\end{pmatrix}, \begin{pmatrix}1&2&3\\3&2&1\end{pmatrix} \right\}
\end{aligned}$$

with signatures

$$\mathrm{sgn}(\pi_1,\pi_2,\pi_3,\pi_4,\pi_5,\pi_6) = (+1,-1,-1,+1,+1,-1)$$

Facts:

- The contributions from π_1 and π_2 are vacuum diagrams (which cancel out due to the linked-cluster-theorem)
- The contributions from π_3 and π_6 are "Baloon"-diagrams / "Hartree"-diagrams.
- The contributions from π_4 and π_5 are "Sunset"-diagrams / "Fock"-diagrams.

We note that

$$\begin{aligned}
A_1 &= (\alpha, \mathrm{i}\omega_n), \qquad A_2 = (\alpha_3, \mathrm{i}\omega_{n_3}), \qquad A_3 = (\alpha_4, \mathrm{i}\omega_{n_4}) \\
B_1 &= (\alpha', \mathrm{i}\omega_n), \qquad B_2 = (\alpha_1, \mathrm{i}\omega_{n_1}), \qquad B_3 = (\alpha_2, \mathrm{i}\omega_{n_2})
\end{aligned}$$

and therefore we obtain

$$
\begin{aligned}
&B_{\pi_3(1)} \equiv B_2 \equiv (\alpha_1, \mathrm{i}\omega_{n_1}), \quad B_{\pi_3(2)} \equiv B_1 \equiv (\alpha', \mathrm{i}\omega_n), \quad B_{\pi_3(3)} \equiv B_3 \equiv (\alpha_2, \mathrm{i}\omega_{n_2}),\\
&B_{\pi_5(1)} \equiv B_3 \equiv (\alpha_2, \mathrm{i}\omega_{n_2}), \quad B_{\pi_5(2)} \equiv B_1 \equiv (\alpha', \mathrm{i}\omega_n), \quad B_{\pi_5(3)} \equiv B_2 \equiv (\alpha_1, \mathrm{i}\omega_{n_1}),\\
&B_{\pi_6(1)} \equiv B_3 \equiv (\alpha_2, \mathrm{i}\omega_{n_2}), \quad B_{\pi_6(2)} \equiv B_2 \equiv (\alpha_1, \mathrm{i}\omega_{n_1}), \quad B_{\pi_6(3)} \equiv B_1 \equiv (\alpha', \mathrm{i}\omega_n),\\
&B_{\pi_4(1)} \equiv B_2 \equiv (\alpha_1, \mathrm{i}\omega_{n_1}), \quad B_{\pi_4(2)} \equiv B_3 \equiv (\alpha_2, \mathrm{i}\omega_{n_2}), \quad B_{\pi_4(3)} \equiv B_1 \equiv (\alpha', \mathrm{i}\omega_n).
\end{aligned}
$$

Baloon-Diagrams

π_3:

This gives then for the first order correction of the Green-function

$$
\begin{aligned}
\mathscr{G}^{\pi_3}_{\alpha\alpha'}(\mathrm{i}\omega_n) &= +\frac{1}{2} \sum_{\substack{\alpha_1,\alpha_2,\alpha_3,\alpha_4 \in \mathscr{A} \\ \omega_{n_1},\omega_{n_2},\omega_{n_3},\omega_{n_4} \in \Omega_\zeta}} \frac{1}{\beta} V_{\alpha_1\alpha_2\alpha_3\alpha_4} \delta_{\omega_{n_1}+\omega_{n_2},\omega_{n_3}+\omega_{n_4}} \mathscr{G}^{\ 0}_{\alpha,\alpha_1}(\mathrm{i}\omega_n) \delta_{\omega_n,\omega_{n_1}} \mathscr{G}^{\ 0}_{\alpha_3\alpha'}(\mathrm{i}\omega_n) \delta_{\omega_{n_3},\omega_n} \mathscr{G}^{\ 0}_{\alpha_4\alpha_2}(\mathrm{i}\omega_{n_2}) \delta_{\omega_{n_2},\omega_{n_4}} \\
&= +\frac{1}{2} \sum_{\substack{\alpha_1,\alpha_2,\alpha_3,\alpha_4 \in \mathscr{A} \\ \omega_{n_1},\omega_{n_2},\omega_{n_3},\omega_{n_4} \in \Omega_\zeta}} \mathscr{G}^{\ 0}_{\alpha,\alpha_1}(\mathrm{i}\omega_n) \delta_{\omega_n,\omega_{n_1}} \frac{1}{\beta} V_{\alpha_1\alpha_2\alpha_3\alpha_4} \delta_{\omega_{n_1}+\omega_{n_2},\omega_{n_3}+\omega_{n_4}} \mathscr{G}^{\ 0}_{\alpha_4\alpha_2}(\mathrm{i}\omega_{n_2}) \delta_{\omega_{n_2},\omega_{n_4}} \mathscr{G}^{\ 0}_{\alpha_3\alpha'}(\mathrm{i}\omega_n) \delta_{\omega_{n_3},\omega_n} \\
&= +\frac{1}{2} \sum_{\substack{\alpha_1,\alpha_2,\alpha_3,\alpha_4 \in \mathscr{A} \\ \omega_{n_1},\omega_{n_2} \in \Omega_\zeta}} \mathscr{G}^{\ 0}_{\alpha,\alpha_1}(\mathrm{i}\omega_n) \delta_{\omega_n,\omega_{n_1}} \frac{1}{\beta} V_{\alpha_1\alpha_2\alpha_3\alpha_4} \delta_{\omega_{n_1}+\omega_{n_2},\omega_n+\omega_{n_2}} \mathscr{G}^{\ 0}_{\alpha_4\alpha_2}(\mathrm{i}\omega_{n_2}) \mathscr{G}^{\ 0}_{\alpha_3\alpha'}(\mathrm{i}\omega_n) \\
&= +\frac{1}{2} \sum_{\substack{\alpha_1,\alpha_2,\alpha_3,\alpha_4 \in \mathscr{A} \\ \omega_{n_2} \in \Omega_\zeta}} \mathscr{G}^{\ 0}_{\alpha,\alpha_1}(\mathrm{i}\omega_n) \frac{1}{\beta} V_{\alpha_1\alpha_2\alpha_3\alpha_4} \mathscr{G}^{\ 0}_{\alpha_4\alpha_2}(\mathrm{i}\omega_{n_2}) \mathscr{G}^{\ 0}_{\alpha_3\alpha'}(\mathrm{i}\omega_n)
\end{aligned}
$$

From this we can read off the self-energy

$$
\Sigma^{\pi_3}_{\alpha_1\alpha_3}(\mathrm{i}\omega_n) = +\frac{1}{2} \sum_{\substack{\alpha_2 \in \mathscr{A} \\ \omega_{n_2} \in \Omega_\zeta}} \frac{1}{\beta} V_{\alpha_1\alpha_2\alpha_3\alpha_2} \mathscr{G}^{\ 0}_{\alpha_2\alpha_2}(\mathrm{i}\omega_{n_2}) = +\frac{1}{2} \sum_{\alpha_2 \in \mathscr{A}} V_{\alpha_1\alpha_2\alpha_3\alpha_2} \mathrm{F}_{\hbar\beta}(\epsilon_{\alpha_2} - \mu) = -\zeta \frac{1}{2} \sum_{\alpha_2 \in \mathscr{A}} V_{\alpha_1\alpha_2\alpha_3\alpha_2} \mathrm{n}^{\zeta}_{\hbar\beta}(\epsilon_{\alpha_2} - \mu) \tag{28.17}
$$

π_6:

This gives then for the first order correction of the Green-function

$$
\begin{aligned}
\mathscr{G}^{\pi_6}_{\alpha\alpha'}(\mathrm{i}\omega_n) &= +\frac{1}{2} \sum_{\substack{\alpha_1,\alpha_2,\alpha_3,\alpha_4 \in \mathscr{A} \\ \omega_{n_1},\omega_{n_2},\omega_{n_3},\omega_{n_4} \in \Omega_\zeta}} \frac{1}{\beta} V_{\alpha_1\alpha_2\alpha_3\alpha_4} \delta_{\omega_{n_1}+\omega_{n_2},\omega_{n_3}+\omega_{n_4}} \mathscr{G}^{\ 0}_{\alpha,\alpha_2}(\mathrm{i}\omega_n) \delta_{\omega_n,\omega_{n_2}} \mathscr{G}^{\ 0}_{\alpha_3,\alpha_1}(\mathrm{i}\omega_{n_3}) \delta_{\omega_{n_3},\omega_{n_1}} \mathscr{G}^{\ 0}_{\alpha_4,\alpha'}(\mathrm{i}\omega_n) \delta_{\omega_{n_4},\omega_n} \\
&= +\frac{1}{2} \sum_{\substack{\alpha_1,\alpha_2,\alpha_3,\alpha_4 \in \mathscr{A} \\ \omega_{n_3} \in \Omega_\zeta}} \frac{1}{\beta} V_{\alpha_1\alpha_2\alpha_3\alpha_4} \delta_{\omega_{n_3}+\omega_n,\omega_{n_3}+\omega_n} \mathscr{G}^{\ 0}_{\alpha,\alpha_2}(\mathrm{i}\omega_n) \mathscr{G}^{\ 0}_{\alpha_3\alpha_1}(\mathrm{i}\omega_{n_3}) \mathscr{G}^{\ 0}_{\alpha_4\alpha'}(\mathrm{i}\omega_n)
\end{aligned}
$$

From this we can read off the self-energy

$$\Sigma^{\pi_6}_{\alpha_2\alpha_4}(\mathrm{i}\omega_n) = +\frac{1}{2}\sum_{\substack{\alpha_3\in\mathscr{A}\\ \omega_{n_3}\in\Omega_\zeta}} \frac{1}{\beta} V_{\alpha_3\alpha_2\alpha_3\alpha_4}\, \mathscr{G}^{\ 0}_{\alpha_3\alpha_3}(\mathrm{i}\omega_{n_3}) = +\frac{1}{2}\sum_{\alpha_3\in\mathscr{A}} V_{\alpha_3\alpha_2\alpha_3\alpha_4}\, \mathrm{F}_{\hbar\beta}(\epsilon_{\alpha_3}-\mu) = -\zeta\frac{1}{2}\sum_{\alpha_3\in\mathscr{A}} V_{\alpha_3\alpha_2\alpha_3\alpha_4}\, \mathrm{n}^{\zeta}_{\hbar\beta}(\epsilon_{\alpha_3}-\mu) \tag{28.18}$$

$\underline{\pi_4}$**:**

This gives then for the first order correction of the Green-function

$$\begin{aligned}\mathscr{G}^{\pi_4}_{\alpha\alpha'}(\mathrm{i}\omega_n) &= -\frac{1}{2}\sum_{\substack{\alpha_1,\alpha_2,\alpha_3,\alpha_4\in\mathscr{A}\\ \omega_{n_1},\omega_{n_2},\omega_{n_3},\omega_{n_4}\in\Omega_\zeta}} \frac{1}{\beta} V_{\alpha_1\alpha_2\alpha_3\alpha_4}\delta_{\omega_{n_1}+\omega_{n_2},\omega_{n_3}+\omega_{n_4}}\mathscr{G}^{\ 0}_{\alpha,\alpha_1}(\mathrm{i}\omega_n)\delta_{\omega_n,\omega_{n_1}}\mathscr{G}^{\ 0}_{\alpha_3\alpha_2}(\mathrm{i}\omega_{n_3})\delta_{\omega_{n_3},\omega_{n_2}}\mathscr{G}^{\ 0}_{\alpha_4\alpha'}(\mathrm{i}\omega_n)\delta_{\omega_{n_4},\omega_n}\\ &= -\frac{1}{2}\sum_{\substack{\alpha_1,\alpha_2,\alpha_3,\alpha_4\in\mathscr{A}\\ \omega_{n_3}\in\Omega_\zeta}} \frac{1}{\beta} V_{\alpha_1\alpha_2\alpha_3\alpha_4}\delta_{\omega_n+\omega_{n_3},\omega_{n_3}+\omega_n}\mathscr{G}^{\ 0}_{\alpha,\alpha_1}(\mathrm{i}\omega_n)\mathscr{G}^{\ 0}_{\alpha_3,\alpha_2}(\mathrm{i}\omega_{n_3})\mathscr{G}^{\ 0}_{\alpha_4,\alpha'}(\mathrm{i}\omega_n)\end{aligned}$$

From this we can read off the self-energy

$$\Sigma^{\pi_4}_{\alpha_1\alpha_4}(\mathrm{i}\omega_n) = -\frac{1}{2}\sum_{\substack{\alpha_3\in\mathscr{A}\\ \omega_{n_3}\in\Omega_\zeta}} \frac{1}{\beta} V_{\alpha_1\alpha_3\alpha_3\alpha_4}\, \mathscr{G}^{\ 0}_{\alpha_3\alpha_3}(\mathrm{i}\omega_{n_3}) = -\frac{1}{2}\sum_{\alpha_3\in\mathscr{A}} V_{\alpha_1\alpha_3\alpha_3\alpha_4}\, \mathrm{F}_{\hbar\beta}(\epsilon_{\alpha_3}-\mu) = +\zeta\frac{1}{2}\sum_{\alpha_3\in\mathscr{A}} V_{\alpha_1\alpha_3\alpha_3\alpha_4}\, \mathrm{n}^{\zeta}_{\hbar\beta}(\epsilon_{\alpha_3}-\mu) \tag{28.19}$$

$\underline{\pi_5}$**:**

This gives then for the first order correction of the Green-function

$$\begin{aligned}\mathscr{G}^{\pi_5}_{\alpha\alpha'}(\mathrm{i}\omega_n) &= -\frac{1}{2}\sum_{\substack{\alpha_1,\alpha_2,\alpha_3,\alpha_4\in\mathscr{A}\\ \omega_{n_1},\omega_{n_2},\omega_{n_3},\omega_{n_4}\in\Omega_\zeta}} \frac{1}{\beta} V_{\alpha_1\alpha_2\alpha_3\alpha_4}\delta_{\omega_{n_1}+\omega_{n_2},\omega_{n_3}+\omega_{n_4}}\mathscr{G}^{\ 0}_{\alpha,\alpha_2}(\mathrm{i}\omega_n)\delta_{\omega_n,\omega_{n_2}}\mathscr{G}^{\ 0}_{\alpha_3\alpha'}(\mathrm{i}\omega_n)\delta_{\omega_{n_3},\omega_n}\mathscr{G}^{\ 0}_{\alpha_4\alpha_1}(\mathrm{i}\omega_{n_4})\delta_{\omega_{n_4},\omega_{n_1}}\\ &= -\frac{1}{2}\sum_{\substack{\alpha_1,\alpha_2,\alpha_3,\alpha_4\in\mathscr{A}\\ \omega_{n_4}\in\Omega_\zeta}} \frac{1}{\beta} V_{\alpha_1\alpha_2\alpha_3\alpha_4}\delta_{\omega_{n_4}+\omega_n,\omega_n+\omega_{n_4}}\mathscr{G}^{\ 0}_{\alpha,\alpha_2}(\mathrm{i}\omega_n)\mathscr{G}^{\ 0}_{\alpha_4\alpha_1}(\mathrm{i}\omega_{n_4})\mathscr{G}^{\ 0}_{\alpha_3\alpha'}(\mathrm{i}\omega_n)\end{aligned}$$

From this we can read off the self-energy

$$\Sigma^{\pi_5}_{\alpha_2\alpha_3}(\mathrm{i}\omega_n) = -\frac{1}{2}\sum_{\substack{\alpha_4\in\mathscr{A}\\ \omega_{n_4}\in\Omega_\zeta}} \frac{1}{\beta} V_{\alpha_4\alpha_3\alpha_3\alpha_4}\, \mathscr{G}^{\ 0}_{\alpha_4\alpha_4}(\mathrm{i}\omega_{n_4}) = -\frac{1}{2}\sum_{\alpha_3\in\mathscr{A}} V_{\alpha_4\alpha_3\alpha_3\alpha_4}\, \mathrm{F}_{\hbar\beta}(\epsilon_{\alpha_4}-\mu) = +\zeta\frac{1}{2}\sum_{\alpha_3\in\mathscr{A}} V_{\alpha_4\alpha_3\alpha_3\alpha_4}\, \mathrm{n}^{\zeta}_{\hbar\beta}(\epsilon_{\alpha_4}-\mu) \tag{28.20}$$

28.3. Self Energy of a Spin-Independent-Interaction between an Electron-Gas and a Phonon-Gas

Proof 28.3 of Theorem 21.3

Notice first, that going over to the field-integral-description of the problem gives the action

$$\begin{aligned} S[\chi,\overline{\chi}] = & \quad S_{\text{el}}[\psi,\overline{\psi}] \quad + \quad S_{\text{ph}}[\phi,\overline{\phi}] \quad + S_{\text{el-ph-int}}[\chi,\overline{\chi}] \\ = & \sum\!\!\!\!\!\!\int \overline{\psi}_{m\mathbf{k}\sigma}(\tau)\left(\partial_\tau + \frac{\epsilon_{m\mathbf{k}\sigma}-\mu}{\hbar}\right)\psi_{m\mathbf{k}\sigma}(\tau) + \sum\!\!\!\!\!\!\int \overline{\phi}_{\mathbf{q}\nu}(\tau)\left(\partial_\tau+\omega_{\mathbf{q},\nu}\right)\phi_{\mathbf{q}\nu}(\tau) + S_{\text{el-ph-int}}[\chi,\overline{\chi}] \end{aligned}$$

with interaction-term

$$S_{\text{el-ph-int}}[\chi,\overline{\chi}] = \sum\!\!\!\!\!\!\int \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\hbar\sqrt{N_p}}\left(\phi_{\mathbf{q}\nu}(\tau)+\overline{\phi}_{-\mathbf{q}\nu}(\tau)\right)\overline{\psi}_{\mathbf{k}+\mathbf{q}m\sigma}(\tau)\psi_{\mathbf{k}n\sigma}(\tau)$$

We will now determine the self-energy of the electronic system.

We will use the following trick: Inverting the Dyson-equation with the von Neumann series on the one hand, and re-expressing the imaginary-time-Green-function with help of the field integral on the other hand, gives the two equations

$$\mathscr{G}_{\alpha,\alpha'}(\mathrm{i}\omega_n) = \sum_{n=0}^{\infty}\left[\left(\mathscr{G}_0\cdot\Sigma\right)^n(\mathrm{i}\omega_n)\cdot\mathscr{G}_0(\mathrm{i}\omega_n)\right]_{\alpha,\alpha'} \tag{28.21}$$

$$\mathscr{G}_{\alpha,\alpha'}(\mathrm{i}\omega_n) = \int_0^{\hbar\beta}\mathrm{d}\tau\,\mathrm{e}^{\mathrm{i}\omega_n\tau}\,\mathscr{G}_{\alpha,\alpha'}(\tau) = \frac{-1}{\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau\,\mathrm{e}^{\mathrm{i}\omega_n\tau}\,\langle\psi_\alpha(\tau)\overline{\psi}_{\alpha'}(0)\rangle \tag{28.22}$$

The self-energy of the electronic Green-function is known to be given as the sum of all the connected irreducible diagrams of the interaction

$$\Sigma(\mathrm{i}\omega_n) = \sum_{j=0}^{\infty}\Sigma^{(j)}(\mathrm{i}\omega_n) \approx 0 + \Sigma^{(2)}(\mathrm{i}\omega_n) + 0 + \mathcal{O}(\mathrm{V}^4), \tag{28.23}$$

whereas the first contribution will turn out to vanish since the interaction can be expanded as a sum of monomials of creation- and annihilation-operators with uneven degree. Inserting this in the upper-equation above and keeping the first non-vanishing terms yields the sets of equations

$$\mathscr{G}_{\alpha,\alpha'}(\mathrm{i}\omega_n) = \mathscr{G}_{\underset{\alpha,\alpha'}{0}}(\mathrm{i}\omega_n) + \left(\mathscr{G}_0\cdot\Sigma^{(2)}\cdot\mathscr{G}_0\right)_{\alpha,\alpha'}(\mathrm{i}\omega_n) \tag{28.24}$$

$$\mathscr{G}_{\alpha,\alpha'}(\mathrm{i}\omega_n) = \frac{-1}{\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau\,\mathrm{e}^{\mathrm{i}\omega_n\tau}\,\langle\psi_\alpha(\tau)\overline{\psi}_{\alpha'}(0)\rangle \tag{28.25}$$

The lower equation can be calculated explicitly with help of the Wick-theorem, linked-cluster-theorem, and the residue-theorem, and then, by comparing the first non-vanishing coefficients with the upper-equation, we can conclude what $\Sigma^{(2)}(i\omega_n)$ must be.

Fact 1: The action, corresponding to this system, is given by the equation above.

Fact 2: The electronic Green-function is written in second order perturbation-theory as

$$\begin{aligned}\underset{\substack{\mathbf{p},\mathbf{p}'\\ \sigma,\sigma'}}{\mathscr{G}_{b,b'}}(\tau) &= \underset{\substack{\mathbf{p},\mathbf{p}'\\ \sigma,\sigma'}}{\mathscr{G}^{(0)}_{b,b'}}(\tau) + \underset{\substack{\mathbf{p},\mathbf{p}'\\ \sigma,\sigma'}}{\mathscr{G}^{(1)}_{b,b'}}(\tau) + \underset{\substack{\mathbf{p},\mathbf{p}'\\ \sigma,\sigma'}}{\mathscr{G}^{(2)}_{b,b'}}(\tau) + \dots \\ &= \underset{\substack{\mathbf{p},\mathbf{p}'\\ \sigma,\sigma'}}{\mathscr{G}_{0\,b,b'}}(\tau) + \quad 0 \quad + \underset{\substack{\mathbf{p},\mathbf{p}'\\ \sigma,\sigma'}}{\mathscr{G}^{(2)}_{b,b'}}(\tau) + \dots\end{aligned}$$

The second contribution reads

$$\begin{aligned}&\underset{\substack{\mathbf{p},\mathbf{p}'\\ \sigma,\sigma'}}{\mathscr{G}^{(2)}_{b,b'}}(\tau) \\ &= \frac{1}{2!}\oint_{\substack{\tau_1,\tau_2\in[0,\hbar\beta]\\ \mu,\mu'\in\{\downarrow,\uparrow\}\\ \mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}'\in Q\\ m,m',n,n'\in\{1,2,\dots\}\\ \nu,\nu'\in\{1,2,\dots,rd\}}} \frac{-1}{\hbar}\frac{g_{mn\nu}(\mathbf{k},\mathbf{q})g_{m'n'\nu'}(\mathbf{k}',\mathbf{q}')}{\hbar^2 N_p}\langle\psi_{\mathbf{p}b\sigma}(\tau)\overline{\psi}_{\mathbf{p}'b'\sigma'}(0)\left(\phi_{\mathbf{q}\nu}(\tau_1)+\overline{\phi}_{-\mathbf{q}\nu}(\tau_1)\right)\overline{\psi}_{\mathbf{k}+\mathbf{q}m\mu}(\tau_1)\psi_{\mathbf{k}n\mu}(\tau_1)\left(\phi_{\mathbf{q}'\nu'}(\tau_2)+\overline{\phi}_{-\mathbf{q}'\nu'}(\tau_2)\right)\overline{\psi}_{\mathbf{k}'+\mathbf{q}'m'\mu'}(\tau_2)\psi_{\mathbf{k}'n'\mu'}(\tau_2)\rangle_0^{\mathrm{CD}}\end{aligned} \tag{28.26}$$

where only [C]onnected [D]iagrams are summed over (linked cluster theorem). We can therefore simply sum over all diagrams and discard the disconnected diagrams.

Fact 3: The correlator in it's decomposition into it's fermionic and bosonic component reads

$$\begin{aligned}&\frac{-1}{\hbar}\langle\psi_{\mathbf{p}b\sigma}(\tau)\overline{\psi}_{\mathbf{p}'b'\sigma'}(0)\left(\phi_{\mathbf{q}\nu}(\tau_1)+\overline{\phi}_{-\mathbf{q}\nu}(\tau_1)\right)\overline{\psi}_{\mathbf{k}+\mathbf{q}m\mu}(\tau_1)\psi_{\mathbf{k}n\mu}(\tau_1)\left(\phi_{\mathbf{q}'\nu'}(\tau_2)+\overline{\phi}_{-\mathbf{q}'\nu'}(\tau_2)\right)\overline{\psi}_{\mathbf{k}'+\mathbf{q}'m'\mu'}(\tau_2)\psi_{\mathbf{k}'n'\mu'}(\tau_2)\rangle_0^{\mathrm{CD}} \\ &= \frac{-1}{\hbar}\langle\psi_{\mathbf{p}b\sigma}(\tau)\overline{\psi}_{\mathbf{p}'b'\sigma'}(0)\overline{\psi}_{\mathbf{k}+\mathbf{q}m\mu}(\tau_1)\psi_{\mathbf{k}n\mu}(\tau_1)\overline{\psi}_{\mathbf{k}'+\mathbf{q}'m'\mu'}(\tau_2)\psi_{\mathbf{k}'n'\mu'}(\tau_2)\rangle_0^{\mathrm{CD}}\langle\left(\phi_{\mathbf{q}\nu}(\tau_1)+\overline{\phi}_{-\mathbf{q}\nu}(\tau_1)\right)\left(\phi_{\mathbf{q}'\nu'}(\tau_2)+\overline{\phi}_{-\mathbf{q}'\nu'}(\tau_2)\right)\rangle_0^{\mathrm{CD}} \\ &= -\langle\psi_{\mathbf{p}b\sigma}(\tau)\psi_{\mathbf{k}n\mu}(\tau_1)\psi_{\mathbf{k}'n'\mu'}(\tau_2)\overline{\psi}_{\mathbf{p}'b'\sigma'}(0)\overline{\psi}_{\mathbf{k}+\mathbf{q}m\mu}(\tau_1)\overline{\psi}_{\mathbf{k}'+\mathbf{q}'m'\mu'}(\tau_2)\rangle_0^{\mathrm{CD}}\cdot\underset{\substack{\mathbf{q},-\mathbf{q}'\\ \nu,\nu'}}{\mathscr{D}_0}(\tau_1-\tau_2)\end{aligned} \tag{28.27}$$

The electronic correlator can now be evaluated with the Wick-theorem. In order to so, we will enumerate all the permutations of the group S_3.

$$\begin{aligned}S_3 &= \left\{\pi_1,\pi_2,\pi_3,\pi_4,\pi_5,\pi_6\right\} \\ &= \left\{\begin{pmatrix}1&2&3\\1&2&3\end{pmatrix},\begin{pmatrix}1&2&3\\1&3&2\end{pmatrix},\begin{pmatrix}1&2&3\\2&1&3\end{pmatrix},\begin{pmatrix}1&2&3\\2&3&1\end{pmatrix},\begin{pmatrix}1&2&3\\3&1&2\end{pmatrix},\begin{pmatrix}1&2&3\\3&2&1\end{pmatrix}\right\}\end{aligned}$$

with signatures

$$\mathrm{sgn}(\pi_1,\pi_2,\pi_3,\pi_4,\pi_5,\pi_6) = (+1,-1,-1,+1,+1,-1)$$

Now we write

$$
\begin{aligned}
&- \langle \psi_{\mathbf{p}b\sigma}(\tau)\psi_{\mathbf{k}n\mu}(\tau_1)\psi_{\mathbf{k}'n'\mu'}(\tau_2)\overline{\psi}_{\mathbf{p}'b'\sigma'}(0)\overline{\psi}_{\mathbf{k}+\mathbf{q}m\mu}(\tau_1)\overline{\psi}_{\mathbf{k}'+\mathbf{q}'m'\mu'}(\tau_2)\rangle_0^{\mathrm{CD}} \\
&\equiv -\langle \psi(A_1)\psi(A_2)\psi(A_3)\overline{\psi}(B_1)\overline{\psi}(B_2)\overline{\psi}(B_3)\rangle_0 \\
&\equiv +\langle \psi(A_1)\psi(A_2)\psi(A_3)\overline{\psi}(B_3)\overline{\psi}(B_2)\overline{\psi}(B_1)\rangle_0 \\
&= +\sum_{\pi\in \mathrm{S}_3} \mathrm{sgn}(\pi)\prod_{l=1}^{3}\langle \psi(A_l)\,\overline{\psi}(B_{\pi(l)})\rangle_0 \\
&= -\hbar^3 \sum_{\pi\in \mathrm{S}_3} \mathrm{sgn}(\pi)\prod_{l=1}^{3}\mathscr{G}_0(A_l, B_{\pi(l)})
\end{aligned}
$$

Facts:

- The contributions from π_1 and π_2 are vacuum diagrams (which cancel out due to the linked-cluster-theorem)
- The contributions from π_3 and π_6 are "Baloon"-diagrams / "Hartree"-diagrams.
- The contributions from π_4 and π_5 are "Sunset"-diagrams / "Fock"-diagrams.

Note that the two Hartree- and Fock-terms don't cancel out, but contribute equally to the series expansion (respectively) which cancels out the prefactor of $1/2!$ from the Taylor-expansion.

We note that

$$
\begin{aligned}
A_1 &= (\mathbf{p}, b, \sigma, \tau), \qquad & A_2 &= (\mathbf{k}, n, \mu, \tau_1), \qquad & A_3 &= (\mathbf{k}', n', \mu', \tau_2) \\
B_1 &= (\mathbf{p}', b', \sigma', 0), \qquad & B_2 &= (\mathbf{k}+\mathbf{q}, m, \mu, \tau_1), \qquad & B_3 &= (\mathbf{k}'+\mathbf{q}', m', \mu', \tau_2)
\end{aligned}
$$

and therefore we obtain

$$
\begin{aligned}
&B_{\pi_3(1)} \equiv B_2 \equiv (\mathbf{q}+\mathbf{k}, m, \mu, \tau_1), \quad B_{\pi_3(2)} \equiv B_1 \equiv (\mathbf{p}', b', \sigma', 0), \quad B_{\pi_3(3)} \equiv B_3 \equiv (\mathbf{k}'+\mathbf{q}', m', \mu', \tau_2), \\
&B_{\pi_4(1)} \equiv B_2 \equiv (\mathbf{k}+\mathbf{q}, m, \mu, \tau_1), \quad B_{\pi_4(2)} \equiv B_3 \equiv (\mathbf{k}'+\mathbf{q}', m', \mu', \tau_2), \quad B_{\pi_4(3)} \equiv B_1 \equiv (\mathbf{p}', b', \sigma', 0).
\end{aligned}
$$

This gives now for the second-order-contribution

$$
\begin{aligned}
\mathscr{G}^{(2)}_{\substack{b,b'\\ \mathbf{p},\mathbf{p}'\\ \sigma,\sigma'}}(\tau) &= -\hbar \iint_{\substack{\tau_1,\tau_2\in[0,\hbar\beta]\\ \mu,\mu'\in\{\downarrow,\uparrow\}\\ \mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}'\in \mathrm{Q}\\ m,m',n,n'\in\{1,2,\dots\}\\ \nu,\nu'\in\{1,2,\dots,rd\}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})g_{m'n'\nu'}(\mathbf{k}',\mathbf{q}')}{N_p}\,\mathscr{D}_{\substack{0\\ \mathbf{q},-\mathbf{q}'\\ \nu,\nu'}}(\tau_1-\tau_2)\sum_{\pi\in\{\pi_3,\pi_4\}}\mathrm{sgn}(\pi)\prod_{l=1}^{3}\mathscr{G}_0(A_l, B_{\pi(l)}) \\
&= \hbar \iint_{\substack{\tau_1,\tau_2\in[0,\hbar\beta]\\ \mu,\mu'\in\{\downarrow,\uparrow\}\\ \mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}'\in \mathrm{Q}\\ m,m',n,n'\in\{1,2,\dots\}\\ \nu,\nu'\in\{1,2,\dots,rd\}}} +\frac{g_{mn\nu}(\mathbf{k},\mathbf{q})g_{m'n'\nu'}(\mathbf{k}',\mathbf{q}')}{N_p}\,\mathscr{G}_{\substack{0\\ \mathbf{p},\mathbf{k}+\mathbf{q}\\ b,m\\ \sigma,\mu}}(\tau-\tau_1)\mathscr{G}_{\substack{0\\ \mathbf{k},\mathbf{p}'\\ n,b'\\ \mu,\sigma'}}(\tau_1-0)\mathscr{G}_{\substack{0\\ \mathbf{k}',\mathbf{k}'+\mathbf{q}'\\ n',m'\\ \mu',\mu'}}(0)\,\mathscr{D}_{\substack{0\\ \mathbf{q},-\mathbf{q}'\\ \nu,\nu'}}(\tau_1-\tau_2) \\
&+ \hbar \iint_{\substack{\tau_1,\tau_2\in[0,\hbar\beta]\\ \mu,\mu'\in\{\downarrow,\uparrow\}\\ \mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}'\in \mathrm{Q}\\ m,m',n,n'\in\{1,2,\dots\}\\ \nu,\nu'\in\{1,2,\dots,rd\}}} -\frac{g_{mn\nu}(\mathbf{k},\mathbf{q})g_{m'n'\nu'}(\mathbf{k}',\mathbf{q}')}{N_p}\,\mathscr{G}_{\substack{0\\ \mathbf{p},\mathbf{k}+\mathbf{q}\\ b,m\\ \sigma,\mu}}(\tau-\tau_1)\mathscr{G}_{\substack{0\\ \mathbf{k},\mathbf{k}'+\mathbf{q}'\\ n,m'\\ \mu,\mu'}}(\tau_1-\tau_2)\mathscr{G}_{\substack{0\\ \mathbf{k}',\mathbf{p}'\\ n',b'\\ \mu',\sigma'}}(\tau_2-0)\,\mathscr{D}_{\substack{0\\ \mathbf{q},-\mathbf{q}'\\ \nu,\nu'}}(\tau_1-\tau_2)
\end{aligned}
$$

$$\equiv \mathscr{G}^{\text{Hartree}}_{\substack{b,b' \\ \mathbf{p},\mathbf{p}' \\ \sigma,\sigma'}}(\tau) \quad + \quad \mathscr{G}^{\text{Fock}}_{\substack{b,b' \\ \mathbf{p},\mathbf{p}' \\ \sigma,\sigma'}}(\tau)$$

In order to compute the self-energy, we compute the Fourier-Matsubara-transform of these functions. We therefore determine $\mathscr{G}(\mathrm{i}\omega_n)$.

Fourier-Matsubara-Component of the Hartree-Contribution

Lemma 28.1 It holds

$$\mathscr{G}^{\text{Hartree}}_{\sigma,\sigma'}(\mathrm{i}\omega_n) = \sum_{\substack{\mu,\mu' \in \{\downarrow,\uparrow\} \\ \mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}' \in \mathrm{Q} \\ m,m',n,n' \in \{1,2,\dots\} \\ \nu,\nu' \in \{1,2,\dots,rd\}}} \mathscr{G}_{\substack{0 \\ \mathbf{p},\mathbf{k}+\mathbf{q} \\ b,m \\ \sigma,\mu}}(\mathrm{i}\omega_n) \left(\frac{1}{\beta} \sum_{\omega_m \in \Omega_{-1}} + \frac{g_{mn\nu}(\mathbf{k},\mathbf{q}) g_{m'n'\nu'}(\mathbf{k}',\mathbf{q}')}{N_p} \mathscr{G}_{\substack{0 \\ \mathbf{k}',\mathbf{k}'+\mathbf{q}' \\ n',m' \\ \mu',\mu'}}(\mathrm{i}\omega_m) \mathscr{D}_{\substack{0 \\ \mathbf{q},-\mathbf{q}' \\ \nu,\nu'}}(0) \right) \mathscr{G}_{\substack{0 \\ \mathbf{k},\mathbf{p}' \\ n,b' \\ \mu,\sigma'}}(\mathrm{i}\omega_n) \tag{28.28}$$

Proof 28.4

We will now focus on the temporal components of the Hartree-contribution to the Green-function. For this we consider the function

$$\widetilde{\mathscr{G}}^{\text{Hartree}}(\tau) = \iint_{[0,\hbar\beta]^2} \mathrm{d}(\tau_1,\tau_2) \underset{\text{I}}{\mathscr{G}_0}(\tau-\tau_1) \underset{\text{II}}{\mathscr{G}_0}(\tau_1-0) \underset{\text{III}}{\mathscr{G}_0}(0) \underset{\text{IV}}{\mathscr{D}_0}(\tau_1-\tau_2) \tag{28.29}$$

and this gives for the Matsubara-components

$$\begin{aligned}
\widetilde{\mathscr{G}}^{\text{Hartree}}(\mathrm{i}\omega_n) &= \int_0^{\hbar\beta} \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\omega_n\tau} \widetilde{\mathscr{G}}^{\text{Hartree}}(\tau) \\
&= \iiint_{[0,\hbar\beta]^3} \mathrm{d}(\tau,\tau_1,\tau_2)\, \mathrm{e}^{\mathrm{i}\omega_n\tau} \underset{\text{I}}{\mathscr{G}_0}(\tau-\tau_1) \underset{\text{II}}{\mathscr{G}_0}(\tau_1-0) \underset{\text{III}}{\mathscr{G}_0}(0) \underset{\text{IV}}{\mathscr{D}_0}(\tau_1-\tau_2) \\
&= \dots
\end{aligned}$$

now we expand the statistical functions according to Lemma TBReferenced and we obtain

$$\begin{aligned}
\dots &= \frac{1}{(\hbar\beta)^4} \sum_{\substack{\omega_{n_4} \in \Omega_{+1} \\ \omega_{n_1},\omega_{n_2},\omega_{n_3} \in \Omega_{-1}}} \iiint_{[0,\hbar\beta]^3} \mathrm{d}(\tau,\tau_1,\tau_2) \mathscr{G}_{\substack{0 \\ \alpha,\xi}}(\mathrm{i}\omega_{n_1}) \mathscr{G}_{\substack{0 \\ \xi',\alpha'}}(\mathrm{i}\omega_{n_2}) \mathscr{G}_{\substack{0 \\ \zeta',\zeta}}(\mathrm{i}\omega_{n_3}) \mathscr{D}_0(\mathrm{i}\omega_{n_4}) \mathrm{e}^{\mathrm{i}\left(\omega_n\tau - \omega_{n_1}(\tau-\tau_1) - \omega_{n_2}\tau_1 - \omega_{n_4}(\tau_1-\tau_2)\right)} \\
&= \sum_{\substack{\omega_{n_4} \in \Omega_{+1} \\ \omega_{n_1,n_2,n_3} \in \Omega_{-1}}} \underset{\text{I}}{\mathscr{G}_0}(\mathrm{i}\omega_{n_1}) \underset{\text{II}}{\mathscr{G}_0}(\mathrm{i}\omega_{n_2}) \underset{\text{III}}{\mathscr{G}_0}(\mathrm{i}\omega_{n_3}) \underset{\text{IV}}{\mathscr{D}_0}(\mathrm{i}\omega_{n_4}) \frac{1}{(\hbar\beta)^4} \iiint_{[0,\hbar\beta]^3} \mathrm{d}(\tau,\tau_1,\tau_2) \mathrm{e}^{\mathrm{i}\left(\omega_n\tau - \omega_{n_1}(\tau-\tau_1) - \omega_{n_2}\tau_1 - \omega_{n_4}(\tau_1-\tau_2)\right)} \\
&= \dots
\end{aligned}$$

and we find for the integral-factor

$$\iiint_{[0,\hbar\beta]^3} \mathrm{d}(\tau,\tau_1,\tau_2)\mathrm{e}^{\mathrm{i}\left(\omega_n\tau-\omega_{n_1}(\tau-\tau_1)-\omega_{n_2}\tau_1-\omega_{n_4}(\tau_1-\tau_2)\right)} = \int_0^{\hbar\beta}\mathrm{d}\tau\,\mathrm{e}^{\mathrm{i}\tau\left(\omega_n-\omega_{n_1}\right)}\int_0^{\hbar\beta}\mathrm{d}\tau_1\,\mathrm{e}^{\mathrm{i}\tau_1\left(\omega_{n_1}-\omega_{n_2}-\omega_{n_4}\right)}\int_0^{\hbar\beta}\mathrm{d}\tau_2\,\mathrm{e}^{\mathrm{i}\tau_2\omega_{n_4}}$$
$$= (\hbar\beta)^3\delta_{\omega_n,\omega_{n_1}}\delta_{\omega_{n_1},\omega_{n_2}}\delta_{\omega_{n_4},0}$$

We use the first, second and third delta-function in order to eliminate the summations over ω_{n_1}, ω_{n_2} and ω_{n_4} respectively. This yields then

$$\widetilde{\mathscr{G}}^{\mathrm{Hartree}}(\mathrm{i}\omega_n) = \ldots = \sum_{\omega_{n_3}\in\Omega_{-1}} \frac{1}{\hbar\beta}\underset{\mathrm{I}}{\mathscr{G}_0}(\mathrm{i}\omega_n)\underset{\mathrm{II}}{\mathscr{G}_0}(\mathrm{i}\omega_n)\underset{\mathrm{III}}{\mathscr{G}_0}(\mathrm{i}\omega_{n_3})\underset{\mathrm{IV}}{\mathscr{D}_0}(0)$$
$$\equiv \underset{\mathrm{I}}{\mathscr{G}_0}(\mathrm{i}\omega_n)\left(\frac{1}{\hbar\beta}\sum_{\omega_{n_3}\in\Omega_{-1}}\underset{\mathrm{III}}{\mathscr{G}_0}(\mathrm{i}\omega_{n_3})\underset{\mathrm{IV}}{\mathscr{D}_0}(0)\right)\underset{\mathrm{II}}{\mathscr{G}_0}(\mathrm{i}\omega_n)$$

or in short:

$$\widetilde{\mathscr{G}}^{\mathrm{Hartree}}(\tau) = \iint_{[0,\hbar\beta]^2}\mathrm{d}(\tau_1,\tau_2)\,\underset{\mathrm{I}}{\mathscr{G}_0}(\tau-\tau_1)\underset{\mathrm{II}}{\mathscr{G}_0}(\tau_1-0)\underset{\mathrm{III}}{\mathscr{G}_0}(0)\underset{\mathrm{IV}}{\mathscr{D}_0}(\tau_1-\tau_2)$$
$$\Rightarrow \quad \widetilde{\mathscr{G}}^{\mathrm{Hartree}}(\mathrm{i}\omega_n) = \underset{\mathrm{I}}{\mathscr{G}_0}(\mathrm{i}\omega_n)\left(\frac{1}{\hbar\beta}\sum_{\omega_{n_3}\in\Omega_{-1}}\underset{\mathrm{III}}{\mathscr{G}_0}(\mathrm{i}\omega_{n_3})\underset{\mathrm{IV}}{\mathscr{D}_0}(0)\right)\underset{\mathrm{II}}{\mathscr{G}_0}(\mathrm{i}\omega_n) \tag{28.30}$$

Using this identity for the Matsubara-component of a function proves the Lemma: We can compute the Fourier-Matsubara-component as

$$\mathscr{G}^{\mathrm{Hartree}}_{\sigma,\sigma'}(\mathrm{i}\omega_n) = \int_0^{\hbar\beta}\mathrm{d}\tau\,\mathscr{G}^{\mathrm{Hartree}}_{\sigma,\sigma'}(\tau)\,\mathrm{e}^{\mathrm{i}\omega_n\tau}$$
$$= \hbar\sum_{\substack{\tau,\tau_1,\tau_2\in[0,\hbar\beta]\\ \mu,\mu'\in\{\downarrow,\uparrow\}\\ \mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}'\in\mathrm{Q}\\ m,m',n,n'\in\{1,2,\ldots\}\\ \nu,\nu'\in\{1,2,\ldots,rd\}}} + \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})g_{m'n'\nu'}(\mathbf{k}',\mathbf{q}')}{N_p}\underset{\substack{\mathbf{p},\mathbf{k}+\mathbf{q}\\ b,m\\ \sigma,\mu}}{\mathscr{G}_0}(\tau-\tau_1)\underset{\substack{\mathbf{k},\mathbf{p}'\\ n,b'\\ \mu,\sigma'}}{\mathscr{G}_0}(\tau_1-0)\underset{\substack{\mathbf{k}',\mathbf{k}'+\mathbf{q}'\\ n',m'\\ \mu',\mu'}}{\mathscr{G}_0}(0)\underset{\substack{\mathbf{q},-\mathbf{q}'\\ \nu,\nu'}}{\mathscr{D}_0}(\tau_1-\tau_2)\,\mathrm{e}^{\mathrm{i}\omega_n\tau}$$
$$= \sum_{\substack{\mu,\mu'\in\{\downarrow,\uparrow\}\\ \mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}'\in\mathrm{Q}\\ m,m',n,n'\in\{1,2,\ldots\}\\ \nu,\nu'\in\{1,2,\ldots,rd\}}} \underset{\substack{\mathbf{p},\mathbf{k}+\mathbf{q}\\ b,m\\ \sigma,\mu}}{\mathscr{G}_0}(\mathrm{i}\omega_n)\left(\frac{1}{\beta}\sum_{\omega_m\in\Omega_{-1}} + \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})g_{m'n'\nu'}(\mathbf{k}',\mathbf{q}')}{N_p}\underset{\substack{\mathbf{k}',\mathbf{k}'+\mathbf{q}'\\ n',m'\\ \mu',\mu'}}{\mathscr{G}_0}(\mathrm{i}\omega_m)\underset{\substack{\mathbf{q},-\mathbf{q}'\\ \nu,\nu'}}{\mathscr{D}_0}(0)\right)\underset{\substack{\mathbf{k},\mathbf{p}'\\ n,b'\\ \mu,\sigma'}}{\mathscr{G}_0}(\mathrm{i}\omega_n)$$

Fourier-Matsubara-Component of the Fock-Contribution

Lemma 28.2 It holds

$$\mathscr{G}^{\text{Fock}}_{\sigma,\sigma'}(\mathrm{i}\omega_n) = \sum_{\substack{\mu,\mu'\in\{\downarrow,\uparrow\}\\ \mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}'\in\mathrm{Q}\\ m,m',n,n'\in\{1,2,\ldots\}\\ \nu,\nu'\in\{1,2,\ldots,rd\}}} \underset{\substack{\mathbf{p},\mathbf{k}+\mathbf{q}\\ b,m\\ \sigma,\mu}}{\mathscr{G}_0}(\mathrm{i}\omega_n)\left(\frac{1}{\beta}\sum_{\omega_{n_2}\in\Omega_{-1}} -\frac{g_{mn\nu}(\mathbf{k},\mathbf{q})g_{m'n'\nu'}(\mathbf{k}',\mathbf{q}')}{N_p}\underset{\substack{\mathbf{k},\mathbf{k}'+\mathbf{q}'\\ n,m'\\ \mu,\mu'}}{\mathscr{G}_0}(\mathrm{i}\omega_{n_2})\underset{\substack{\mathbf{q},-\mathbf{q}'\\ \nu,\nu'}}{\mathscr{D}_0}(\mathrm{i}(\omega_n-\omega_{n_2}))\right)\underset{\substack{\mathbf{k}',\mathbf{p}'\\ n',b'\\ \mu',\sigma'}}{\mathscr{G}_0}(\mathrm{i}\omega_n) \tag{28.31}$$

Proof 28.5

We will now focus on the temporal components of the Fock-contribution to the Green-function. For this we consider the function

$$\widetilde{\mathscr{G}}^{\text{Fock}}(\tau) = \iint_{[0,\hbar\beta]^2} \mathrm{d}(\tau_1,\tau_2)\underset{\text{I}}{\mathscr{G}_0}(\tau-\tau_1)\underset{\text{II}}{\mathscr{G}_0}(\tau_1-\tau_2)\underset{\text{III}}{\mathscr{G}_0}(\tau_2)\underset{\text{IV}}{\mathscr{D}_0}(\tau_1-\tau_2) \tag{28.32}$$

and this gives for the Matsubara-components

$$\begin{aligned}\widetilde{\mathscr{G}}^{\text{Fock}}(\mathrm{i}\omega_n) &= \int_0^{\hbar\beta}\mathrm{d}\tau\,\mathrm{e}^{\mathrm{i}\omega_n\tau}\widetilde{\mathscr{G}}^{\text{Fock}}(\tau)\\ &= \iiint_{[0,\hbar\beta]^3}\mathrm{d}(\tau,\tau_1,\tau_2)\,\mathrm{e}^{\mathrm{i}\omega_n\tau}\underset{\text{I}}{\mathscr{G}_0}(\tau-\tau_1)\underset{\text{II}}{\mathscr{G}_0}(\tau_1-\tau_2)\underset{\text{III}}{\mathscr{G}_0}(\tau_2)\underset{\text{IV}}{\mathscr{D}_0}(\tau_1-\tau_2)\\ &= \ldots\end{aligned}$$

now we expand the statistical functions according to Lemma TBReferenced and we obtain

$$\begin{aligned}\ldots &= \sum_{\substack{\omega_{n_1},n_2,n_3\in\Omega_{-1}\\ \omega_{n_4}\in\Omega_{+1}}}\underset{\text{I}}{\mathscr{G}_0}(\omega_{n_1})\underset{\text{II}}{\mathscr{G}_0}(\omega_{n_2})\underset{\text{III}}{\mathscr{G}_0}(\omega_{n_3})\underset{\text{IV}}{\mathscr{D}_0}(\omega_{n_4})\frac{1}{(\hbar\beta)^4}\iiint_{[0,\hbar\beta]^3}\mathrm{d}(\tau,\tau_1,\tau_2)\mathrm{e}^{\mathrm{i}\left(\omega_n\tau-\omega_{n_1}(\tau-\tau_1)-\omega_{n_2}(\tau_1-\tau_2)-\omega_{n_3}\tau_2-\omega_{n_4}(\tau_1-\tau_2)\right)}\\ &= \ldots\end{aligned}$$

and we find for the integral-factor

$$\begin{aligned}&\iiint_{[0,\hbar\beta]^3}\mathrm{d}(\tau,\tau_1,\tau_2)\mathrm{e}^{\mathrm{i}\left(\omega_n\tau-\omega_{n_1}(\tau-\tau_1)-\omega_{n_2}(\tau_1-\tau_2)-\omega_{n_3}\tau_2-\omega_{n_4}(\tau_1-\tau_2)\right)}\\ &= \int_0^{\hbar\beta}\mathrm{d}\tau\,\mathrm{e}^{\mathrm{i}\tau\left(\omega_n-\omega_{n_1}\right)}\int_0^{\hbar\beta}\mathrm{d}\tau_1\,\mathrm{e}^{\mathrm{i}\tau_1\left(\omega_{n_1}-\omega_{n_2}-\omega_{n_4}\right)}\int_0^{\hbar\beta}\mathrm{d}\tau_2\,\mathrm{e}^{\mathrm{i}\tau_2\left(\omega_{n_2}-\omega_{n_3}+\omega_{n_4}\right)}\\ &= (\hbar\beta)^3\delta_{\omega_n,\omega_{n_1}}\delta_{\omega_{n_1},\omega_{n_2}+\omega_{n_4}}\delta_{\omega_{n_2}+\omega_{n_4},\omega_{n_3}}\end{aligned}$$

We use the first delta-function to eliminate the summation over ω_{n_1}. The second delta-function can be simplified according to

$$\begin{aligned}\delta_{\omega_{n_1},\omega_{n_2}+\omega_{n_4}} &= \delta_{\omega_{n_2},\omega_{n_1}-\omega_{n_4}} \\ &= \delta_{\omega_{n_2},\omega_{n_1}-\omega_{n_3}+\omega_{n_2}} \\ &= \delta_{\omega_{n_3},\omega_{n_1}}\end{aligned}$$

and will eliminate the summation over ω_{n_3}. For the third delta-relation we simplify it to

$$\delta_{\omega_{n_2}+\omega_{n_4},\omega_{n_3}} = \delta_{\omega_{n_4},\omega_{n_3}-\omega_{n_2}}$$

and we will use this to eliminate the summation over ω_{n_4}.

This yields then

$$\begin{aligned}\widetilde{\mathscr{G}}^{\text{Fock}}(\mathrm{i}\omega_n) = \ldots &= \sum_{\omega_{n_2}\in\Omega_{-1}} \frac{1}{\hbar\beta} \underset{\text{I}}{\mathscr{G}_0}(\omega_n)\underset{\text{II}}{\mathscr{G}_0}(\omega_{n_2})\underset{\text{III}}{\mathscr{G}_0}(\omega_n)\underset{\text{IV}}{\mathscr{D}_0}(\mathrm{i}(\omega_n-\omega_{n_2})) \\ &\equiv \underset{\text{I}}{\mathscr{G}_0}(\omega_n)\left(\frac{1}{\hbar\beta}\sum_{\omega_{n_2}\in\Omega_{-1}} \underset{\text{II}}{\mathscr{G}_0}(\omega_{n_2})\underset{\text{IV}}{\mathscr{D}_0}(\mathrm{i}(\omega_n-\omega_{n_2}))\right)\underset{\text{III}}{\mathscr{G}_0}(\omega_n)\end{aligned}$$

Using this identity for the Matsubara-component of a function proves the Lemma: We can compute the Fourier-Matsubara-component as

$$\begin{aligned}\mathscr{G}^{\text{Fock}}_{\sigma,\sigma'}(\mathrm{i}\omega_n) &= \int_0^{\hbar\beta} \mathrm{d}\tau\, \mathscr{G}^{\text{Fock}}_{\sigma,\sigma'}(\tau)\,\mathrm{e}^{\mathrm{i}\omega_n\tau} \\ &= \hbar \sum_{\substack{\tau,\tau_1,\tau_2\in[0,\hbar\beta]\\ \mu,\mu'\in\{\downarrow,\uparrow\}\\ \mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}'\in\mathrm{Q}\\ m,m',n,n'\in\{1,2,\ldots\}\\ \nu,\nu'\in\{1,2,\ldots,rd\}}} -\frac{g_{mn\nu}(\mathbf{k},\mathbf{q})g_{m'n'\nu'}(\mathbf{k}',\mathbf{q}')}{N_p}\, \underset{\substack{\mathbf{p},\mathbf{k}+\mathbf{q}\\ b,m\\ \sigma,\mu}}{\mathscr{G}_0}(\tau-\tau_1)\underset{\substack{\mathbf{k},\mathbf{k}'+\mathbf{q}'\\ n,m'\\ \mu,\mu'}}{\mathscr{G}_0}(\tau_1-\tau_2)\underset{\substack{\mathbf{k}',\mathbf{p}'\\ n',b'\\ \mu',\sigma'}}{\mathscr{G}_0}(\tau_2-0)\underset{\substack{\mathbf{q},-\mathbf{q}'\\ \nu,\nu'}}{\mathscr{D}_0}(\tau_1-\tau_2)\,\mathrm{e}^{\mathrm{i}\omega_n\tau} \\ &= \sum_{\substack{\mu,\mu'\in\{\downarrow,\uparrow\}\\ \mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}'\in\mathrm{Q}\\ m,m',n,n'\in\{1,2,\ldots\}\\ \nu,\nu'\in\{1,2,\ldots,rd\}}} \underset{\substack{\mathbf{p},\mathbf{k}+\mathbf{q}\\ b,m\\ \sigma,\mu}}{\mathscr{G}_0}(\mathrm{i}\omega_n)\left(\frac{1}{\beta}\sum_{\omega_{n_2}\in\Omega_{-1}} -\frac{g_{mn\nu}(\mathbf{k},\mathbf{q})g_{m'n'\nu'}(\mathbf{k}',\mathbf{q}')}{N_p}\, \underset{\substack{\mathbf{k},\mathbf{k}'+\mathbf{q}'\\ n,m'\\ \mu,\mu'}}{\mathscr{G}_0}(\mathrm{i}\omega_{n_2})\underset{\substack{\mathbf{q},-\mathbf{q}'\\ \nu,\nu'}}{\mathscr{D}_0}(\mathrm{i}(\omega_n-\omega_{n_2}))\right)\underset{\substack{\mathbf{k}',\mathbf{p}'\\ n',b'\\ \mu',\sigma'}}{\mathscr{G}_0}(\mathrm{i}\omega_n).\end{aligned} \tag{28.33}$$

which proves the lemma.

Continuation of the Initial Proof

Continuing with the initial proof, we obtained in total

$$
\begin{aligned}
\mathscr{G}^{(2)}_{\substack{b,b'\\ \mathbf{p},\mathbf{p}'\\ \sigma,\sigma'}}(\mathrm{i}\omega_n) &= \mathscr{G}^{\mathrm{Hartree}}_{\sigma,\sigma'}(\mathrm{i}\omega_n) \quad + \quad \mathscr{G}^{\mathrm{Fock}}_{\sigma,\sigma'}(\mathrm{i}\omega_n) \\
&\equiv \sum_{\substack{\mu,\mu'\in\{\downarrow,\uparrow\}\\ \mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}'\in \mathrm{Q}\\ m,m',n,n'\in\{1,2,\dots\}\\ \nu,\nu'\in\{1,2,\dots,rd\}}} \mathscr{G}_{\substack{0\\ \mathbf{p},\mathbf{k}+\mathbf{q}\\ b,m\\ \sigma,\mu}}(\mathrm{i}\omega_n)\left(\frac{1}{\beta}\sum_{\omega_m\in\Omega_{-1}} + \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})g_{m'n'\nu'}(\mathbf{k}',\mathbf{q}')}{N_p}\mathscr{G}_{\substack{0\\ \mathbf{k}',\mathbf{k}'+\mathbf{q}'\\ n',m'\\ \mu',\mu}}(\mathrm{i}\omega_m)\mathscr{D}_{\substack{0\\ \mathbf{q},-\mathbf{q}'\\ \nu,\nu'}}(0)\right)\mathscr{G}_{\substack{0\\ \mathbf{k},\mathbf{p}'\\ n,b'\\ \mu,\sigma'}}(\mathrm{i}\omega_n) \\
&+ \sum_{\substack{\mu,\mu'\in\{\downarrow,\uparrow\}\\ \mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}'\in \mathrm{Q}\\ m,m',n,n'\in\{1,2,\dots\}\\ \nu,\nu'\in\{1,2,\dots,rd\}}} \mathscr{G}_{\substack{0\\ \mathbf{p},\mathbf{k}+\mathbf{q}\\ b,m\\ \sigma,\mu}}(\mathrm{i}\omega_n)\left(\frac{1}{\beta}\sum_{\omega_{n_2}\in\Omega_{-1}} - \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})g_{m'n'\nu'}(\mathbf{k}',\mathbf{q}')}{N_p}\,\mathscr{G}_{\substack{0\\ \mathbf{k},\mathbf{k}'+\mathbf{q}'\\ n,m'\\ \mu,\mu'}}(\mathrm{i}\omega_{n_2})\,\mathscr{D}_{\substack{0\\ \mathbf{q},-\mathbf{q}'\\ \nu,\nu'}}(\mathrm{i}(\omega_n-\omega_{n_2}))\right)\mathscr{G}_{\substack{0\\ \mathbf{k}',\mathbf{p}'\\ n',b'\\ \mu',\sigma'}}(\mathrm{i}\omega_n) \\
&\overset{\mathbf{q}\mapsto\mathbf{q}-\mathbf{k}}{=} \sum_{\substack{\mathbf{k},\mathbf{q}\in \mathrm{Q}\\ \mu\in\{\downarrow,\uparrow\}\\ m,n,\in\{1,2,\dots\}}} \mathscr{G}_{\substack{0\\ \mathbf{p},\mathbf{q}\\ b,m\\ \sigma,\mu}}(\mathrm{i}\omega_n)\left(\frac{1}{\beta}\sum_{\substack{\mathbf{k}',\mathbf{q}'\in \mathrm{Q}\\ \mu'\in\{\downarrow,\uparrow\}\\ m',n'\in\{1,2,\dots\}\\ \nu,\nu'\in\{1,2,\dots,rd\}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q}-\mathbf{k})g_{m'n'\nu'}(\mathbf{k}',\mathbf{q}')}{N_p}\mathscr{D}_{\substack{0\\ \mathbf{q}-\mathbf{k},-\mathbf{q}'\\ \nu,\nu'}}(0)\sum_{\omega_m\in\Omega_{-1}}\mathscr{G}_{\substack{0\\ \mathbf{k}',\mathbf{k}'+\mathbf{q}'\\ n',m'\\ \mu',\mu}}(\mathrm{i}\omega_m)\right)\mathscr{G}_{\substack{0\\ \mathbf{k},\mathbf{p}'\\ n,b'\\ \mu,\sigma'}}(\mathrm{i}\omega_n) \\
&+ \sum_{\substack{\mathbf{k}',\mathbf{q}\in \mathrm{Q}\\ \mu,\mu'\in\{\downarrow,\uparrow\}\\ m,n'\in\{1,2,\dots\}}} \mathscr{G}_{\substack{0\\ \mathbf{p},\mathbf{q}\\ b,m\\ \sigma,\mu}}(\mathrm{i}\omega_n)\left(\sum_{\substack{\mathbf{k},\mathbf{q}'\in \mathrm{Q}\\ m',n\in\{1,2,\dots\}\\ \nu,\nu'\in\{1,2,\dots,rd\}}}\frac{1}{\beta}\sum_{\omega_{n_2}\in\Omega_{-1}} - \frac{g_{mn\nu}(\mathbf{k},\mathbf{q}-\mathbf{k})g_{m'n'\nu'}(\mathbf{k}',\mathbf{q}')}{N_p}\,\mathscr{G}_{\substack{0\\ \mathbf{k},\mathbf{k}'+\mathbf{q}'\\ n,m'\\ \mu,\mu'}}(\mathrm{i}\omega_{n_2})\,\mathscr{D}_{\substack{0\\ \mathbf{q}-\mathbf{k},-\mathbf{q}'\\ \nu,\nu'}}(\mathrm{i}(\omega_n-\omega_{n_2}))\right)\mathscr{G}_{\substack{0\\ \mathbf{k}',\mathbf{p}'\\ n',b'\\ \mu',\sigma'}}(\mathrm{i}\omega_n) \\
&= \sum_{\substack{\mathbf{k},\mathbf{q}\in \mathrm{Q}\\ \mu\in\{\downarrow,\uparrow\}\\ m,n,\in\{1,2,\dots\}}} \mathscr{G}_{\substack{0\\ \mathbf{p},\mathbf{q}\\ b,m\\ \sigma,\mu}}(\mathrm{i}\omega_n)\;\Sigma^{\mathrm{Hartree}}_{\substack{\mathbf{q},\mathbf{k}\\ m,n\\ \mu,\mu}}(\mathrm{i}\omega_n)\;\mathscr{G}_{\substack{0\\ \mathbf{k},\mathbf{p}'\\ n,b'\\ \mu,\sigma'}}(\mathrm{i}\omega_n) \quad + \quad \sum_{\substack{\mathbf{k}',\mathbf{q}\in \mathrm{Q}\\ \mu\in\{\downarrow,\uparrow\}\\ m,n,\in\{1,2,\dots\}}} \mathscr{G}_{\substack{0\\ \mathbf{p},\mathbf{q}\\ b,m\\ \sigma,\mu}}(\mathrm{i}\omega_n)\;\Sigma^{\mathrm{Fock}}_{\substack{\mathbf{q},\mathbf{k}'\\ m,n'\\ \mu,\mu'}}(\mathrm{i}\omega_n)\;\mathscr{G}_{\substack{0\\ \mathbf{k}',\mathbf{p}'\\ n',b'\\ \mu',\sigma'}}(\mathrm{i}\omega_n)
\end{aligned}
\tag{28.34}
$$

In the next step we will perform the Matsubara-summations and simplify the self-energy expressions.

The Hartree-Contribution

Now since $\mathscr{G}_0$ is diagonal (in bands and wave-vectors) we see that only the $\mathbf{q}' = 0$ and $m' = n'$ summand contributes. Since $\mathscr{D}_0$ is diagonal in branches and wave-vectors only the $\nu = \nu'$ and $\mathbf{k} = \mathbf{q}$ summands contribute. This gives the simplification

$$
\Sigma^{\mathrm{Hartree}}_{\substack{\mathbf{q},\mathbf{k}\\ m,n\\ \mu,\mu'}}(\mathrm{i}\omega_n) = \delta_{\mu,\mu'}\frac{1}{\beta}\sum_{\substack{\mathbf{k}'\in \mathrm{Q}\\ \mu'\in\{\downarrow,\uparrow\}\\ m'\in\{1,2,\dots\}\\ \nu\in\{1,2,\dots,rd\}}} + \frac{g_{mn\nu}(\mathbf{k},0)g_{m'm'\nu}(\mathbf{k}',0)}{N_p}\mathscr{D}_{\substack{0\\ \mathbf{0},\mathbf{0}\\ \nu,\nu}}(0)\sum_{\omega_m\in\Omega_{-1}}\mathscr{G}_{\substack{0\\ \mathbf{k}',\mathbf{k}'\\ m',m'\\ \mu',\mu'}}(\mathrm{i}\omega_m)\delta_{\mathbf{q},\mathbf{k}} \tag{28.35}
$$

Therefore this contribution to the self-energy is diagonal in wave-vectors but not in the bands.

We now evaluate the summation over Matsubara-frequencies with the Residue-theorem. Omitting convergence-generating factors for notational simplicity, this gives with Corollary 15.22

$$
\frac{1}{\beta}\sum_{\omega_m\in\Omega_{-1}}\mathscr{G}_{\substack{0\\ \mathbf{k}',\mathbf{k}'\\ m',m'\\ \mu',\mu'}}(\mathrm{i}\omega_m) = \frac{1}{\hbar\beta}\sum_{\omega_m\in\Omega_{-1}}\frac{1}{\mathrm{i}\omega_m - \left(\epsilon_{m'\mu'\mathbf{k}'}-\mu\right)/\hbar} = \mathrm{F}_\beta(\epsilon_{m'\mu'\mathbf{k}'}-\mu) \tag{28.36}
$$

yielding as final expression

$$\Sigma^{\text{Hartree}}_{\substack{0\\ \mathbf{q},\mathbf{k}\\ m,n\\ \mu,\mu'}}(\mathrm{i}\omega_n) = \delta_{\mu,\mu'} \sum_{\substack{\mathbf{k}'\in \mathrm{Q}\\ \mu'\in\{\downarrow,\uparrow\}\\ m'\in\{1,2,\dots\}\\ \nu\in\{1,2,\dots,rd\}}} \frac{g_{mn\nu}(\mathbf{k},0)g_{m'm'\nu}(\mathbf{k}',0)}{N_p} \mathscr{D}^{\ 0}_{\substack{\mathbf{0},\mathbf{0}\\ \nu,\nu}}(0)\,\mathrm{F}_\beta(\epsilon_{m'\mu'\mathbf{k}'}-\mu)\delta_{\mathbf{q},\mathbf{k}} \tag{28.37}$$

The Fock-Contribution

Using now again the diagonality of the unperturbed Green-functions we obtain for the Fock-contribution to the self-energy

$$\begin{aligned}
\Sigma^{\text{Fock}}_{\substack{\mathbf{q},\mathbf{k}'\\ m,n'\\ \mu,\mu'}}(\mathrm{i}\omega_n) &= \sum_{\substack{\mathbf{k},\mathbf{q}'\in\mathrm{Q}\\ m',n\in\{1,2,\dots\}\\ \nu,\nu'\in\{1,2,\dots,rd\}}} \frac{1}{\beta}\sum_{\omega_{n_2}\in\Omega_{-1}} -\frac{g_{mn\nu}(\mathbf{k},\mathbf{q}-\mathbf{k})g_{m'n'\nu'}(\mathbf{k}',\mathbf{q}')}{N_p}\, \mathscr{G}^{\ 0}_{\substack{\mathbf{k},\mathbf{k}'+\mathbf{q}'\\ n,m'\\ \mu,\mu'}}(\mathrm{i}\omega_{n_2})\, \mathscr{D}^{\ 0}_{\substack{\mathbf{q}-\mathbf{k},-\mathbf{q}'\\ \nu,\nu'}}(\mathrm{i}(\omega_n-\omega_{n_2}))\\
&= \sum_{\substack{\mathbf{q}'\in\mathrm{Q}\\ m',n\in\{1,2,\dots\}\\ \nu\in\{1,2,\dots,rd\}}} \frac{1}{\beta}\sum_{\omega_{n_2}\in\Omega_{-1}} -\frac{g_{mn\nu}(\mathbf{k}'+\mathbf{q}',\mathbf{q}-(\mathbf{k}'+\mathbf{q}'))g_{m'n'\nu'}(\mathbf{k}',\mathbf{q}')}{N_p}\, \mathscr{G}^{\ 0}_{\substack{\mathbf{k}'+\mathbf{q}',\mathbf{k}'+\mathbf{q}'\\ n,m'\\ \mu,\mu'}}(\mathrm{i}\omega_{n_2})\, \mathscr{D}^{\ 0}_{\substack{\mathbf{q}-(\mathbf{k}'+\mathbf{q}'),-\mathbf{q}'\\ \nu,\nu}}(\mathrm{i}(\omega_n-\omega_{n_2}))\\
&= \sum_{\substack{\mathbf{q}'\in\mathrm{Q}\\ m',n\in\{1,2,\dots\}\\ \nu\in\{1,2,\dots,rd\}}} \frac{1}{\beta}\sum_{\omega_{n_2}\in\Omega_{-1}} -\frac{g_{mn\nu}(\mathbf{k}'+\mathbf{q}',\mathbf{q}-(\mathbf{k}'+\mathbf{q}'))g_{m'n'\nu'}(\mathbf{k}',\mathbf{q}')}{N_p}\, \mathscr{G}^{\ 0}_{\substack{\mathbf{k}'+\mathbf{q}',\mathbf{k}'+\mathbf{q}'\\ n,m'\\ \mu,\mu'}}(\mathrm{i}\omega_{n_2})\, \mathscr{D}^{\ 0}_{\substack{-\mathbf{q}',-\mathbf{q}'\\ \nu,\nu}}(\mathrm{i}(\omega_n-\omega_{n_2}))\delta_{\mathbf{q}-(\mathbf{k}'+\mathbf{q}'),-\mathbf{q}'}\\
&= \sum_{\substack{\mathbf{q}'\in\mathrm{Q}\\ m',n\in\{1,2,\dots\}\\ \nu\in\{1,2,\dots,rd\}}} \frac{1}{\beta}\sum_{\omega_{n_2}\in\Omega_{-1}} -\frac{g_{mn\nu}(\mathbf{k}'+\mathbf{q}',-\mathbf{q}')g_{m'n'\nu'}(\mathbf{k}',\mathbf{q}')}{N_p}\, \mathscr{G}^{\ 0}_{\substack{\mathbf{k}'+\mathbf{q}',\mathbf{k}'+\mathbf{q}'\\ n,m'\\ \mu,\mu'}}(\mathrm{i}\omega_{n_2})\, \mathscr{D}^{\ 0}_{\substack{-\mathbf{q}',-\mathbf{q}'\\ \nu,\nu}}(\mathrm{i}(\omega_n-\omega_{n_2}))\delta_{\mathbf{q},\mathbf{k}'}\\
&= \sum_{\substack{\mathbf{q}'\in\mathrm{Q}\\ m',n\in\{1,2,\dots\}\\ \nu\in\{1,2,\dots,rd\}}} \frac{1}{\beta}\sum_{\omega_{n_2}\in\Omega_{-1}} -\frac{g^*_{nm\nu}(\mathbf{k}',\mathbf{q}')g_{m'n'\nu'}(\mathbf{k}',\mathbf{q}')}{N_p}\, \mathscr{G}^{\ 0}_{\substack{\mathbf{k}'+\mathbf{q}',\mathbf{k}'+\mathbf{q}'\\ n,m'\\ \mu,\mu'}}(\mathrm{i}\omega_{n_2})\, \mathscr{D}^{\ 0}_{\substack{-\mathbf{q}',-\mathbf{q}'\\ \nu,\nu}}(\mathrm{i}(\omega_n-\omega_{n_2}))\delta_{\mathbf{q},\mathbf{k}'}\\
&= \sum_{\substack{\mathbf{q}'\in\mathrm{Q}\\ n\in\{1,2,\dots\}\\ \nu\in\{1,2,\dots,rd\}}} \frac{1}{\beta}\sum_{\omega_{n_2}\in\Omega_{-1}} -\frac{g_{nn'\nu'}(\mathbf{k}',\mathbf{q}')g^*_{nm\nu}(\mathbf{k}',\mathbf{q}')}{N_p}\, \mathscr{G}^{\ 0}_{\substack{\mathbf{k}'+\mathbf{q}',\mathbf{k}'+\mathbf{q}'\\ n,n\\ \mu,\mu'}}(\mathrm{i}\omega_{n_2})\, \mathscr{D}^{\ 0}_{\substack{\mathbf{q}',\mathbf{q}'\\ \nu,\nu}}(\mathrm{i}(\omega_n-\omega_{n_2}))\delta_{\mathbf{q},\mathbf{k}'}\\
&= \sum_{\substack{\mathbf{q}'\in\mathrm{Q}\\ n\in\{1,2,\dots\}\\ \nu\in\{1,2,\dots,rd\}}} -\frac{g_{nn'\nu'}(\mathbf{k}',\mathbf{q}')g^*_{nm\nu}(\mathbf{k}',\mathbf{q}')}{N_p}\delta_{\mathbf{q},\mathbf{k}'}\delta_{\mu,\mu'}\frac{1}{\beta}\sum_{\omega_{n_2}\in\Omega_{-1}} \mathscr{G}^{\ 0}_{\substack{\mathbf{k}'+\mathbf{q}',\mathbf{k}'+\mathbf{q}'\\ n,n\\ \mu,\mu}}(\mathrm{i}\omega_{n_2})\, \mathscr{D}^{\ 0}_{\substack{\mathbf{q}',\mathbf{q}'\\ \nu,\nu}}(\mathrm{i}(\omega_n-\omega_{n_2}))
\end{aligned} \tag{28.38}$$

Note that we used $\omega_\nu(-\mathbf{q}) = \omega_\nu(\mathbf{q})$ in the last step. We now evaluate the summation over Matsubara-frequencies with the Residue-theorem. Omitting convergence-generating factors for notational simplicity, this confronts us with the task of evaluating the sum

$$\begin{aligned}
\frac{1}{\beta}\sum_{\omega_{n_2}\in\Omega_{-1}} \mathscr{G}^{\ 0}_{\substack{\mathbf{q}'+\mathbf{k}',\mathbf{q}'+\mathbf{k}'\\ n,n\\ \mu,\mu}}(\mathrm{i}\omega_{n_2})\, \mathscr{D}^{\ 0}_{\substack{\mathbf{q}',\mathbf{q}'\\ \nu,\nu}}(\mathrm{i}(\omega_n-\omega_{n_2})) &= \frac{1}{\hbar^2\beta}\sum_{\omega_{n_2}\in\Omega_{-1}} \frac{1}{\mathrm{i}\omega_{n_2}-(\epsilon_{n\mu\mathbf{q}'+\mathbf{k}'}-\mu)/\hbar}\,\frac{-2\omega_\nu(\mathbf{q}')}{(\omega_n-\omega_{n_2})^2+\omega_\nu^2(\mathbf{q}')}\\
&\overset{\text{Corollary 15.23}}{=} \frac{-1}{\hbar}\left[\frac{\mathrm{B}_{\hbar\beta}(\omega_\nu(\mathbf{q}'))+\mathrm{F}_\beta(\xi_{\mathbf{q}'+\mathbf{k}'n\mu})}{\mathrm{i}\omega_n-\xi_{\mathbf{q}'+\mathbf{k}'n\mu}/\hbar+\omega_\nu(\mathbf{q}')}+\frac{\mathrm{B}_{\hbar\beta}(\omega_\nu(\mathbf{q}'))+1-\mathrm{F}_\beta(\xi_{\mathbf{q}'+\mathbf{k}'n\mu})}{\mathrm{i}\omega_n-\xi_{\mathbf{q}'+\mathbf{k}'n\mu}/\hbar-\omega_\nu(\mathbf{q}')}\right]
\end{aligned} \tag{28.39}$$

whereas we introduced the variable $\xi_{\mathbf{q}'+\mathbf{k}'n\mu} = \epsilon_{\mathbf{q}'+\mathbf{k}'n\mu} - \mu$.

In total we obtain the final expression

$$\Sigma^{\text{Fock}}_{\substack{\mathbf{q},\mathbf{k}'\\ m,n'\\ \mu,\mu'}}(\mathrm{i}\omega_n) = \sum_{\substack{\mathbf{q}'\in\mathrm{Q}\\ n\in\{1,2,\dots\}\\ \nu\in\{1,2,\dots,rd\}}} \frac{g_{nn'\nu'}(\mathbf{k}',\mathbf{q}')g^*_{nm\nu}(\mathbf{k}',\mathbf{q}')}{N_p}\delta_{\mathbf{q},\mathbf{k}'}\delta_{\mu,\mu'}\left[\frac{\mathrm{B}_\beta(\hbar\omega_\nu(\mathbf{q}'))+\mathrm{F}_\beta(\xi_{\mathbf{q}'+\mathbf{k}'n\mu})}{\mathrm{i}\hbar\omega_n-\xi_{\mathbf{q}'+\mathbf{k}'n\mu}+\hbar\omega_\nu(\mathbf{q}')}+\frac{\mathrm{B}_\beta(\hbar\omega_\nu(\mathbf{q}'))+1-\mathrm{F}_\beta(\xi_{\mathbf{q}'+\mathbf{k}'n\mu})}{\mathrm{i}\hbar\omega_n-\xi_{\mathbf{q}'+\mathbf{k}'n\mu}-\hbar\omega_\nu(\mathbf{q}')}\right] \tag{28.40}$$

28.4. Polarization of a Spin-Independent-Interaction between an Electron-Gas and a Phonon-Gas

Proof 28.6 of Theorem 21.4 From PHYSICAL REVIEW B 76, 165108 2007 („03“ in the phonon-folder) and / or Computer Physics Communications 209 (2016) 116–133 („04“ in the EPW-folder.)

We will use the following trick: Inverting the Dyson-equation with the von Neumann series on the one hand, and re-expressing the imaginary-time-phononic-Green-function with help of the field integral on the other hand, gives the two equations

$$\mathscr{D}_{\substack{\mathbf{p},\mathbf{p}'\\ \pi,\pi'}}(\mathrm{i}\omega_n) = \sum_{n=0}^{\infty}\left[\left(\mathscr{D}_0\cdot\Pi\right)^n(\mathrm{i}\omega_n)\cdot\mathscr{D}_0(\mathrm{i}\omega_n)\right]_{\substack{\mathbf{p},\mathbf{p}'\\ \pi,\pi'}} \tag{28.41}$$

$$\mathscr{D}_{\substack{\mathbf{p},\mathbf{p}'\\ \pi,\pi'}}(\mathrm{i}\omega_n) = \int_0^{\hbar\beta}\mathrm{d}\tau\,\mathrm{e}^{\mathrm{i}\omega_n\tau}\,\mathscr{D}_{\substack{\mathbf{p},\mathbf{p}'\\ \pi,\pi'}}(\tau) = \frac{-1}{\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau\,\mathrm{e}^{\mathrm{i}\omega_n\tau}\left\langle A_{\mathbf{p}\pi}(\tau)A_{-\mathbf{p}'\pi'}(0)\right\rangle \tag{28.42}$$

The polarization of the phononic Green-function will be a series in the interaction-parameters

$$\Pi(\mathrm{i}\omega_n) = \sum_{j=0}^{\infty}\Pi^{(j)}(\mathrm{i}\omega_n) \approx 0 + \Pi^{(2)}(\mathrm{i}\omega_n) + 0 + \mathcal{O}(\mathrm{V}^4), \tag{28.43}$$

whereas the first contribution will turn out to vanish since the interaction can be expanded as a sum of monomials of creation- and annihilation-operators with uneven degree. Inserting this in the upper-equation above and keeping the first non-vanishing terms yields the sets of equations

$$\mathscr{D}_{\substack{\mathbf{p},\mathbf{p}'\\ \pi,\pi'}}(\mathrm{i}\omega_n) = \mathscr{D}_{\substack{0\\ \mathbf{p},\mathbf{p}'\\ \pi,\pi'}}(\mathrm{i}\omega_n) + \left(\mathscr{D}_0\cdot\Pi^{(2)}\cdot\mathscr{D}_0\right)_{\substack{\mathbf{p},\mathbf{p}'\\ \pi,\pi'}}(\mathrm{i}\omega_n) \tag{28.44}$$

$$\mathscr{D}_{\substack{\mathbf{p},\mathbf{p}'\\ \pi,\pi'}}(\mathrm{i}\omega_n) = \frac{-1}{\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau\,\mathrm{e}^{\mathrm{i}\omega_n\tau}\left\langle A_{\mathbf{p}\pi}(\tau)A_{-\mathbf{p}'\pi'}(0)\right\rangle \tag{28.45}$$

The lower equation can be calculated explicitly with help of the Wick-theorem, linked-cluster-theorem, and the residue-theorem, and then, by comparing the first non-vanishing coefficients with the upper-equation, we can conclude what $\Pi^{(2)}(\mathrm{i}\omega_n)$ must be.

Fact 1: The action, corresponding to this system, is given by the equation above.

Fact 2: The phononic Green-function is written in second order perturbation-theory as

$$\begin{aligned}\mathscr{D}_{\substack{\mathbf{p},\mathbf{p}'\\ \pi,\pi'}}(\tau) &= \mathscr{D}^{(0)}_{\substack{\mathbf{p},\mathbf{p}'\\ \pi,\pi'}}(\tau) + \mathscr{D}^{(1)}_{\substack{\mathbf{p},\mathbf{p}'\\ \pi,\pi'}}(\tau) + \mathscr{D}^{(2)}_{\substack{\mathbf{p},\mathbf{p}'\\ \pi,\pi'}}(\tau) + \dots \\ &= \mathscr{D}_{0\ \substack{\mathbf{p},\mathbf{p}'\\ \pi,\pi'}}(\tau) + \quad 0 \quad + \mathscr{D}^{(2)}_{\substack{\mathbf{p},\mathbf{p}'\\ \pi,\pi'}}(\tau) + \dots\end{aligned}$$

The second contribution reads

$$\frac{1}{2!}\oint_{\substack{\tau_1,\tau_2\in[0,\hbar\beta]\\ \mu,\mu'\in\{\downarrow,\uparrow\}\\ \mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}'\in\mathrm{Q}\\ m,m',n,n'\in\{1,2,\dots\}\\ \nu,\nu'\in\{1,2,\dots,rd\}}} \frac{-1}{\hbar}\frac{g_{mn\nu}(\mathbf{k},\mathbf{q})g_{m'n'\nu'}(\mathbf{k}',\mathbf{q}')}{\hbar^2 N_p}\langle A_{\mathbf{p}\pi}(\tau)A_{-\mathbf{p}'\pi'}(0)A_{\mathbf{q}\nu}(\tau_1)\overline{\psi}_{\mathbf{k}+\mathbf{q}m\mu}(\tau_1)\psi_{\mathbf{k}n\mu}(\tau_1)A_{\mathbf{q}'\nu'}(\tau_2)\overline{\psi}_{\mathbf{k}'+\mathbf{q}'m'\mu'}(\tau_2)\psi_{\mathbf{k}'n'\mu'}(\tau_2$$

where only [C]onnected [D]iagrams are summed over (linked cluster theorem). We can therefore simply sum over all diagrams and discard the disconnected diagrams.

$$\begin{aligned}&\langle A_{\mathbf{p}\pi}(\tau)A_{-\mathbf{p}'\pi'}(0)A_{\mathbf{q}\nu}(\tau_1)\overline{\psi}_{\mathbf{k}+\mathbf{q}m\mu}(\tau_1)\psi_{\mathbf{k}n\mu}(\tau_1)A_{\mathbf{q}'\nu'}(\tau_2)\overline{\psi}_{\mathbf{k}'+\mathbf{q}'m'\mu'}(\tau_2)\psi_{\mathbf{k}'n'\mu'}(\tau_2)\rangle_0^{\mathrm{CD}} \\ &= \langle A_{\mathbf{p}\pi}(\tau)A_{-\mathbf{p}'\pi'}(0)A_{\mathbf{q}\nu}(\tau_1)A_{\mathbf{q}'\nu'}(\tau_2)\rangle_0^{\mathrm{CD}}\,\langle\overline{\psi}_{\mathbf{k}+\mathbf{q}m\mu}(\tau_1)\psi_{\mathbf{k}n\mu}(\tau_1)\overline{\psi}_{\mathbf{k}'+\mathbf{q}'m'\mu'}(\tau_2)\psi_{\mathbf{k}'n'\mu'}(\tau_2)\rangle_0^{\mathrm{CD}}\end{aligned}$$

Computing the correlator of the phononic Green-functions yields two non-trivial contributions. Computing the correlator of the electronic Green-functions yields two more non-trivial contributions.

We therefore consider the correlator

$$\begin{aligned}\langle\overline{\psi}_{\mathbf{k}+\mathbf{q}m\mu}(\tau_1)\psi_{\mathbf{k}n\mu}(\tau_1)\overline{\psi}_{\mathbf{k}'+\mathbf{q}'m'\mu'}(\tau_2)\psi_{\mathbf{k}'n'\mu'}(\tau_2)\rangle_0 &= -\langle\psi_{\mathbf{k}n\mu}(\tau_1)\psi_{\mathbf{k}'n'\mu'}(\tau_2)\overline{\psi}_{\mathbf{k}+\mathbf{q}m\mu}(\tau_1)\overline{\psi}_{\mathbf{k}'+\mathbf{q}'m'\mu'}(\tau_2)\rangle_0 \\ &= -\langle\psi(A_1)\psi(A_2)\overline{\psi}(B_2)\overline{\psi}(B_1)\rangle_0 \\ &= -\sum_{\pi\in\mathrm{S}_2}\mathrm{sign}(\pi)\prod_{l=1}^{2}\langle\psi(A_l)\overline{\psi}(B_{\pi(l)})\rangle_0 \\ &= -\hbar^2\sum_{\pi\in\mathrm{S}_2}\mathrm{sign}(\pi)\prod_{l=1}^{2}\mathscr{G}_0(A_l,B_{\pi(l)}) \\ &= \dots\end{aligned}$$

The electronic correlator can now be evaluated with the Wick-theorem. In order to so, we will enumerate all the permutations of the group S_3.

$$\mathrm{S}_2 = \{\pi_1,\pi_2\} = \left\{\begin{pmatrix}1&2\\1&2\end{pmatrix},\begin{pmatrix}1&2\\2&1\end{pmatrix}\right\} \quad \text{with signatures} \quad \mathrm{sgn}(\pi_1,\pi_2) = (+1,-1). \tag{28.46}$$

this gives

$$\dots = -\hbar^2\left(\mathscr{G}_{0\ \substack{\mathbf{k},\mathbf{k}'+\mathbf{q}'\\ n,m'\\ \mu,\mu'}}(\tau_1-\tau_2)\mathscr{G}_{0\ \substack{\mathbf{k}',\mathbf{k}+\mathbf{q}\\ n',m\\ \mu',\mu}}(\tau_2-\tau_1) - \mathscr{G}_{0\ \substack{\mathbf{k},\mathbf{k}+\mathbf{q}\\ n,m\\ \mu,\mu}}(\tau_1-\tau_1)\mathscr{G}_{0\ \substack{\mathbf{k}',\mathbf{k}'+\mathbf{q}'\\ n',m'\\ \mu',\mu'}}(\tau_2-\tau_2)\right)$$

Now we turn to the phononic correlators

$$\begin{aligned}\langle A_{\mathbf{p}\pi}(\tau)A_{-\mathbf{p}'\pi'}(0)A_{\mathbf{q}\nu}(\tau_1)A_{\mathbf{q}'\nu'}(\tau_2)\rangle_0 &\equiv \langle A(x_1)A(x_2)A(x_3)A(x_4)\rangle_0 \\ &= \sum_{\substack{\text{Pairings of}\\ \{x_1,\dots,x_4\}}} \langle A(x_{k_1})A(x_{k_2})\rangle_0\langle A(x_{k_3})A(x_{k_4})\rangle_0 \\ &= \dots\end{aligned}$$

which gives [cf. Altland]

$$\begin{aligned}\dots &= \langle A(x_1)A(x_2)\rangle_0\langle A(x_3)A(x_4)\rangle_0 + \langle A(x_1)A(x_3)\rangle_0\langle A(x_2)A(x_4)\rangle_0 + +\langle A(x_1)A(x_4)\rangle_0\langle A(x_2)A(x_3)\rangle_0 \\ &= \langle A_{\mathbf{p}\pi}(\tau)A_{-\mathbf{p}'\pi'}(0)\rangle_0\langle A_{\mathbf{q}\nu}(\tau_1)A_{\mathbf{q}'\nu'}(\tau_2)\rangle_0 + \langle A_{\mathbf{p}\pi}(\tau)A_{\mathbf{q}\nu}(\tau_1)\rangle_0\langle A_{-\mathbf{p}'\pi'}(0)A_{\mathbf{q}'\nu'}(\tau_2)\rangle_0 + +\langle A_{\mathbf{p}\pi}(\tau)A_{\mathbf{q}'\nu'}(\tau_2)\rangle_0\langle A_{-\mathbf{p}'\pi'}(0)A_{\mathbf{q}} \\ &= \hbar^2\left(\mathscr{D}^{\ 0}_{\substack{\pi,\pi'\\ \mathbf{p},\mathbf{p}'}}(\tau)\mathscr{D}^{\ 0}_{\substack{\nu,\nu'\\ \mathbf{q},-\mathbf{q}'}}(\tau_1-\tau_2) + \mathscr{D}^{\ 0}_{\substack{\pi,\nu\\ \mathbf{p},-\mathbf{q}}}(\tau-\tau_1)\mathscr{D}^{\ 0}_{\substack{\pi',\nu'\\ -\mathbf{p},-\mathbf{q}'}}(-\tau_2) + \mathscr{D}^{\ 0}_{\substack{\pi,\nu'\\ \mathbf{p},-\mathbf{q}'}}(\tau-\tau_2)\mathscr{D}^{\ 0}_{\substack{\pi',\nu\\ -\mathbf{p}',-\mathbf{q}}}(-\tau_1)\right)\end{aligned}$$

whereas the first term will not contribute since it does not resemble a one particle irreducible diagram (or something like that... external vertices are not connected to inner ones...).

This gives us the intermediate result

$$\begin{aligned}\mathscr{D}^{(2)}_{\substack{\mathbf{p},\mathbf{p}'\\ \pi,\pi'}}(\tau) = \sum\!\!\!\!\!\!\int_{\substack{\tau_1,\tau_2\in[0,\hbar\beta]\\ \mu,\mu'\in\{\downarrow,\uparrow\}\\ \mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}'\in\mathrm{Q}\\ m,m',n,n'\in\{1,2,\dots\}\\ \nu,\nu'\in\{1,2,\dots,rd\}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})g_{m'n'\nu'}(\mathbf{k}',\mathbf{q}')}{2\hbar^{-1}N_p}&\left(\mathscr{G}^{\ 0}_{\substack{\mathbf{k},\mathbf{k}'+\mathbf{q}'\\ n,m'\\ \mu,\mu'}}(\tau_1-\tau_2)\mathscr{G}^{\ 0}_{\substack{\mathbf{k}',\mathbf{k}+\mathbf{q}\\ n',m\\ \mu',\mu}}(\tau_2-\tau_1) - \mathscr{G}^{\ 0}_{\substack{\mathbf{k},\mathbf{k}+\mathbf{q}\\ n,m\\ \mu,\mu}}(\tau_1-\tau_1)\mathscr{G}^{\ 0}_{\substack{\mathbf{k}',\mathbf{k}'+\mathbf{q}'\\ n',m'\\ \mu',\mu'}}(\tau_2-\tau_2)\right) \\ &\times\left(\mathscr{D}^{\ 0}_{\substack{\pi,\nu\\ \mathbf{p},-\mathbf{q}}}(\tau-\tau_1)\mathscr{D}^{\ 0}_{\substack{\pi',\nu'\\ -\mathbf{p},-\mathbf{q}'}}(-\tau_2) + \mathscr{D}^{\ 0}_{\substack{\pi,\nu'\\ \mathbf{p},-\mathbf{q}'}}(\tau-\tau_2)\mathscr{D}^{\ 0}_{\substack{\pi',\nu\\ -\mathbf{p}',-\mathbf{q}}}(-\tau_1)\right)\end{aligned}$$

This yields four contributions to the phonon-propagator, which we enumerate with

- $(1)-(i)$
- $(1)-(ii)$
- $(2)-(i)$
- $(2)-(ii)$

We now consider a generic (periodic) function of the type

$$\mathscr{F}(\tau) = \iint_{[0,\hbar\beta]^2} \mathrm{d}(\tau_1,\tau_2)\,\mathscr{D}(\tau-\tau_{k_1})\mathscr{D}(\tau_{k_2})\mathscr{G}(\tau_{k_3}-\tau_{k_4})\mathscr{G}(\tau_{k_5}-\tau_{k_6}) \tag{28.47}$$

The Matsubara-component of this function reads

$$\begin{aligned}\mathscr{F}(\mathrm{i}\omega_n) &= \iiint_{[0,\hbar\beta]^3} \mathrm{d}(\tau,\tau_1,\tau_2)\, \mathscr{D}(\tau-\tau_{k_1})\mathscr{D}(\tau_{k_2})\mathscr{G}(\tau_{k_3}-\tau_{k_4})\mathscr{G}(\tau_{k_5}-\tau_{k_6})\mathrm{e}^{\mathrm{i}\omega_n\tau} \\ &= \frac{1}{(\hbar\beta)^4} \sum_{\substack{\omega_{n_1},\omega_{n_2}\in\Omega_{+1} \\ \omega_{n_3},\omega_{n_4}\in\Omega_{-1}}} \mathscr{D}(\mathrm{i}\omega_{n_1})\mathscr{D}(\mathrm{i}\omega_{n_2})\mathscr{G}(\mathrm{i}\omega_{n_3})\mathscr{G}(\mathrm{i}\omega_{n_4}) \iiint_{[0,\hbar\beta]^3} \mathrm{d}(\tau,\tau_1,\tau_2)\mathrm{e}^{\mathrm{i}\tau(\omega_n-\omega_{n_1})+\mathrm{i}\tau_{k_1}\omega_{n_1}-\mathrm{i}\tau_{k_2}\omega_{n_2}-\mathrm{i}(\tau_{k_3}-\tau_{k_4})\omega_{n_3}-\mathrm{i}\omega_{n_4}(\tau_{k_5}-}\end{aligned}$$

We now compute the Matsubara-component of each contribution individually and sum up the results afterwards.

ToBeContinued.

29. Appendix - B-Sides

29.1. The Many-Body-Formalism for Indistinguishable Particles: Second Quantization - Operator Formalism

29.1.1. The Fock-Space

The construction of many-body Hilbert-spaces for indistinguishable particles is way more tedious. The initial situation (which one encounters quite naturally in typical materials) is as follows.

Notation 29.1 Let $\mathcal{H} = \text{span}_{\mathbb{C}}\{|1\rangle, |2\rangle, \dots |\text{d}_{\mathcal{H}}\rangle\}$ be a single-particle Hilbert-space with (not neccessarily, oftentimes orthonormal) basis and corresponding wavefunctions / state-vectors with coordinates x

$$\langle\, x \,|\, i \,\rangle \equiv \psi_i(x). \tag{29.1}$$

whereas $\langle\ ,\ \rangle$ refers to the scalarproduct on $\mathcal{H}$.

Note. Almost all of the following formulas need an *orthonormal* basis, $\langle i|j\rangle = \delta_{ij}$: the completeness relations, the overlaps with $\prod_k \text{n}_k!$, the normalization of the quasi-occupation-number-states, the action of the annihilation-operators (Kronecker-deltas) and the commutation relations. [38, p. 4, 8] make the same assumption: "whenever the symbol $|\alpha_1 \dots \alpha_N\rangle$ is utilized, the basis $\{|\alpha_i\rangle\}$ is orthonormal". We assume this from now on. For a non-orthonormal basis, every δ_{ij} below has to be replaced by $\langle i|j\rangle$ (e.g. $[c_i, c_j^\dagger]_\zeta = \langle i|j\rangle$), and the completeness relations need the dual basis. Moreover, $|x\rangle$ is not an element of $\mathcal{H}$ but a generalized position eigenstate (cf. Section 29.8); $\psi_i(x) = \langle x|i\rangle$ is the coordinate representation of $|i\rangle$.

Notation 29.2 In this section we denote $N \in \mathbb{N}_0$ to be a natural number.

Definition 29.3 We define the *unsymmetrized (and unphysical) N-particle-Hilbert-space* $\mathscr{H}_N$ as tensor product

$$\mathscr{H}_N = \mathcal{H} \otimes \mathcal{H} \otimes \cdots \otimes \mathcal{H}. \tag{29.2}$$

(N factors, [38, Eq. (1.26)]; for $N = 0$ we set $\mathscr{H}_0 := \mathbb{C}$.)

Remark 29.3.1 This is not the Hilbert-space that one is allowed to work with. Only a subspace of it (depending on the "statistics" of the particles at hand) is relevant for computations.

Important Spanning Set / Basis 1 (of $\mathscr{H}_N$)

Corollary 29.4 A basis of $\mathscr{H}_N$ is given by the set

$$\mathscr{B}_{\mathscr{H}_N} \equiv \left\{ |i_1, i_2, \dots, i_N) \equiv |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_N\rangle \mid i_j \in \{1, \dots, \mathrm{d}_{\mathcal{H}}\} \right\} \tag{29.3}$$

Proof 29.4 See introductory lectures about tensor-products.

Remark 29.4.1 Recall that the *scalar-product* between two basis-vectors is defined as

$$\begin{aligned}(i_1, i_2, \dots, i_N \mid j_1, j_2, \dots, j_N) &\equiv \left(\langle i_1| \otimes \langle i_2| \otimes \dots \otimes \langle i_N|\right) \left(|j_1\rangle \otimes |j_2\rangle \otimes \dots \otimes |j_N\rangle\right) \\ &\equiv \langle i_1 \mid j_1\rangle\langle i_2 \mid j_2\rangle \cdots \langle i_N \mid j_N\rangle\end{aligned}$$

and by sesqui-linearity thus on the entire Hilbert-space.

Remark 29.4.2 Recall that the basis yields a *completeness relation* on $\mathscr{H}_N$ given through projectors as

$$1_{\mathscr{H}_N} \equiv \sum_{i_1, i_2, \dots, i_N = 1}^{\mathrm{d}_{\mathcal{H}}} |i_1, i_2, \dots, i_N)(i_1, i_2, \dots, i_N|. \tag{29.4}$$

(This needs an orthonormal basis $\{|i\rangle\}$ of $\mathcal{H}$, [38, Eq. (1.30)]; then $\{|i_1, \dots, i_N)\}$ is an orthonormal basis of $\mathscr{H}_N$ by the previous Remark.)

Notation 29.5 We write for the value of a wavefunction at some coordinate-tuple

$$\begin{aligned}\psi_{i_1, i_2, \dots, i_N}(x_1, x_2, \dots, x_N) &\equiv (x_1, x_2, \dots, x_N \mid i_1, i_2, \dots, i_N), \\ &\equiv \left(\langle x_1| \otimes \langle x_2| \otimes \dots \otimes \langle x_N|\right) \left(|i_1\rangle \otimes |i_2\rangle \otimes \dots \otimes |i_N\rangle\right), \\ &\equiv \psi_{i_1}(x_1)\psi_{i_2}(x_2) \cdots \psi_{i_N}(x_N).\end{aligned}$$

Definition 29.6 For $\zeta \in \{-1, +1\}$, and $N \in \mathbb{N}_0$ we define the *ζ-Fock-subspaces* $\mathscr{F}_\zeta^N$ as

$$\begin{aligned}\mathscr{F}_\zeta^0 &= \mathbb{C}, \\ \mathscr{F}_\zeta^N &= \left\{ \psi \in \mathscr{H}_N \mid \forall \pi \in \mathrm{S}_N : \psi(x_{\pi(1)}, \dots, x_{\pi(N)}) = \mathrm{sign}(\pi)^{1-\theta(\zeta)} \psi(x_1, \dots, x_N) \right\} \quad \text{for } N \geq 1.\end{aligned} \tag{29.5}$$

Remark 29.6.1 It might seem redundant to consider a subspace with zero-particles. This has computational reasons. It will later turn out, that it is easier to compute observables, when one is working in the grand-canonical ensemble, which makes this construction (mathematically) neat.

Remark 29.6.2 We remark that the dimensions of the individual subspaces can be written explicitly in terms of N, ζ and $\mathrm{d}_{\mathcal{H}}$. We will compute them in Theorem 7.7. At this point we simply state the result that in the case of fermions (i.e. $\zeta = -1$) there is an $N_{\max} \equiv N_{\max}(\mathrm{d}_{\mathcal{H}}) \in \mathbb{N}$ such that $\mathscr{F}_{\zeta}^{N} = \{0\}$ for all $N > N_{\max}$.

Completion. Explicitly, $N_{\max} = \mathrm{d}_{\mathcal{H}}$, and (with the occupation-number-states below as a basis) $\dim \mathscr{F}_{-1}^{N} = \binom{\mathrm{d}_{\mathcal{H}}}{N}$ (choose N distinct occupied states), $\dim \mathscr{F}_{+1}^{N} = \binom{\mathrm{d}_{\mathcal{H}}+N-1}{N}$ (number of $(\mathrm{n}_1, \dots, \mathrm{n}_{\mathrm{d}_{\mathcal{H}}}) \in \mathbb{N}_0^{\mathrm{d}_{\mathcal{H}}}$ with $\sum_k \mathrm{n}_k = N$).

Lemma 29.7 We define the *statistical-symmetrization-operator* as linear mapping

$$\begin{aligned} \mathrm{P}_{\zeta} : \mathscr{H}_N &\to \mathscr{F}_{\zeta}^{N} \\ \psi &\mapsto \mathrm{P}_{\zeta}\,\psi \end{aligned}$$

as

$$\left(\mathrm{P}_{\zeta}\,\psi\right)(x_1, x_2, \dots, x_N) := \frac{1}{N!} \sum_{\pi \in \mathrm{S}_N} \mathrm{sign}(\pi)^{1-\theta(\zeta)}\, \psi(x_{\pi(1)}, x_{\pi(2)}, \dots, x_{\pi(N)}). \tag{29.6}$$

Proof 29.7 We have to prove that

$$\left(\mathrm{P}_{\zeta}\,\psi\right)(x_{\sigma(1)}, \dots, x_{\sigma(N)}) = \mathrm{sign}(\sigma)^{1-\theta(\zeta)} \left(\mathrm{P}_{\zeta}\,\psi\right)(x_1, \dots, x_N) \tag{29.7}$$

which is easy to see after relabeling the summations and since $\mathrm{sign}(\sigma) = \mathrm{sign}(\sigma^{-1})$.

Details. Abbreviate $s(\pi) \equiv \mathrm{sign}(\pi)^{1-\theta(\zeta)}$, which is multiplicative, $s(\pi\circ\rho) = s(\pi)s(\rho)$, with $s(\pi^{-1}) = s(\pi)$. With $y_l \equiv x_{\sigma(l)}$ we have $y_{\pi(l)} = x_{\sigma(\pi(l))}$, hence, substituting $\rho = \sigma\circ\pi$ (a bijection of S_N for fixed σ),

$$\begin{aligned} (\mathrm{P}_{\zeta}\,\psi)(y_1, \dots, y_N) &= \frac{1}{N!} \sum_{\pi} s(\pi)\psi(x_{\sigma(\pi(1))}, \dots, x_{\sigma(\pi(N))}) \\ &= \frac{1}{N!} \sum_{\rho} s(\sigma^{-1}\circ\rho)\psi(x_{\rho(1)}, \dots, x_{\rho(N)}) = s(\sigma)(\mathrm{P}_{\zeta}\,\psi)(x_1, \dots, x_N). \end{aligned}$$

Corollary 29.8 The statistical-symmetrization-operator is a projector, i.e. it holds $\mathrm{P}_{\zeta} \circ \mathrm{P}_{\zeta} = \mathrm{P}_{\zeta}$.

Proof 29.8 See Appendix, p. 637.

Lemma 29.9 The statistical symmetrization-operator P_{ζ} acts as the identity on the subspace $\mathscr{F}_{\zeta}^{N}$, i.e.

$$\forall \psi \in \mathscr{F}_{\zeta}^{N} \,:\, \mathrm{P}_{\zeta}\,\psi \equiv 1_{\mathscr{F}_{\zeta}^{N}}\psi = \psi \tag{29.8}$$

Proof 29.9 Using the symmetry-property in Equation (29.5) we obtain a sum of $N!$ identical contributions which cancels out the prefactor in Equation (29.6).

Theorem 29.10 It follows

$$\mathrm{P}_{+1}\,\mathrm{P}_{-1} = \mathrm{P}_{-1}\,\mathrm{P}_{+1} = 0 \tag{29.9}$$

Proof 29.10 We compute for example

$$\begin{aligned}\left(\mathrm{P}_{+1}\,\mathrm{P}_{-1}\,\psi\right)(x_1,\ldots,x_N) &= \frac{1}{N!}\sum_{\pi\in \mathrm{S}_N}\left(\mathrm{P}_{-1}\,\psi\right)(x_{\pi(1)},\ldots,x_{\pi(N)}) \\ &= \frac{1}{N!}\left(\sum_{\pi\in \mathrm{S}_N}\mathrm{sign}(\pi)\right)\left(\mathrm{P}_{-1}\,\psi\right)(x_1,\ldots,x_N) \\ &= 0\end{aligned}$$

Correction note. The Theorem holds only for $N \geq 2$. The second equation sign uses $\mathrm{P}_{-1}\,\psi \in \mathscr{F}^N_{-1}$, i.e. $(\mathrm{P}_{-1}\,\psi)(x_{\pi(1)},\ldots) = \mathrm{sign}(\pi)(\mathrm{P}_{-1}\,\psi)(x_1,\ldots)$. The last equation sign uses $\sum_{\pi\in \mathrm{S}_N}\mathrm{sign}(\pi) = 0$, which is true only for $N \geq 2$: the even and the odd permutations are in bijection via $\pi \mapsto (1\,2)\circ\pi$. For $N \in \{0,1\}$ one has $\mathrm{S}_N = \{\mathrm{id}\}$, hence $\mathrm{P}_{+1} = \mathrm{P}_{-1} = 1_{\mathscr{H}_N}$ and $\mathrm{P}_{+1}\,\mathrm{P}_{-1} = 1 \neq 0$ (a single particle is both a "Boson" and a "Fermion" state, $\mathscr{F}^1_{+1} = \mathscr{F}^1_{-1} = \mathcal{H}$). The second product $\mathrm{P}_{-1}\,\mathrm{P}_{+1}$ is computed in the same way, with the roles of $\mathrm{sign}(\pi)$ and 1 exchanged.

Lemma 29.11 For *pure tensor-product states* $|\psi\rangle$, i.e. states that can be written as

$$|\psi\rangle = \bigotimes_{j=1}^{N}|\psi_j\rangle \tag{29.10}$$

for some $|\psi_j\rangle \in \mathcal{H}$, it follows

$$\mathrm{P}_\zeta\,|\psi\rangle = \frac{1}{N!}\sum_{\pi\in \mathrm{S}_N}\mathrm{sign}(\pi)^{1-\theta(\zeta)}\bigotimes_{j=1}^{N}|\psi_{\pi(j)}\rangle \tag{29.11}$$

and one obtains *Slater-determinants* and *permanents* for the coordinate representations as

$$(x_1,x_2,\ldots,x_N\,|\,\mathrm{P}_\zeta\,|\,\psi\,\rangle = \frac{1}{N!}\begin{vmatrix}\langle x_1|\psi_1\rangle_{\mathcal{H}} & \cdots & \langle x_1|\psi_N\rangle_{\mathcal{H}} \\ \vdots & \ddots & \vdots \\ \langle x_n|\psi_1\rangle_{\mathcal{H}} & \cdots & \langle x_n|\psi_n\rangle_{\mathcal{H}}\end{vmatrix}_\zeta . \tag{29.12}$$

Note. In the last row n has to be N, i.e. the entries are $\langle x_N|\psi_1\rangle, \dots, \langle x_N|\psi_N\rangle$. The symbol $|M|_\zeta$ for an $N \times N$-matrix M is not defined yet; it is the "ζ-determinant" [38, Eqs. (1.47), (1.48)]

$$|M|_\zeta := \sum_{\pi\in \mathrm{S}_N} \mathrm{sign}(\pi)^{1-\theta(\zeta)} M_{1,\pi(1)} M_{2,\pi(2)} \cdots M_{N,\pi(N)} = \begin{cases} \det(M), & \zeta = -1 \text{ (Slater-determinant)} \\ \mathrm{Per}(M), & \zeta = +1 \text{ (permanent)} \end{cases}$$

applied to $M_{lm} = \langle x_l|\psi_m\rangle$. Indeed, Equation (29.11) gives $(x_1, \dots, x_N|\,\mathrm{P}_\zeta\,|\psi\rangle = \frac{1}{N!}\sum_\pi \mathrm{sign}(\pi)^{1-\theta(\zeta)} \prod_l \langle x_l|\psi_{\pi(l)}\rangle = \frac{1}{N!}|M|_\zeta$.

Proof 29.11 See Appendix, p. 638.

Definition 29.12 For a permutation $\pi \in \mathrm{S}_N$ we define its *action on a product-state*

$$|\psi\rangle = \bigotimes_{j=1}^{N} |\psi_j\rangle \tag{29.13}$$

as

$$\pi|\psi\rangle := \bigotimes_{j=1}^{N} |\psi_{\pi(j)}\rangle \tag{29.14}$$

Lemma 29.13 Now the statistical symmetrization-operator can be written for pure states as

$$\mathrm{P}_\zeta := \frac{1}{N!}\sum_{\pi\in \mathrm{S}_N} \mathrm{sign}(\pi)^{1-\theta(\zeta)}\,\pi \tag{29.15}$$

Proof 29.13 Follows with Equation (29.11).

Remark 29.13.1 Notice that by linear extension this is equation can be used to act on any state in $\mathscr{H}_N$ (since every element can be expandend w.r.t. the basis in Equation (29.3).

Note. "Pure states" in the Lemma means pure tensor-product states as in Equation (29.10), not pure states in the sense of density matrices. The well-defined way to read the Definition is: define π on the basis vectors, $\pi|i_1, \dots, i_N) := |i_{\pi(1)}, \dots, i_{\pi(N)})$, and extend it linearly; by multilinearity of $\otimes$ this reproduces the Definition on all product states. With this definition $\pi(\sigma|\psi\rangle) = (\sigma\circ\pi)|\psi\rangle$, i.e. the action is a right action (the map from S_N to the operators on $\mathscr{H}_N$ is an anti-homomorphism). This does not matter for P_ζ, because the sum runs over the whole group and $\mathrm{sign}(\pi) = \mathrm{sign}(\pi^{-1})$.

Lemma 29.14 The statistical symmtrization-operator P_ζ is hermitian w.r.t. the scalar-product on $\mathscr{H}_N$.

Proof 29.14 See Appendix, p. 639.

Important Spanning Set / Basis 2 (of $\mathscr{F}_\zeta^N$)

Definition 29.15 For $i_1, \dots, i_N \in \{1, 2, \dots, \mathrm{d}_H\}$, we define *auxiliary-states* as

$$\begin{aligned} |i_1, i_2, \dots, i_N\} &= \frac{\mathrm{P}_\zeta}{N!^{-1/2}} |i_1, i_2, \dots, i_N) \\ &= \frac{1}{\sqrt{N!}} \sum_{\pi \in \mathrm{S}_N} \mathrm{sign}(\pi)^{1-\theta(\zeta)} |i_{\pi(1)}\rangle \otimes |i_{\pi(2)}\rangle \otimes \cdots \otimes |i_{\pi(N)}\rangle. \end{aligned} \tag{29.16}$$

Remark 29.15.1 Notice that in the special case of $N = 1$ one finds $|i\} = |i)$.

Remark 29.15.2 Introducing these states is a bit problematic from a pedagogical perspective, since they **only** serve in order to introduce the so-called „occupation number states“ later on (which will turn out to be the basis of states that we are **actually** interested in working with).

Lemma 29.16 The auxiliary-states have the property

$$\forall \sigma \in \mathrm{S}_N \ : \ |i_{\sigma(1)}, i_{\sigma(2)}, \dots, i_{\sigma(N)}\} = \mathrm{sign}(\sigma)^{1-\theta(\zeta)} |i_1, i_2, \dots, i_N\} \tag{29.17}$$

Proof 29.16 We prove this theorem by referring to the coordinate representation of the auxiliary-states. We therefore consider $\sigma \in \mathrm{S}_N$ and we compute

$$\begin{aligned} (x_1, x_2, \dots, x_N | i_{\sigma(1)}, i_{\sigma(2)}, \dots, i_{\sigma(N)}\} &= \frac{1}{\sqrt{N!}} \sum_{\pi \in \mathrm{S}_N} \mathrm{sign}(\pi)^{1-\theta(\zeta)} \prod_{l=1}^{N} \langle x_l | i_{\pi(\sigma(l))}\rangle \\ &= \mathrm{sign}(\sigma)^{1-\theta(\zeta)} \frac{1}{\sqrt{N!}} \sum_{\pi \in \mathrm{S}_N} \mathrm{sign}(\pi\circ\sigma)^{1-\theta(\zeta)} \prod_{l=1}^{N} \langle x_l | i_{\pi(\sigma(l))}\rangle \\ &= \mathrm{sign}(\sigma)^{1-\theta(\zeta)} (x_1, x_2, \dots, x_N | i_1, i_2, \dots, i_N\} \end{aligned}$$

which proves the Lemma.

Note. With $j_m \equiv i_{\sigma(m)}$ the l-th factor of $|j_{\pi(1)}\rangle \otimes \cdots \otimes |j_{\pi(N)}\rangle$ is $|i_{\sigma(\pi(l))}\rangle$, so the first line should read $\langle x_l | i_{\sigma(\pi(l))}\rangle$ (composition $\sigma\circ\pi$, not $\pi\circ\sigma$), and the second line $\mathrm{sign}(\sigma\circ\pi)^{1-\theta(\zeta)}$. The argument is the same: substitute $\rho = \sigma\circ\pi$ and use $\mathrm{sign}(\pi) = \mathrm{sign}(\sigma)\,\mathrm{sign}(\sigma\circ\pi)$. The result is unchanged. Alternatively, without coordinates: $|i_{\sigma(1)}, \dots\} = \sqrt{N!}\,\mathrm{P}_\zeta\,\sigma|i_1, \dots) = \sqrt{N!}\ \mathrm{sign}(\sigma)^{1-\theta(\zeta)}\,\mathrm{P}_\zeta\,|i_1, \dots)$, since $\mathrm{P}_\zeta\,\sigma = \mathrm{sign}(\sigma)^{1-\theta(\zeta)}\,\mathrm{P}_\zeta$ (relabel the sum).

Remark 29.16.1 Notice that this implies in the fermionic case (i.e. $\zeta = -1$) that if $i_j = i_{j'}$ for some $j, j' \in \{1, \dots, N\}$, then $|i_1, i_2, \dots, i_N\} = 0$.

Corollary 29.17 One obtains the completeness relation on $\mathscr{F}_\zeta^N$ as

$$1_{\mathscr{F}_\zeta^N} \equiv \frac{1}{N!} \sum_{i_1,\dots,i_N=1}^{\mathrm{d}_\mathcal{H}} |i_1,\dots,i_N\}\{i_1,\dots,i_N|. \tag{29.18}$$

Proof 29.17 We compute

$$\begin{aligned}
\frac{1}{N!} \sum_{i_1,\dots,i_N=1}^{\mathrm{d}_\mathcal{H}} |i_1,\dots,i_N\}\{i_1,\dots,i_N| &= \frac{1}{N!} \sum_{i_1,\dots,i_N=1}^{\mathrm{d}_\mathcal{H}} \sqrt{N!}\,\mathrm{P}_\zeta\ |i_1,\dots,i_N)(i_1,\dots,i_N|\ \sqrt{N!}\,\mathrm{P}_\zeta \\
&= \mathrm{P}_\zeta \left[\sum_{i_1,\dots,i_N=1}^{\mathrm{d}_\mathcal{H}} |i_1,\dots,i_N)(i_1,\dots,i_N| \right] \mathrm{P}_\zeta \\
&= \mathrm{P}_\zeta\ 1_{\mathscr{H}_N}\ \mathrm{P}_\zeta \\
&= \mathrm{P}_\zeta \\
&= 1_{\mathscr{F}_\zeta^N}\ .
\end{aligned}$$

whereas we used Equation (29.4), the fact that P_ζ is a projector (cf. Corollary 29.8) and that it acts as the identity on $\mathscr{F}_\zeta^N$ (cf. Lemma 29.9).

(In the first equation sign one also needs the hermiticity $\mathrm{P}_\zeta^\dagger = \mathrm{P}_\zeta$, Lemma 29.14, to write the bra as $\{i| = \sqrt{N!}\,(i|\,\mathrm{P}_\zeta$. The last equation sign means: as an operator on $\mathscr{H}_N$, P_ζ is the orthogonal projector onto $\mathscr{F}_\zeta^N$, i.e. its restriction to $\mathscr{F}_\zeta^N$ is $1_{\mathscr{F}_\zeta^N}$. Cf. [38, Eq. (1.40)].)

Lemma 29.18 It follows

$$\{i_1, i_2, \dots, i_N \,|\, j_1, j_2, \dots, j_N\} = \sum_{\pi\in \mathrm{S}_N} \mathrm{sign}(\pi)^{1-\theta(\zeta)} \prod_{k=1}^{N} \langle i_k \,|\, j_{\pi(k)}\rangle \tag{29.19}$$

Proof 29.18 We compute straightforwardly

$$\begin{aligned}
\{i_1, i_2, \dots, i_N \,|\, j_1, j_2, \dots, j_N\} &= N!(i_1, i_2, \dots, i_N|\,\mathrm{P}_\zeta^2\,|j_1, j_2, \dots, j_N) \\
&= N!(i_1, i_2, \dots, i_N|\,\mathrm{P}_\zeta\,|j_1, j_2, \dots, j_N) \\
&= \sum_{\pi\in \mathrm{S}_N} \mathrm{sign}(\pi)^{1-\theta(\zeta)} (i_1, \dots, i_N|\,\left(|j_{\pi(1)}\rangle \otimes |j_{\pi(2)}\rangle \otimes \cdots \otimes |j_{\pi(N)}\rangle\right)) \\
&= \sum_{\pi\in \mathrm{S}_N} \mathrm{sign}(\pi)^{1-\theta(\zeta)} \prod_{k=1}^{N} \langle i_k \,|\, j_{\pi(k)}\rangle \\
&= \sum_{\pi\in \mathrm{S}_N} \mathrm{sign}(\pi)^{1-\theta(\zeta)}\, \langle i_1 \,|\, j_{\pi(1)}\rangle \langle i_2 \,|\, j_{\pi(2)}\rangle \cdots \langle i_N \,|\, j_{\pi(N)}\rangle
\end{aligned} \tag{29.20}$$

Remark 29.18.1 Notice that the auxiliary states in Definition 29.15 are not a basis, because of Lemma 29.16, but they form an overcomplete set, because of Corollary 29.17. Because of Lemma 29.18 it is evident that these states form an *overcomplete set*.

Correction note. The last sentence is not what Lemma 29.18 shows. "Overcomplete" means: the set spans $\mathscr{F}_\zeta^N$ (Corollary 29.17), but it is linearly dependent (Lemma 29.16: permuted index tuples give the same vector up to a sign, and for Fermions some vectors vanish). Lemma 29.18 (together with the next Corollary) shows instead that the states are *not normalized*, $\{i_1 \dots i_N | i_1 \dots i_N\} = \prod_k \mathrm{n}_k!$, and that the states with non-decreasing (Bosons) resp. strictly increasing (Fermions) indices $i_1 \leq \dots \leq i_N$ resp. $i_1 < \dots < i_N$ are mutually orthogonal and form a basis.

Definition 29.19 For each $k \in \{1, 2, \dots, \mathrm{d}_{\mathcal{H}}\}$, we introduce the *occupation-numbers of a state w.r.t. a basis* as functions

$$\begin{aligned} \mathrm{n}_k : \{1, \dots, \mathrm{d}_{\mathcal{H}}\}^N &\longrightarrow \mathbb{N}_0 \\ (i_1, \dots, i_N) \equiv i &\mapsto \mathrm{n}_k(i_1, \dots, i_N) := \sum_{l=1}^{N} \delta_{i_l,k} \equiv \mathrm{n}_k, \end{aligned}$$

whereas we define $\mathrm{n}_k(\bullet) \equiv 0$ for $N = 0$.

(Correction: the codomain is $\mathbb{N}_0$, since $\mathrm{n}_k = 0$ is possible.)

Remark 29.19.1 Notice that this implies with Remark 29.16.1 that in the fermionic case (i.e. $\zeta = -1$) it holds $\mathrm{n}_k \in \{0, 1\}$ for all $k \in \{1, 2, \dots, \mathrm{d}_{\mathcal{H}}\}$.

Note. More precisely: n_k is defined for every index tuple, also for Fermions (e.g. $\mathrm{n}_1(1, 1) = 2$). What Remark 29.16.1 implies is: for $\zeta = -1$, $|i_1, \dots, i_N\} \neq 0$ only if $\mathrm{n}_k(i_1, \dots, i_N) \in \{0, 1\}$ for all k (Pauli principle, [38, Eq. (1.39)]).

Corollary 29.20 The overlap between different vectors is given by

$$\{i_1, i_2, \dots, i_N \mid j_1, j_2, \dots, j_N\} = \begin{cases} \mathrm{sign}(\sigma)^{1-\theta(\zeta)} \prod_{k=1}^{\mathrm{d}_{\mathcal{H}}} \mathrm{n}_k! & \text{if } \exists\, \sigma \in \mathrm{S}_N \ : \ (i_1, i_2, \dots, i_N) = (j_{\sigma(1)}, \dots, j_{\sigma(N)}) \\ 0 & \text{otherwise.} \end{cases}$$

Correction note. (i) This needs an orthonormal basis. (ii) For Fermions the formula is only correct if all $\mathrm{n}_k \in \{0, 1\}$ (then $\prod_k \mathrm{n}_k! = 1$ and the overlap is $\mathrm{sign}(\sigma)$, [38, Eq. (1.43a)]). If some $\mathrm{n}_k \geq 2$, then $|j_1, \dots, j_N\} = 0$ and the overlap is 0, not $\pm \prod_k \mathrm{n}_k!$. (iii) For Bosons $\mathrm{sign}(\sigma)^{1-\theta(\zeta)} = 1$, and the result is [38, Eq. (1.43b)]. Both cases are summarized in [38, Eq. (1.45)].

Proof 29.20 If the numbers $i_1, \dots, i_N$ are *not* a permutation of the numbers $j_1, \dots, j_N$, then there is in the right hand side of Equation (29.19) for each summand at least one factor which is zero, such that the entire sum vanishes. We divide the rest of the proof into two cases.

Case 1: $\zeta = -1$:

Then it follows with Remarks 29.19.1 and 29.16.1 that if the numbers are a permutation of each other, i.e. if there is some $\sigma \in \mathrm{S}_N$ such that $(i_1, i_2, \dots, i_N) = (j_{\sigma(1)}, \dots, j_{\sigma(N)})$, then only one summand contributes in Equation (29.19), yielding the result from Equation (29.18) as

$$\begin{aligned} \{i_1, i_2, \dots, i_N \mid j_1, j_2, \dots, j_N\} &= \sum_{\pi \in \mathrm{S}_N} \operatorname{sign}(\pi) \prod_{k=1}^{N} \langle i_k \mid j_{\pi(k)} \rangle \\ &= \sum_{\pi \in \mathrm{S}_N} \operatorname{sign}(\pi) \prod_{k=1}^{N} \langle j_{\sigma(k)} \mid j_{\pi(k)} \rangle \\ &= \operatorname{sign}(\sigma) \sum_{\pi \in \mathrm{S}_N} \operatorname{sign}(\sigma^{-1} \circ \pi) \prod_{k=1}^{N} \langle i_k \mid j_{(\sigma^{-1} \circ \pi)(k)} \rangle \\ &= \operatorname{sign}(\sigma) \end{aligned} \tag{29.21}$$

since there is only one permutation that contributes to the sum.

Correction note. The third line is not correct as written: it changes $\langle j_{\sigma(k)} | j_{\pi(k)} \rangle$ into $\langle i_k | j_{(\sigma^{-1}\circ\pi)(k)} \rangle$. Correctly: since the $j_1, \dots, j_N$ are pairwise distinct (otherwise both sides vanish, cf. the note after the Corollary) and the basis is orthonormal, $\prod_k \langle j_{\sigma(k)} | j_{\pi(k)} \rangle = \prod_k \delta_{\sigma(k),\pi(k)} = \delta_{\pi,\sigma}$. Hence the sum over π gives $\operatorname{sign}(\sigma)$ directly. The reference "Equation (29.18)" means Lemma 29.18, Equation (29.19).

Case 2: $\zeta = +1$:

For bosons, we use Lemma 29.16 in order to write $\{i_1, i_2, \dots, i_N \mid = \{j_1, j_2, \dots, j_N \mid$ and we obtain with Equation (29.18) then the overlap as

$$\begin{aligned} \{i_1, i_2, \dots, i_N \mid j_1, j_2, \dots, j_N\} &= \{j_1, j_2, \dots, j_N \mid j_1, j_2, \dots, j_N\} \\ &= \sum_{\pi \in \mathrm{S}_N} \prod_{k=1}^{N} \langle j_k \mid j_{\pi(k)} \rangle \\ &= \dots \end{aligned} \tag{29.22}$$

the only permutations that contribute are now those, where identical j_k are being mapped onto each other. For each $k \in \{1, 2, \dots, \mathrm{d}_{\mathcal{H}}\}$ there are $\mathrm{n}_k!$ such permutations, which yields the result.

Completion of the "…". With an orthonormal basis, $\prod_k \langle j_k | j_{\pi(k)} \rangle = \prod_k \delta_{j_k, j_{\pi(k)}} \in \{0, 1\}$. It equals 1 exactly if π lies in the stabilizer $\mathrm{Stab}(j) = \{\pi \in \mathrm{S}_N \mid j_{\pi(k)} = j_k \ \forall k\}$, i.e. if π only permutes positions with equal entries. Hence

$$\dots = |\operatorname{Stab}(j)| = \left| \mathrm{S}_{\mathrm{n}_1} \times \mathrm{S}_{\mathrm{n}_2} \times \cdots \times \mathrm{S}_{\mathrm{n}_{\mathrm{d}_{\mathcal{H}}}} \right| = \prod_{k=1}^{\mathrm{d}_{\mathcal{H}}} \mathrm{n}_k!,$$

because the n_k positions with entry k can be permuted among themselves independently for each k. (Here $\mathrm{n}_k = \mathrm{n}_k(j_1, \dots, j_N) = \mathrm{n}_k(i_1, \dots, i_N)$, [38, Eq. (1.43b)].)

Important Spanning Set / Basis 3 (of $\mathscr{F}_\zeta^N$)

Definition 29.21 For $i_1, \dots, i_N \in \{1, 2, \dots, \mathrm{d}_{\mathcal{H}}\}$, we define the *quasi-occupation-number-states* as

$$
\begin{aligned}
|\, i_1, i_2, \dots, i_N\rangle &\equiv \frac{1}{\sqrt{\prod_{k=1}^{\mathrm{d}_{\mathcal{H}}} \mathrm{n}_k!}} |i_1, i_2, \dots, i_N\} \\
&\equiv \frac{1}{\sqrt{N! \prod_{k=1}^{\mathrm{d}_{\mathcal{H}}} \mathrm{n}_k!}} \sum_{\pi \in \mathrm{S}_N} \mathrm{sign}(\pi)^{1-\theta(\zeta)}\, |i_{\pi(1)}\rangle \otimes |i_{\pi(2)}\rangle \otimes \cdots \otimes |i_{\pi(N)}\rangle
\end{aligned}
\tag{29.23}
$$

with occupation-numbers as $\forall k \in \{1, 2, \dots, \mathrm{d}_{\mathcal{H}}\} \;:\; \mathrm{n}_k \equiv \mathrm{n}_k(i_1, \dots, i_N)$.

(This is [38, Eq. (1.46)]. For an orthonormal basis these states are normalized, $\langle i_1, \dots, i_N | i_1, \dots, i_N\rangle = 1$, by the previous Corollary, unless they vanish, which happens exactly for Fermions with some $\mathrm{n}_k \geq 2$.)

Remark 29.21.1 Notice that these states give *Slater-determinants* and *permanents* in the coordinate representation, i.e.

$$
(x_1, \dots, x_N | i_1, \dots, i_N\rangle = \frac{1}{\sqrt{N! \prod_k \mathrm{n}_k!}} \sum_{\pi \in \mathrm{S}_N} \mathrm{sign}(\pi)^{1-\theta(\zeta)} \prod_{l=1}^{N} \psi_{i_{\pi(l)}}(x_l) = \frac{1}{\sqrt{N! \prod_k \mathrm{n}_k!}} \begin{vmatrix} \psi_{i_1}(x_1) & \cdots & \psi_{i_N}(x_1) \\ \vdots & \ddots & \vdots \\ \psi_{i_1}(x_N) & \cdots & \psi_{i_N}(x_N) \end{vmatrix}_{\zeta},
$$

with $|\cdot|_\zeta$ the permanent ($\zeta = +1$) resp. determinant ($\zeta = -1$) from the note after Lemma 29.11. For Fermions $\prod_k \mathrm{n}_k! = 1$, and one obtains the normalized Slater-determinant $\frac{1}{\sqrt{N!}} \det(\psi_{i_m}(x_l))$, [38, Eqs. (1.49a), (1.49b)]. (In [38, Eq. (1.49a)] the occupation numbers in the prefactor should be those of the state $|\beta_1 \dots \beta_N\rangle$, i.e. $\prod n_\beta!$.)

Corollary 29.22 One obtains the completeness relation

$$
1_{\mathscr{F}_\zeta^N} \equiv \sum_{i_1, i_2, \dots, i_N = 1}^{\mathrm{d}_{\mathcal{H}}} \frac{\prod_{k=1}^{\mathrm{d}_{\mathcal{H}}} \mathrm{n}_k!}{N!} |i_1, i_2, \dots, i_N\rangle\langle i_1, i_2, \dots, i_N| \tag{29.24}
$$

with occupation-numbers as $\forall k \in \{1, 2, \dots, \mathrm{d}_{\mathcal{H}}\} \;:\; \mathrm{n}_k \equiv \mathrm{n}_k(i_1, \dots, i_N)$.

Proof 29.22 Follows from the completeness relation in Corollary 29.17.

(Insert $|i\}\{i| = \prod_k \mathrm{n}_k!\, |i\rangle\langle i|$ with $i = (i_1, \dots, i_N)$, which follows from Equation (29.23); cf. [38, Eq. (1.51)].)

TBD: Overlap between different quasi-occupation-number-states and relation to Slater-determinants and permanents.

Corollary 29.23 Let $|\beta_1, \dots, \beta_N\rangle$ and $|\alpha_1, \dots, \alpha_N\rangle$ be quasi-occupation-number-states with occupation numbers $\mathrm{n}_k(\beta)$ and $\mathrm{n}_k(\alpha)$. Then [38, Eqs. (1.47), (1.50)]

$$
\begin{aligned}
(\beta_1, \dots, \beta_N | \alpha_1, \dots, \alpha_N\rangle &= \frac{1}{\sqrt{N! \prod_k \mathrm{n}_k(\alpha)!}} \Big| \langle \beta_l | \alpha_m \rangle \Big|_\zeta, \\
\langle \beta_1, \dots, \beta_N | \alpha_1, \dots, \alpha_N\rangle &= \frac{1}{\sqrt{\prod_k \mathrm{n}_k(\beta)! \prod_k \mathrm{n}_k(\alpha)!}} \Big| \langle \beta_l | \alpha_m \rangle \Big|_\zeta,
\end{aligned}
$$

with the ζ-determinant $|M|_\zeta$ of the $N \times N$-matrix $M_{lm} = \langle \beta_l | \alpha_m \rangle$. In particular, for an orthonormal basis: if $(\beta_1, \dots, \beta_N) = (\alpha_{\sigma(1)}, \dots, \alpha_{\sigma(N)})$ for some $\sigma \in \mathrm{S}_N$, then $\langle \beta | \alpha \rangle = \mathrm{sign}(\sigma)^{1-\theta(\zeta)}$ (for non-vanishing states); otherwise $\langle \beta | \alpha \rangle = 0$. Hence two quasi-occupation-number-states are either equal up to a sign (same occupation numbers) or orthogonal (different occupation numbers).

Proof 29.23 By Definition 29.15 and Lemma 29.11,

$$(\beta|\alpha\rangle = \frac{\sqrt{N!}}{\sqrt{\prod_k \mathrm{n}_k(\alpha)!}} (\beta| \, \mathrm{P}_\zeta \, |\alpha) = \frac{\sqrt{N!}}{\sqrt{\prod_k \mathrm{n}_k(\alpha)!}} \frac{1}{N!} \sum_\pi \mathrm{sign}(\pi)^{1-\theta(\zeta)} \prod_l \langle \beta_l | \alpha_{\pi(l)} \rangle = \frac{1}{\sqrt{N! \prod_k \mathrm{n}_k(\alpha)!}} \Big| \langle \beta_l | \alpha_m \rangle \Big|_\zeta .$$

The second identity follows in the same way from Lemma 29.18, $\langle \beta | \alpha \rangle = \{\beta|\alpha\} / \sqrt{\prod_k \mathrm{n}_k(\beta)! \prod_k \mathrm{n}_k(\alpha)!}$. For an orthonormal basis, the overlap Corollary gives $\{\beta|\alpha\} = \mathrm{sign}(\sigma)^{1-\theta(\zeta)} \prod_k \mathrm{n}_k!$ with $\mathrm{n}_k(\beta) = \mathrm{n}_k(\alpha) = \mathrm{n}_k$, resp. 0. The coordinate representation in the Remark above is the special case of the first identity with $\langle \beta_l | \to \langle x_l |$.

29.1.2. Creation- and Annihilation-Operators

Definition 29.24 In the zero-particle subspace $\mathscr{F}_\zeta^0 = \mathbb{C}$, we introduce *the vacuum-state* as

$$|0\rangle \equiv |\mathrm{vac.}\rangle \equiv 1 \in \mathbb{C}.$$

(The vacuum is a normalized state, $\langle 0|0\rangle = 1$, and must be distinguished from the zero vector of the Fock space, [38, p. 11].)

Definition 29.25 *(Missing so far.)* The *ζ-Fock-space* is the orthogonal direct sum of the ζ-Fock-subspaces [38, Eqs. (1.66), (1.67)]

$$\mathscr{F}_\zeta := \bigoplus_{N=0}^\infty \mathscr{F}_\zeta^N, \qquad \langle \psi | \phi \rangle_{\mathscr{F}_\zeta} := \sum_{N=0}^\infty \langle \psi_N | \phi_N \rangle_{\mathscr{H}_N} \quad \text{for} \quad \psi = (\psi_N)_N, \ \phi = (\phi_N)_N,$$

i.e. states with different particle numbers are orthogonal. For Fermions the sum ends at $N = \mathrm{d}_\mathcal{H}$. For Bosons it is infinite, and $\mathscr{F}_{+1}$ consists of the sequences with $\sum_N \|\psi_N\|^2 < \infty$ (Hilbert-space direct sum). A general state, e.g. $\frac{1}{2}|0\rangle + \frac{1}{\sqrt{2}}|\lambda\rangle + \frac{1}{2}|\lambda\mu\rangle$, is a superposition of different particle numbers [38, Eq. (1.68)].

Remark 29.25.1 Notice that with this supplement, we can extend the completeness-relation in Equation (29.24) to the entire Fock-space $\mathscr{F}_\zeta$ as

$$1_{\mathscr{F}_\zeta} = \sum_{N=0}^\infty \sum_{i_1, i_2, \dots, i_N = 1}^{\mathrm{d}_\mathcal{H}} \frac{\prod_{k=1}^{\mathrm{d}_\mathcal{H}} \mathrm{n}_k!}{N!} |i_1, i_2, \dots, i_N\rangle\langle i_1, i_2, \dots, i_N|. \tag{29.25}$$

with occupation-numbers as $\forall k \in \{1, 2, \dots, \mathrm{d}_\mathcal{H}\} \ : \ \mathrm{n}_k \equiv \mathrm{n}_k(i_1, \dots, i_N)$.

(The $N = 0$ term is $|0\rangle\langle 0|$, with the convention that the empty sum over $i_1, \dots, i_N$ has exactly one term, the empty tuple, and $0! = 1$. This is [38, Eq. (1.69)]. It uses Definition 29.25: $1_{\mathscr{F}_\zeta} = \sum_N 1_{\mathscr{F}_\zeta^N}$, because the subspaces are mutually orthogonal.)

Definition 29.26 For each $k \in \{1, \dots, \mathrm{d}_{\mathcal{H}}\}$ we introduce a mapping as the *(particle-)creation-operators*

$$\begin{aligned} c_k^\dagger : \mathscr{F}_\zeta^N &\to \mathscr{F}_\zeta^{N+1} \\ |\psi\rangle &\mapsto c_k^\dagger |\psi\rangle \end{aligned}$$

by specifying its action on the overcomplete basis in Equation (29.15) and extending its definition by linearity on the entire Fock-space. We define for the states

$$\begin{aligned} c_k^\dagger |0\rangle &\equiv |k\}, \\ c_k^\dagger |i_1, i_2, \dots, i_N\} &\equiv |k, i_1, i_2, \dots, i_N\} \end{aligned} \tag{29.26}$$

Note on well-definedness (gap). Since the states $|i_1, \dots, i_N\}$ are linearly dependent (they are a spanning set, not a basis), one has to check that this prescription defines a linear map. It does, because it agrees with the manifestly linear and well-defined formula

$$c_k^\dagger \psi = \sqrt{N+1}\; \mathrm{P}_\zeta^{(N+1)} \left(|k\rangle \otimes \psi \right) \qquad \text{for } \psi \in \mathscr{F}_\zeta^N. \tag{29.27}$$

Indeed, $\mathrm{P}_\zeta^{(N+1)}(1_{\mathcal{H}} \otimes \mathrm{P}_\zeta^{(N)}) = \mathrm{P}_\zeta^{(N+1)}$, because $1 \otimes \mathrm{P}_\zeta^{(N)}$ averages over the subgroup of S_{N+1} fixing the first slot, and $\mathrm{P}_\zeta^{(N+1)}\, \sigma = \mathrm{sign}(\sigma)^{1-\theta(\zeta)}\, \mathrm{P}_\zeta^{(N+1)}$. Hence

$$\sqrt{N+1}\; \mathrm{P}_\zeta^{(N+1)} \left(|k\rangle \otimes \sqrt{N!}\, \mathrm{P}_\zeta^{(N)} |i_1, \dots, i_N) \right) = \sqrt{(N+1)!}\; \mathrm{P}_\zeta^{(N+1)} |k, i_1, \dots, i_N) = |k, i_1, \dots, i_N\},$$

and for $N = 0$: $\mathrm{P}_\zeta^{(1)} |k\rangle = |k\}$. The same formula defines $c^\dagger(\varphi)$ for every $|\varphi\rangle \in \mathcal{H}$ (replace $|k\rangle$ by $|\varphi\rangle$); it is linear in φ, $c^\dagger(\varphi) = \sum_k \langle k|\varphi\rangle c_k^\dagger$, and $c^\dagger(\varphi)|i_1, \dots, i_N\} = |\varphi, i_1, \dots, i_N\}$, where the curly states are defined for arbitrary single-particle vectors by the same formula as in Definition 29.15. On $\mathscr{F}_\zeta$ the operator acts componentwise in N. This is [38, Eq. (1.63a)].

Remark 29.26.1 Since these operators are mappings from the N-particle Hilbert-space to the $N+1$-particle Hilbert-space, the name "creation-operators" becomes evident.

Remark 29.26.2 Another thing to notice is that this definition / prefactor-convention is not unique within the literature. We are following the prefactor-convention from [Negele, Orland] in contrast to [TBD].

Note. Only the *states* are normalized differently; the operator $c_k^\dagger$ is the same in all standard references, cf. Equation (29.27). On the unnormalized states $|\dots\}$ it acts without prefactor [38, Eq. (1.63a)]; on normalized states the factor $\sqrt{\mathrm{n}_k + 1}$ appears (next Corollary), as in the occupation-number definitions of e.g. [4, p. 44]. "The absence of factors of N or n_λ in Eq. (1.70a) is the reason for the definition of the states $|\ \}$" [38, p. 12]. For Fermions, the references differ in the order convention of the occupation-number-states, which only changes signs.

Corollary 29.27 It follows

$$c_k^\dagger |i_1, i_2, \dots, i_N\rangle = \sqrt{\mathrm{n}_k + 1}\, |k, i_1, i_2, \dots, i_N\rangle \tag{29.28}$$

with occupation-numbers as $\forall k \in \{1, 2, \dots, \mathrm{d}_{\mathcal{H}}\} \ :\ \mathrm{n}_k \equiv \mathrm{n}_k(i_1, \dots, i_N)$.

Proof 29.27 Follows immediately by considering the respective definitions: We have

$$\begin{aligned} c_k^\dagger |i_1, i_2, \dots, i_N\rangle &\overset{\text{Eq. (29.23)}}{=} \frac{1}{\sqrt{\prod_{k=1}^{\mathrm{d}_\mathcal{H}} \mathrm{n}_k!}} c_k^\dagger |i_1, i_2, \dots, i_N\} \\ &\overset{\text{Eq. (29.26)}}{=} \frac{1}{\sqrt{\prod_{k=1}^{\mathrm{d}_\mathcal{H}} \mathrm{n}_k!}} |k, i_1, i_2, \dots, i_N\} \\ &\overset{\text{Eq. (29.23)}}{=} \sqrt{\mathrm{n}_k + 1}\, |k, i_1, i_2, \dots, i_N\rangle \end{aligned} \tag{29.29}$$

with occupation-numbers $\mathrm{n}_k \equiv \mathrm{n}_k(i_1, \dots, i_N)$.

Note. Correct ([38, Eq. (1.63b)]), but the product index clashes with the fixed creation index k; write $\prod_l \mathrm{n}_l!$. The last step uses $\mathrm{n}_l(k, i_1, \dots, i_N) = \mathrm{n}_l(i_1, \dots, i_N) + \delta_{lk}$, i.e. $\prod_l \mathrm{n}_l(k, i)! = (\mathrm{n}_k + 1) \prod_l \mathrm{n}_l(i)!$. For Fermions with $\mathrm{n}_k = 1$ both sides vanish, since $|k, i_1, \dots, i_N\rangle = 0$; this is [38, Eq. (1.64)].

Remark 29.27.1 By repeated application of Corollary 29.27 one finds that any basis-vector can be rewritten as a product of particle creations on the vacuum-state as

$$|i_1, i_2, \dots, i_N\} = c_{i_1}^\dagger \cdots c_{i_N}^\dagger |0\rangle \quad \Longleftrightarrow \quad |i_1, i_2, \dots, i_N\rangle = \frac{1}{\sqrt{\prod_{k=1}^{\mathrm{d}_\mathcal{H}} \mathrm{n}_k!}} c_{i_1}^\dagger \cdots c_{i_N}^\dagger |0\rangle \tag{29.30}$$

with occupation-numbers $\mathrm{n}_k \equiv \mathrm{n}_k(i_1, \dots, i_N)$.

(The first identity follows by repeated application of Definition (29.26) itself, starting with $c_{i_N}^\dagger |0\rangle = |i_N\}$; the second one then by Equation (29.23), cf. [38, Eq. (1.70)]. Hence the creation operators generate $\mathscr{F}_\zeta$ from the vacuum.)

Corollary 29.28 One obtains the statistical commutation relations for the creation-operators

$$c_\lambda^\dagger c_\mu^\dagger - \zeta c_\mu^\dagger c_\lambda^\dagger \equiv [c_\lambda^\dagger, c_\mu^\dagger]_\zeta = 0 \tag{29.31}$$

Proof 29.28 We compute

$$\begin{aligned} c_\lambda^\dagger c_\mu^\dagger |i_1, i_2, \dots, i_N\} &= c_\lambda^\dagger |\mu, i_1, i_2, \dots, i_N\} = |\lambda, \mu, i_1, i_2, \dots, i_N\} \\ &= \zeta |\mu, \lambda, i_1, i_2, \dots, i_N\} = \zeta c_\mu^\dagger |\lambda, i_1, i_2, \dots, i_N\} = \zeta c_\mu^\dagger c_\lambda^\dagger |i_1, i_2, \dots, i_N\} \end{aligned} \tag{29.32}$$

Now rearranging terms yields the desired result.

Definition 29.29 We introduce the *particle-annihilation-operators* $\{c_1, \dots c_{\mathrm{d}_\mathcal{H}}\}$ as the hermitian-adjoints of the creation-operators $\{c_1^\dagger, \dots c_{\mathrm{d}_\mathcal{H}}^\dagger\}$ w.r.t. the scalar-product on the Fock-space.

Note. The adjoint can be written down explicitly. From Equation (29.27), the hermiticity of P_ζ and $\mathrm{P}_\zeta\,\psi = \psi$ for $\psi \in \mathscr{F}_\zeta^{N+1}$ we get $\langle\psi|c_k^\dagger\phi\rangle = \sqrt{N+1}\,\langle\psi|k\otimes\phi\rangle$ for $\phi \in \mathscr{F}_\zeta^N$, hence

$$c_k\psi = \sqrt{N+1}\,\big(\langle k|\otimes 1_{\mathscr{H}_N}\big)\psi \qquad \text{for } \psi \in \mathscr{F}_\zeta^{N+1}, \qquad c_k|0\rangle = 0,$$

i.e. c_k contracts the first slot with $\langle k|$ [38, Eqs. (1.75), (1.76)]. It maps $\mathscr{F}_\zeta^{N+1}$ into $\mathscr{F}_\zeta^N$, since the symmetry in the remaining slots is preserved. For Fermions all operators are bounded (finite dimension). For Bosons $c_k^\dagger$ is unbounded on the infinite-dimensional $\mathscr{F}_{+1}$, and all statements are understood on the dense subspace of states with finitely many particles.

Lemma 29.30 It follows

$$c_\lambda c_\mu - \zeta c_\mu c_\lambda \equiv [c_\lambda, c_\mu]_\zeta = 0 \tag{29.33}$$

Proof 29.30 Follows immediately from taking the hermitian adjoint of Equation (29.31).

Lemma 29.31 For the action of the hermitian adjoint it follows

$$c_j|i_1, i_2, \dots, i_N\} = \sum_{k=1}^{N} \zeta^{k-1}\delta_{j,i_k}|i_1, \dots i_{k-1}, i_{k+1}, \dots, i_N\} \equiv \sum_{k=1}^{N} \zeta^{k-1}\delta_{j,i_k}|i_1, \dots \hat{i}_k, \dots, i_N\}. \tag{29.34}$$

Proof 29.31 We prove this identity, by taking an arbitrary state $\{j_2, \dots, j_n|$ and compute the overlap of the two two sides of the equation. This gives

$$\begin{aligned}\{j_2, \dots, j_n|c_j|i_1, i_2, \dots, i_N\} &= \{j, j_2, \dots, j_n|i_1, i_2, \dots, i_N\} \\ &\overset{j\equiv j_1,\text{Lemma (29.18)}}{=} \sum_{\pi\in \mathrm{S}_N} \mathrm{sign}(\pi)^{1-\theta(\zeta)} \prod_{k=1}^{N} \langle j_k|i_{\pi(k)}\rangle \\ &= \dots\end{aligned} \tag{29.35}$$

In order to proceed, we have to make some considerations about the permutations $\pi \in \mathrm{S}_N$:

Intermezzo

Every permutation in $\pi \in \mathrm{S}_N$ is uniquely determined after one specifies

1. the image of the first element, i.e. $\pi(1) = k$ for some $k \in \{1, 2, \dots, N\}$ and
2. the permutation of the remaining $N-1$ elements.

For some $\tau \in \mathrm{S}_{N-1}$ that is acting bijectively on the set $\{2, \dots, N\}$, we define …

- a *natural embedding* $\iota : \mathrm{S}_{N-1} \longrightarrow \mathrm{S}_N$ with $\iota(\tau) = \widetilde{\tau}$ as

$$\begin{aligned} \widetilde{\tau}(1) &= 1 \qquad , \\ \widetilde{\tau}(i) &= \tau(i) \quad \text{if } i > 1, \end{aligned} \tag{29.36}$$

- for each $k \in \{1, 2, \dots, N\}$ a *canonical insertion map* $\iota_k : \mathrm{S}_{N-1} \longrightarrow \mathrm{S}_N$ with $\iota_k(\tau) = \pi$ as

$$\begin{aligned} \pi(1) &= k, \\ \pi(i) &= \tau(i) - 1 \quad \text{if } i \geq 2 \ \wedge \ \tau(i) \leq k, \\ \pi(i) &= \tau(i) \qquad \text{if } i \geq 2 \ \wedge \ \tau(i) > k. \end{aligned} \tag{29.37}$$

Then it follows that

$$\pi = \iota_k(\tau) = (k \ k-1) \cdots (2 \ 1) \circ \iota(\tau) \quad \text{ and } \ \mathrm{sign}(\pi) = \mathrm{sign}(\iota_k(\tau)) = \mathrm{sign}(\tau) \cdot (-1)^{k-1}. \tag{29.38}$$

This gives a disjoint union of the symmetric group S_N as

$$S_N = \bigsqcup_{k=1}^{N} \iota_k(\mathrm{S}_{N-1}). \tag{29.39}$$

which allows us to reorder the sum in Equation (29.35) by summing over permutations $\tau \in \mathrm{S}_{N-1}$

$$\begin{aligned} \dots &= \sum_{k=1}^{N} \sum_{\tau \in \mathrm{S}_{N-1}} \mathrm{sign}(\iota_k(\tau))^{1-\theta(\zeta)} \prod_{l=1}^{N} \langle j_l | i_{\iota_k(\tau)(l)} \rangle \\ &= \sum_{k=1}^{N} \underbrace{(-1)^{(k-1)(1-\theta(\zeta))}}_{=\zeta^{k-1}} \sum_{\tau \in \mathrm{S}_{N-1}} \mathrm{sign}(\tau)^{1-\theta(\zeta)} \underbrace{\langle j_1 | i_{\iota_k(\tau)(1)} \rangle}_{=\langle j_1 | i_k \rangle = \delta_{j,i_k}} \prod_{l=2}^{N} \langle j_l | i_{\iota_k(\tau)(l)} \rangle \\ &= \sum_{k=1}^{N} \zeta^{k-1} \delta_{j,i_k} \sum_{\tau \in \mathrm{S}_{N-1}} \mathrm{sign}(\tau)^{1-\theta(\zeta)} \prod_{l=2}^{N} \langle j_l | i_{\tau(l)} \rangle \\ &= \sum_{k=1}^{N} \zeta^{k-1} \delta_{j,i_k} \{ j_2, \dots, j_N | i_1, \dots i_{k-1}, i_{k+1}, \dots, i_N \} \\ &= \sum_{k=1}^{N} \zeta^{k-1} \delta_{j,i_k} \{ j_2, \dots, j_N | i_1, \dots \hat{i}_k, \dots, i_N \} \end{aligned} \tag{29.40}$$

Since this equation holds for any vector $\{j_2, \dots, j_N\}$, we can conclude that the identity claimed in the Lemma is correct.

Correction notes.

- The Lemma holds for $N \geq 1$ and an orthonormal basis ($\delta_{j,i_k} = \langle j | i_k \rangle$). For $N = 0$ one has $c_j |0\rangle = 0$ [38, Eq. (1.76a)], since $\langle \psi | c_j | 0 \rangle = \langle c_j^\dagger \psi | 0 \rangle = 0$ for all ψ (the state $c_j^\dagger \psi$ has at least one particle).
- In the proof, $\{j_2, \dots, j_n|$ has to be $\{j_2, \dots, j_N|$ (an $(N-1)$-particle state). The first equation sign is

$$\{ j_2 \dots | c_j | i \} = (\{ i | c_j^\dagger | j_2 \dots \})^* = (\{ i | j, j_2, \dots \})^* = \{ j, j_2, \dots | i \}.$$

- In the third-to-last line, $i_{\tau(l)}$ has to be read as $i'_{\tau(l)}$, where $(i'_2, \dots, i'_N) := (i_1, \dots, \hat{i}_k, \dots, i_N)$ is the tuple with i_k removed (relabelled to the positions $2, \dots, N$). Indeed $\iota_k(\tau)(l) = f_k(\tau(l))$ with the order-preserving bijection $f_k : \{2, \dots, N\} \to \{1, \dots, N\} \setminus \{k\}$, $f_k(m) = m-1$ for $m \leq k$, $f_k(m) = m$ for $m > k$, and $i'_m = i_{f_k(m)}$. Only then the sum over τ is the overlap $\{j_2, \dots, j_N | i_1, \dots, \hat{i}_k, \dots, i_N\}$ of Lemma 29.18 (for $N-1$ particles). The Intermezzo itself is correct: $(k\ k{-}1) \cdots (2\ 1)$ maps $1 \mapsto k$ and $m \mapsto m-1$ for $2 \leq m \leq k$, consists of $k-1$ transpositions, and $\operatorname{sign}(\iota(\tau)) = \operatorname{sign}(\tau)$.
- The last sentence uses that the states $\{j_2, \dots, j_N|$ span $\mathscr{F}_\zeta^{N-1}$ (Corollary 29.17). A two-line alternative proof: with the explicit form of c_j from the note after the Definition of the annihilation-operators, $c_j|i\} = \frac{\sqrt{N}}{\sqrt{N!}} \sum_\pi \operatorname{sign}(\pi)^{1-\theta(\zeta)} \langle j | i_{\pi(1)} \rangle \bigotimes_{l \geq 2} |i_{\pi(l)}\rangle$. Grouping the permutations by $k = \pi(1)$ as in the Intermezzo gives the claim, since $\sqrt{N}\sqrt{(N-1)!}/\sqrt{N!} = 1$. This is [38, Eq. (1.78a)].

Corollary 29.32 Analogously one finds

$$c_j|i_1, i_2, \dots, i_N\rangle = \frac{1}{\sqrt{n_j}} \sum_{k=1}^{N} \zeta^{k-1} \delta_{j,i_k} |i_1, \dots i_{k-1}, i_{k+1}, \dots, i_N\rangle = \frac{1}{\sqrt{n_j}} \sum_{k=1}^{N} \zeta^{k-1} \delta_{j,i_k} |i_1, \dots \hat{i}_k, \dots, i_N\rangle \tag{29.41}$$

Proof 29.32 Follows immediately with Equation (29.23) and the previous Lemma.

(Details and caveat: every non-vanishing term has $i_k = j$, so the remaining tuple has occupation numbers $\mathrm{n}_l - \delta_{lj}$, and $|\dots \hat{i}_k \dots\} = \sqrt{\prod_l \mathrm{n}_l! / \mathrm{n}_j}\, |\dots \hat{i}_k \dots\rangle$. Dividing by $\sqrt{\prod_l \mathrm{n}_l!}$ gives the factor $1/\sqrt{\mathrm{n}_j}$, [38, Eq. (1.78b)]. Here $n_j \equiv \mathrm{n}_j(i_1, \dots, i_N)$, and the formula is meant for $\mathrm{n}_j \geq 1$; for $\mathrm{n}_j = 0$ all Kronecker-deltas vanish and $c_j|i_1, \dots, i_N\rangle = 0$.)

Theorem 29.33 In total, we arrive at creation- and annihilation-operators $\left\{c_1, c_1^\dagger, c_2, c_2^\dagger, \dots, c_{\mathrm{d}_\mathcal{H}}, c_{\mathrm{d}_\mathcal{H}}^\dagger\right\}$ obey the statistics-dependent commutation-relations

$$\left[c_i, c_j\right]_\zeta = \left[c_i^\dagger, c_j^\dagger\right]_\zeta = 0, \qquad \left[c_i, c_j^\dagger\right]_\zeta = \delta_{i,j}$$

Proof 29.33

- TBD, cf. Negele, Orland page 15.

Proof [38, Eqs. (1.80)–(1.83)]. The first two relations were shown above. Let $|\alpha_1, \dots, \alpha_n\}$ be any auxiliary state. Applying the previous Lemma to the $(n+1)$-tuple $(\mu, \alpha_1, \dots, \alpha_n)$, where μ sits at position 1 and α_i at position $i+1$, gives

$$c_\lambda c_\mu^\dagger |\alpha_1, \dots, \alpha_n\} = c_\lambda |\mu, \alpha_1, \dots, \alpha_n\} = \delta_{\lambda\mu} |\alpha_1, \dots, \alpha_n\} + \sum_{i=1}^{n} \zeta^i \delta_{\lambda\alpha_i} |\mu, \alpha_1, \dots, \hat{\alpha}_i, \dots, \alpha_n\},$$

while the Lemma (for the n-tuple) and the Definition of $c_\mu^\dagger$ give

$$c_\mu^\dagger c_\lambda |\alpha_1, \dots, \alpha_n\} = \sum_{i=1}^{n} \zeta^{i-1} \delta_{\lambda\alpha_i} |\mu, \alpha_1, \dots, \hat{\alpha}_i, \dots, \alpha_n\}.$$

Since $\zeta^i = \zeta \cdot \zeta^{i-1}$, the sum in the first equation is $\zeta c_\mu^\dagger c_\lambda |\alpha_1, \dots, \alpha_n\}$, i.e. $(c_\lambda c_\mu^\dagger - \zeta c_\mu^\dagger c_\lambda)|\alpha_1, \dots, \alpha_n\} = \delta_{\lambda\mu}|\alpha_1, \dots, \alpha_n\}$. For $n = 0$: $c_\lambda c_\mu^\dagger|0\rangle = c_\lambda|\mu\} = \delta_{\lambda\mu}|0\rangle$ and $c_\mu^\dagger c_\lambda|0\rangle = 0$. Since the auxiliary states and $|0\rangle$ span $\mathscr{F}_\zeta$, the operator identity $[c_\lambda, c_\mu^\dagger]_\zeta = \delta_{\lambda\mu}$ follows. For $\zeta = +1$ this is a commutator, for $\zeta = -1$ an anti-commutator. ■

TBD: Basis Change etc according to page 15...

Theorem 29.34 *(Basis change, [38, pp. 15f., Eqs. (1.84)–(1.89)].)* Let $\{|\tilde{\alpha}\rangle\}$ be another basis of $\mathcal{H}$, $|\tilde{\alpha}\rangle = \sum_\alpha \langle\alpha|\tilde{\alpha}\rangle\,|\alpha\rangle$, where $\{|\alpha\rangle\}$ is the orthonormal basis used so far. Then the creation- and annihilation-operators of the states $|\tilde{\alpha}\rangle$, i.e. $c_{\tilde{\alpha}}^\dagger \equiv c^\dagger(\tilde{\alpha})$ from the note after Equation (29.26), are

$$c_{\tilde{\alpha}}^\dagger = \sum_\alpha \langle\alpha|\tilde{\alpha}\rangle\, c_\alpha^\dagger, \qquad c_{\tilde{\alpha}} = \sum_\alpha \langle\tilde{\alpha}|\alpha\rangle\, c_\alpha,$$

and they satisfy

$$[c_{\tilde{\beta}}, c_{\tilde{\alpha}}^\dagger]_\zeta = \langle\tilde{\beta}|\tilde{\alpha}\rangle, \qquad [c_{\tilde{\alpha}}^\dagger, c_{\tilde{\beta}}^\dagger]_\zeta = [c_{\tilde{\alpha}}, c_{\tilde{\beta}}]_\zeta = 0.$$

Hence the transformation is canonical (the commutation relations are preserved) if and only if the new basis is orthonormal as well. In particular, for the (generalized) position states $|x\rangle$ (including spin) one obtains the *field operators*

$$\hat{\psi}^\dagger(x) = \sum_\alpha \langle\alpha|x\rangle c_\alpha^\dagger = \sum_\alpha \psi_\alpha^*(x) c_\alpha^\dagger, \qquad \hat{\psi}(x) = \sum_\alpha \psi_\alpha(x) c_\alpha,$$

$$[\hat{\psi}(x), \hat{\psi}^\dagger(y)]_\zeta = \delta(x-y), \qquad [\hat{\psi}(x), \hat{\psi}(y)]_\zeta = [\hat{\psi}^\dagger(x), \hat{\psi}^\dagger(y)]_\zeta = 0.$$

Proof 29.34 The map $\varphi \mapsto c^\dagger(\varphi)$ is linear (Equation (29.27)), which gives the first formula [38, Eq. (1.85)]; the second one is its adjoint (the coefficients get complex conjugated). The commutators follow from bilinearity and the commutation relations of the c_α:

$$[c_{\tilde{\beta}}, c_{\tilde{\alpha}}^\dagger]_\zeta = \sum_{\alpha,\beta} \langle\tilde{\beta}|\beta\rangle\langle\alpha|\tilde{\alpha}\rangle [c_\beta, c_\alpha^\dagger]_\zeta = \sum_\alpha \langle\tilde{\beta}|\alpha\rangle\langle\alpha|\tilde{\alpha}\rangle = \langle\tilde{\beta}|\tilde{\alpha}\rangle,$$

using the completeness $\sum_\alpha |\alpha\rangle\langle\alpha| = 1_\mathcal{H}$. For the field operators insert $|\tilde{\alpha}\rangle = |x\rangle$ and $\langle y|x\rangle = \delta(x-y)$; since $|x\rangle \notin \mathcal{H}$, $\hat{\psi}(x)$ is an operator-valued distribution (cf. Section 29.8). ■

Important Spanning Set / Basis 4 (of $\mathscr{F}_\zeta^N$)

Definition 29.35 We consider a state $|i_1, i_2, \dots, i_N\rangle$. We denote its occupation-numbers $\mathrm{n}_1, \mathrm{n}_2, \dots, \mathrm{n}_{\mathrm{d}_\mathcal{H}}$ with occupation-number-operators as usual $\forall k \in \{1, 2, \dots, \mathrm{d}_\mathcal{H}\} : \mathrm{n}_k \equiv \mathrm{n}_k(i_1, \dots, i_N)$. Then we introduce the *occupation-number-representation* of the state a.k.a. *occupation-number-states* as

$$|\,\mathrm{n}_1, \mathrm{n}_2, \dots, \mathrm{n}_{\mathrm{d}_\mathcal{H}}\rangle_{\mathrm{occ}} := |i_1, i_2, \dots, i_N\rangle \in \mathscr{F}_\zeta^N. \tag{29.42}$$

Remark 29.35.1 Usually one drops the index "occ" in the notation as it is clear from the context which states one is referring to, i.e.

$$|\,\mathrm{n}_1, \mathrm{n}_2, \dots, \mathrm{n}_{\mathrm{d}_\mathcal{H}}\rangle_{\mathrm{occ}} \equiv |\,\mathrm{n}_1, \mathrm{n}_2, \dots, \mathrm{n}_{\mathrm{d}_\mathcal{H}}\rangle. \tag{29.43}$$

Remark 29.35.2 Notice that this is a *many-to-one-correspondence*.

Correction note (well-definedness). Because of this many-to-one correspondence, the Definition is well-defined for Bosons only: all tuples with the same occupation numbers give the same state $|i_1,\dots,i_N\rangle$. For Fermions the state changes its sign under a reordering of $(i_1,\dots,i_N)$ (Lemma 29.16), so a convention is needed. The standard one, which is also the one that produces the sign $\zeta^{\sum_{l<j}\mathrm{n}_l}$ in the next Corollary, is to take the *ordered* tuple $i_1 \le i_2 \le \dots \le i_N$ (for Fermions $i_1 < \dots < i_N$):

$$|\,\mathrm{n}_1,\dots,\mathrm{n}_{\mathrm{d}_\mathcal{H}}\rangle := |\,\underbrace{1,\dots,1}_{\mathrm{n}_1},\underbrace{2,\dots,2}_{\mathrm{n}_2},\dots\rangle = \frac{1}{\sqrt{\prod_k \mathrm{n}_k!}}(c_1^\dagger)^{\mathrm{n}_1}(c_2^\dagger)^{\mathrm{n}_2}\cdots(c_{\mathrm{d}_\mathcal{H}}^\dagger)^{\mathrm{n}_{\mathrm{d}_\mathcal{H}}}|0\rangle,$$

with $\mathrm{n}_k \in \mathbb{N}_\zeta$, where $\mathbb{N}_{+1} := \mathbb{N}_0$ and $\mathbb{N}_{-1} := \{0,1\}$ (this also defines the symbol $\mathbb{N}_\zeta$ used in the Theorem below). Dropping the index "occ" is dangerous, e.g. $|1,1\rangle$ could mean $(i_1,i_2)=(1,1)$ or $(\mathrm{n}_1,\mathrm{n}_2)=(1,1)$.

Corollary 29.36 One obtains the simple formulae,

$$\begin{aligned} c_j|\,\mathrm{n}_1,\mathrm{n}_2,\dots,\mathrm{n}_{\mathrm{d}_\mathcal{H}}\rangle &= \sqrt{\mathrm{n}_j} && |\,\mathrm{n}_1,\mathrm{n}_2,\dots,\mathrm{n}_{j-1},\mathrm{n}_j-1,\mathrm{n}_{j+1},\dots,\mathrm{n}_{\mathrm{d}_\mathcal{H}}\rangle \\ c_j^\dagger|\,\mathrm{n}_1,\mathrm{n}_2,\dots,\mathrm{n}_{\mathrm{d}_\mathcal{H}}\rangle &= \sqrt{\mathrm{n}_j+1}\,\zeta^{\sum_{l=1}^{j-1}\mathrm{n}_l} && |\,\mathrm{n}_1,\mathrm{n}_2,\dots,\mathrm{n}_{j-1},\mathrm{n}_j+1,\mathrm{n}_{j+1},\dots,\mathrm{n}_{\mathrm{d}_\mathcal{H}}\rangle \end{aligned} \tag{29.44}$$

whereas the state on the r.h.s. is defined as 0 for $\mathrm{n}_j = 0$.

Correction note. The first formula is missing the same sign as the second one. With the ordering convention above, the correct formulae are

$$\begin{aligned} c_j|\dots,\mathrm{n}_j,\dots\rangle &= \zeta^{\sum_{l=1}^{j-1}\mathrm{n}_l}\sqrt{\mathrm{n}_j}\,|\dots,\mathrm{n}_j-1,\dots\rangle, \\ c_j^\dagger|\dots,\mathrm{n}_j,\dots\rangle &= \zeta^{\sum_{l=1}^{j-1}\mathrm{n}_l}\sqrt{\mathrm{n}_j+1}\,|\dots,\mathrm{n}_j+1,\dots\rangle. \end{aligned}$$

For Bosons the sign is 1 [38, Eq. (1.79a)]. For Fermions, $c_j|\dots 1_j\dots\rangle = (-1)^{\sum_{l<j}\mathrm{n}_l}|\dots 0_j\dots\rangle$, which is [38, Eq. (1.79b)] with $(-1)^{i-1}$, i = position of j in the ordered tuple. Moreover, for Fermions the right-hand side of the second line has to be read as 0 for $\mathrm{n}_j = 1$, since $\mathrm{n}_j+1 = 2 \notin \mathbb{N}_{-1}$ (Pauli principle, [38, Eq. (1.64)]).

Proof 29.36

- TBD, cf. Negele, Orland page 14 and Altland page 44.

Proof of the corrected formulae. Write $|\,\mathrm{n}\rangle = \frac{1}{\sqrt{\prod_k \mathrm{n}_k!}}|i_1,\dots,i_N\}$ with the ordered tuple, in which the entries j occupy the positions $s_j+1,\dots,s_j+\mathrm{n}_j$, $s_j := \sum_{l<j}\mathrm{n}_l$.

Creation operator. $c_j^\dagger|i_1,\dots,i_N\} = |j,i_1,\dots,i_N\}$. Moving j from position 1 past the s_j entries smaller than j (to the position just before the other entries j) needs s_j transpositions. By Lemma 29.16 this gives ζ^{s_j} times the ordered auxiliary state of $\mathrm{n}+e_j$. Normalizing with $\sqrt{\prod_k(\mathrm{n}+e_j)_k!} = \sqrt{\mathrm{n}_j+1}\sqrt{\prod_k \mathrm{n}_k!}$ gives the second line.

Annihilation operator. By the Lemma on the action of c_j, $c_j|i_1,\dots,i_N\} = \sum_k \zeta^{k-1}\delta_{j,i_k}|\dots\hat{i}_k\dots\}$. The non-vanishing terms are $k = s_j+1,\dots,s_j+\mathrm{n}_j$. Removing any one of the equal entries j gives the same ordered tuple of $\mathrm{n}-e_j$. For Bosons all n_j terms are equal with $\zeta^{k-1}=1$, which gives $\mathrm{n}_j\,|\,\mathrm{n}-e_j\}$; for Fermions there is one term with $\zeta^{k-1}=\zeta^{s_j}$. In both cases $c_j|i\} = \zeta^{s_j}\,\mathrm{n}_j\,|\,\mathrm{n}-e_j\}$ (curly, ordered). Dividing by $\sqrt{\prod_k \mathrm{n}_k!}$ and using $\sqrt{\prod_k(\mathrm{n}-e_j)_k!} = \sqrt{\prod_k \mathrm{n}_k!/\,\mathrm{n}_j}$ gives $\zeta^{s_j}\sqrt{\mathrm{n}_j}\,|\,\mathrm{n}-e_j\rangle$. For $\mathrm{n}_j = 0$ there is no term, so the result is 0. ■

Theorem 29.37 The occupation number states are an orthonormal basis of the Fock-space, i.e. one has the orthonormality condition

$$\langle n_1, n_2, \dots, n_{\mathrm{d}_{\mathcal{H}}} | n'_1, n'_2, \dots, n'_{\mathrm{d}_{\mathcal{H}}} \rangle = \prod_{l=1}^{\mathrm{d}_{\mathcal{H}}} \delta_{n_l, n'_l} \tag{29.45}$$

and the resolution of identity

$$\sum_{n_1, \dots, n_{\mathrm{d}_{\mathcal{H}}} \in \mathbb{N}_\zeta} |n_1, n_2, \dots, n_{\mathrm{d}_{\mathcal{H}}}\rangle\langle n_1, n_2, \dots, n_{\mathrm{d}_{\mathcal{H}}}| = 1_{\mathscr{F}_\zeta} \tag{29.46}$$

Proof 29.37

- Cf. Negele, Orland page 22, Nolting 2 page 277, Schwabl 2 page 1 onwards. [38, p. 22], [41, Sect. 8.3, p. 277], [48, Chapter 1, p. 1 ff.]

The second identity (resolution of identity) follows from Equation (29.25) and the fact that each occupation-number-state appears $\frac{N!}{\prod_k n_k!}$ times in the sum.

Completion. (The relevant equations of [38] are (1.45), (1.51) on p. 7 f. and (1.69) on p. 12; p. 22 is about coherent states.) *Orthonormality.* By the ordering convention, $|\,\mathrm{n}\rangle = |i\rangle$ and $|\,\mathrm{n}'\rangle = |i'\rangle$ with ordered tuples i, i'. If $\mathrm{n} \neq \mathrm{n}'$, then either the particle numbers differ (orthogonal subspaces, Definition 29.25), or i is not a permutation of i'; in both cases $\langle \mathrm{n}\,|\,\mathrm{n}'\rangle = 0$ by Corollary 29.23. If $\mathrm{n} = \mathrm{n}'$, then $i = i'$ and $\langle i|i\rangle = \{i|i\}/\prod_k \mathrm{n}_k! = 1$ (for Fermions $\mathrm{n}_k \in \{0,1\}$). *Resolution of identity.* In Equation (29.25), all $N!/\prod_k \mathrm{n}_k!$ tuples with the same occupation numbers give $|i\rangle\langle i| = (\pm 1)^2 |\,\mathrm{n}\rangle\langle \mathrm{n}\,|$. For Fermions, tuples with some $\mathrm{n}_k \geq 2$ give $|i\rangle = 0$. Summing over N gives the sum over all $\mathrm{n} \in \mathbb{N}_\zeta^{\mathrm{d}_\mathcal{H}}$. Together with orthonormality this shows that $\{|\,\mathrm{n}\rangle\}$ is an orthonormal basis.

29.1.3. Operators on the Fock-Space

29.1.3.1. 1-Body-Operators

Corollary 29.38 We define the number-operator $n_j \equiv a_j^\dagger a_j$, which counts the "number of particles in a given state"

$$n_j |n_1, n_2, \ldots, n_{\mathrm{d}_\mathcal{H}}\rangle = n_j |n_1, n_2, \ldots, n_{\mathrm{d}_\mathcal{H}}\rangle \tag{29.47}$$

whereas on the l.h.s. of the equation n_j represents an operator, and on the r.h.s. of the equation it represents a number.

(Notation: $a_j \equiv c_j$; the letter a is used for the same operators as in [38]. Cf. [38, Eqs. (1.90)–(1.92)].)

Proof 29.38 TBD.

With the corrected formulae for the occupation-number-states and $s_j = \sum_{l<j} \mathrm{n}_l$, which is the same for $|\,\mathrm{n}\rangle$ and $|\,\mathrm{n} - e_j\rangle$,

$$c_j^\dagger c_j |\,\mathrm{n}\rangle = \zeta^{s_j} \sqrt{\mathrm{n}_j}\, c_j^\dagger |\,\mathrm{n} - e_j\rangle = \zeta^{2s_j} \sqrt{\mathrm{n}_j}\sqrt{\mathrm{n}_j}\,|\,\mathrm{n}\rangle = \mathrm{n}_j\,|\,\mathrm{n}\rangle,$$

also for $\mathrm{n}_j = 0$. Alternatively, on auxiliary states, with $i = (i_1, \ldots, i_N)$,

$$c_j^\dagger c_j |i\} = \sum_k \zeta^{k-1} \delta_{j,i_k} |j, i_1, \ldots \hat{i}_k \ldots, i_N\} = \sum_k \delta_{j,i_k} |i\} = \mathrm{n}_j(i)|i\},$$

since moving j back to position k gives another ζ^{k-1} [38, Eq. (1.91)]. Consequently the total number operator satisfies $\sum_j c_j^\dagger c_j |i\} = \big(\sum_j \mathrm{n}_j(i)\big)|i\} = N|i\}$, i.e. it is $N \cdot 1$ on $\mathscr{F}_\zeta^N$. ■

Remark 29.38.1 Analog one also introduces the operator for the total number of particles

$$N = \sum_{j=1}^{\mathrm{d}_\mathcal{H}} n_j. \tag{29.48}$$

Lemma 29.39 *(Auxiliary result for the proofs below.)* For arbitrary single-particle vectors write $|\varphi_1,\dots,\varphi_N\} := \sqrt{N!}\,\mathrm{P}_\zeta(|\varphi_1\rangle\otimes\cdots\otimes|\varphi_N\rangle)$, which is multilinear in the φ's. For $1\le r\le N$ and indices $\lambda_1,\dots,\lambda_r$, $\mu_1,\dots,\mu_r$ one has

$$c^\dagger_{\lambda_1}\cdots c^\dagger_{\lambda_r} c_{\mu_r}\cdots c_{\mu_1}|\alpha_1,\dots,\alpha_N\} = \sum_{\substack{a_1,\dots,a_r\in\{1,\dots,N\}\\ \text{pairwise distinct}}} \Big(\prod_{s=1}^{r}\delta_{\mu_s,\alpha_{a_s}}\Big)|\alpha_1,\dots,\alpha_N\}_{a_1\to\lambda_1,\dots,a_r\to\lambda_r},$$

where the last state is $|\alpha_1,\dots,\alpha_N\}$ with the entry at position a_s replaced by λ_s ($s=1,\dots,r$). In words: the operator replaces, in all possible ways, particles in the states $\mu_1,\dots,\mu_r$ by particles in the states $\lambda_1,\dots,\lambda_r$, and no signs appear.

Proof 29.39 Induction on r. For $r=1$, the Lemma on the action of c_μ gives

$$c^\dagger_\lambda c_\mu|\alpha\} = \sum_a \zeta^{a-1}\delta_{\mu,\alpha_a}|\lambda,\alpha_1,\dots,\hat\alpha_a,\dots,\alpha_N\}.$$

Moving λ from position 1 to position a needs $a-1$ transpositions, so $|\lambda,\dots\hat\alpha_a\dots\} = \zeta^{a-1}|\alpha\}_{a\to\lambda}$ (Lemma 29.16), and $\zeta^{2(a-1)}=1$. For $r\to r+1$: first apply c_{μ_1}, which gives $\sum_{a_1}\zeta^{a_1-1}\delta_{\mu_1,\alpha_{a_1}}|\dots\hat\alpha_{a_1}\dots\}$. Then use the induction hypothesis for $c^\dagger_{\lambda_2}\cdots c_{\mu_2}$ on the $(N-1)$-particle state; its positions correspond to $a_2,\dots\in\{1,\dots,N\}\setminus\{a_1\}$. Finally, $c^\dagger_{\lambda_1}$ puts λ_1 in front, and moving it to position a_1 compensates ζ^{a_1-1} as for $r=1$. ∎

Theorem 29.40 One can write for a one-body-operator U that acts on occupation-number-states

$$U = \frac{1}{1!}\sum_{i,j=1}^{\mathrm{d}_\mathcal{H}}\langle\, i\,|\,U\,|\,j\,\rangle\, c^\dagger_i c_j \tag{29.49}$$

Note (missing definition). "One-body-operator" means [38, Eq. (1.53)]: for a single-particle operator u on $\mathcal{H}$ one sets $U^{(N)} := \sum_{l=1}^N u_l$ on $\mathscr{H}_N$, where $u_l = 1\otimes\cdots\otimes u\otimes\cdots\otimes 1$ acts on the l-th factor, and $U := \bigoplus_N U^{(N)}$ (with $U^{(0)}=0$). $U^{(N)}$ commutes with all permutations, hence with P_ζ, and maps $\mathscr{F}_\zeta^N$ into itself. In the formula, $\langle i|U|j\rangle \equiv \langle i|u|j\rangle$ is the single-particle matrix element in an orthonormal basis [38, Eqs. (1.95)–(1.97)].

Proof 29.40

- TBD, cf. Negele, Orland page 17.

Proof (direct, without the detour over the diagonal basis used in [38]). By Lemma 29.39 with $r=1$, multilinearity, and completeness $\sum_i |i\rangle\langle i|u|\alpha_a\rangle = u|\alpha_a\rangle$:

$$\begin{aligned}\sum_{i,j}\langle i|u|j\rangle c^\dagger_i c_j|\alpha_1,\dots,\alpha_N\} &= \sum_{a=1}^N\sum_i\langle i|u|\alpha_a\rangle|\alpha_1,\dots,\alpha_N\}_{a\to i} = \sum_{a=1}^N|\alpha_1,\dots,u\alpha_a,\dots,\alpha_N\}\\ &= \sqrt{N!}\,\mathrm{P}_\zeta\,U^{(N)}|\alpha_1,\dots,\alpha_N) = U\,|\alpha_1,\dots,\alpha_N\},\end{aligned}$$

where the last step uses $[U^{(N)},\mathrm{P}_\zeta]=0$. Both sides vanish on $|0\rangle$, and the auxiliary states span $\mathscr{F}_\zeta$, which proves the operator identity. In the field-operator representation (Theorem 29.34) this gives e.g. [38, Eqs. (1.98)–(1.100)]

$$T = \int \mathrm{d}x\,\hat\psi^\dagger(x)\Big(-\frac{\hbar^2}{2m}\nabla^2\Big)\hat\psi(x), \qquad W = \int \mathrm{d}x\,W(x)\,\hat\psi^\dagger(x)\hat\psi(x),$$

and with $u=1$ the total number operator $N=\sum_j c^\dagger_j c_j$. ∎

29.1.3.2. 2-Body-Operators

Theorem 29.41 One can write for a two-body-operator V that acts on occupation-number-states

$$V = \frac{1}{2!} \sum_{i,j,k,l} \langle\, i\,, j \,|\, U \,|\, k\,, l \,\rangle\, c_i^\dagger c_j^\dagger c_l c_k \tag{29.50}$$

Correction note. (i) The operator in the matrix element is V, not U. (ii) The matrix element is taken between *unsymmetrized* product states, $(i,j|v|k,l) := (\langle i|\otimes\langle j|)\, v\, (|k\rangle\otimes|l\rangle)$, written with round brackets in [38, Eq. (1.107a)]. With the (anti)symmetrized states one has $\{i,j|v|k,l\} = (i,j|v|k,l) + \zeta(i,j|v|l,k)$, and the prefactor would be $\frac{1}{4}$ instead of $\frac{1}{2}$ [38, Eq. (1.107b)]. (iii) The order $c_l c_k$ (reversed w.r.t. k,l) is essential; with $c_k c_l$ one gets an extra factor ζ. (iv) Missing definition [38, Eqs. (1.56), (1.57)]: a two-body operator is $V^{(N)} = \sum_{1\le a<b\le N} v_{ab} = \frac{1}{2}\sum_{a\neq b} v_{ab}$ on $\mathscr{H}_N$, where v acts on $\mathscr{H}_2$, commutes with the exchange of the two particles, and v_{ab} acts on the factors a and b.

Proof 29.41

- TBD, cf. Negele, Orland page 18.

Proof. By Lemma 29.39 with $r = 2$, $(\lambda_1,\lambda_2,\mu_1,\mu_2) = (i,j,k,l)$, so that $c_i^\dagger c_j^\dagger c_l c_k$ appears, and by completeness of $\{|i,j)\}$ in $\mathscr{H}_2$:

$$\begin{aligned}
&\frac{1}{2}\sum_{i,j,k,l} (i,j|v|k,l)\, c_i^\dagger c_j^\dagger c_l c_k |\alpha_1,\dots,\alpha_N\} \\
&= \frac{1}{2}\sum_{a\neq b}\sum_{i,j} (i,j|v|\alpha_a,\alpha_b)\, |\alpha_1,\dots,\alpha_N\}_{a\to i,\, b\to j} \\
&= \frac{1}{2}\sum_{a\neq b} \sqrt{N!}\, \mathrm{P}_\zeta\, v_{ab}|\alpha_1,\dots,\alpha_N) = \sqrt{N!}\, \mathrm{P}_\zeta\, V^{(N)}|\alpha_1,\dots,\alpha_N) = V|\alpha_1,\dots,\alpha_N\},
\end{aligned}$$

using $[V^{(N)}, \mathrm{P}_\zeta] = 0$. For $N \le 1$ both sides vanish. For a local interaction, $(x_1,x_2|v|x_3,x_4) = \delta(x_1-x_3)\delta(x_2-x_4)v(x_1-x_2)$, this gives [38, Eq. (1.108)]

$$V = \frac{1}{2}\int \mathrm{d}x\, \mathrm{d}y\, v(x-y)\, \hat\psi^\dagger(x)\hat\psi^\dagger(y)\hat\psi(y)\hat\psi(x).$$

The normal ordered form $\hat\psi^\dagger\hat\psi^\dagger\hat\psi\hat\psi$ automatically excludes the self-interaction: $\frac{1}{2}\int v\,\hat n(x)\hat n(y) = V + \frac{1}{2}v(0)N$. ■

29.1.3.3. n-Body-Operators

Theorem 29.42 For an n-body-operator L we write

$$L = \sum_{\substack{i_1<\dots<i_n \\ j_1<j_2<\dots<j_{n-1}<j_n}} L^{i_1,\dots,i_n}_{j_1,\dots,j_n}\, a_{i_1}^\dagger \cdots a_{i_n}^\dagger a_{j_1}\cdots a_{j_n},$$

with $L^{i_1,\dots,i_n}_{j_1,\dots,j_n} \in \mathbb{C}$ being defined through the scalar-product (and omitting units for notational simplicity).

Correction note. As stated, the formula is only correct for Fermions. For Bosons the restriction to strictly ordered indices drops all terms with repeated indices (e.g. $c_1^\dagger c_1^\dagger c_1 c_1$ in a two-body interaction). The general formula, valid for both statistics, is [38, Eq. (1.110)]

$$L = \frac{1}{n!} \sum_{\lambda_1,\dots,\lambda_n} \sum_{\mu_1,\dots,\mu_n} (\lambda_1, \dots, \lambda_n | l | \mu_1, \dots, \mu_n)\, c_{\lambda_1}^\dagger \cdots c_{\lambda_n}^\dagger c_{\mu_n} \cdots c_{\mu_1}, \tag{29.51}$$

with the unsymmetrized matrix element of the n-particle operator l (cf. the Definition of m-body-operators below) and the annihilation-operators in *reversed* order. For Fermions, grouping the $n!^2$ orderings of (λ, μ) gives the ordered form of the Theorem with $L^{i_1\dots i_n}_{j_1\dots j_n} = (-1)^{n(n-1)/2} \langle i_1, \dots, i_n | l | j_1, \dots, j_n \rangle$ (normalized antisymmetrized states, $i_1 < \dots < i_n$, $j_1 < \dots < j_n$). The sign comes from reversing $c_{j_n} \cdots c_{j_1}$ into $c_{j_1} \cdots c_{j_n}$. Also: $a \equiv c$.

Proof 29.42

- TBD, cf. Negele, Orland page 19.

Proof of Equation (29.51). Exactly as for two-body-operators. By Lemma 29.39 with $r = n$, the right-hand side acting on $|\alpha_1, \dots, \alpha_N\}$ gives $\frac{1}{n!} \sum_{a_1,\dots,a_n \text{ distinct}} \sqrt{N!}\, \mathrm{P}_\zeta\; l_{a_1\dots a_n} |\alpha_1, \dots, \alpha_N)$. Here we used completeness in $\mathscr{H}_n$, and $l_{a_1\dots a_n}$ acts on the factors $a_1, \dots, a_n$. This is $\sqrt{N!}\, \mathrm{P}_\zeta\, L^{(N)} |\alpha) = L |\alpha\}$ by the Definition below and $[L^{(N)}, \mathrm{P}_\zeta] = 0$. For $N < n$ both sides vanish. The only bookkeeping difficulty, the counting of n-tuples of equal states for Bosons [38, Problem 1.1], is taken care of by the sum over distinct positions a_s, not states. ■

Definition 29.43 An operator R on the many-particle-Hilbert-space is called an m-body-operator if it can be written in the following way

$$R | i_1, i_2, \dots, i_N) =: \frac{1}{m!} \sum_{1 \le n_1 \ne n_2 \ne \dots \ne n_m \le \mathrm{d}_\mathcal{H}} R_{n_1,n_2,\dots,n_m} | i_1, i_2, \dots, i_N) \tag{29.52}$$

Correction note. The summation indices label *particles*, not single-particle states: they run over $\{1, \dots, N\}$, not $\{1, \dots, \mathrm{d}_\mathcal{H}\}$, and they have to be *pairwise* distinct. The chain $n_1 \ne n_2 \ne \dots$ would only exclude neighbouring coincidences. Moreover, $R_{n_1\dots n_m}$ has to be specified: it is a fixed operator r on $\mathscr{H}_m$, acting on the factors $n_1, \dots, n_m$ of $\mathscr{H}_N$ (in this order). The correct definition [38, Eq. (1.61)] reads

$$R^{(N)} | i_1, \dots, i_N) := \frac{1}{m!} \sum_{\substack{a_1,\dots,a_m \in \{1,\dots,N\} \\ \text{pairwise distinct}}} r_{a_1\dots a_m} | i_1, \dots, i_N), \qquad R := \bigoplus_N R^{(N)},$$

with $R^{(N)} = 0$ for $N < m$. For $m = 1$ and $m = 2$ this gives the one- and two-body-operators above.

Lemma 29.44 For any permutation $\pi \in \mathrm{S}_N$ one finds

$$\left(i_1, i_2, \dots, i_N | R | i'_1, i'_2, \dots, i'_N\right) = \left(i_{\pi(1)}, i_{\pi(2)}, \dots, i_{\pi(N)} | R | i'_{\pi(1)}, i'_{\pi(2)}, \dots, i'_{\pi(N)}\right) \tag{29.53}$$

Proof 29.44

- TBD, cf. Negele, Orland p. 10.

Proof (for R as in the corrected Definition; [38, Eq. (1.52)] states it for every operator describing indistinguishable particles). Let $T_\pi|i_1,\dots,i_N\rangle := |i_{\pi(1)},\dots,i_{\pi(N)}\rangle$; T_π maps the orthonormal basis onto itself and is therefore unitary. $T_\pi^\dagger r_{a_1\dots a_m} T_\pi$ is r acting on the relabeled factors $\pi(a_1),\dots,\pi(a_m)$, and the sum over all ordered tuples of pairwise distinct positions is invariant under this relabeling. Hence $T_\pi^\dagger R^{(N)} T_\pi = R^{(N)}$, and $(i_\pi|R|i'_\pi) = (i|T_\pi^\dagger R T_\pi|i') = (i|R|i')$. The same argument shows $[R^{(N)}, \mathrm{P}_\zeta] = 0$, which was used in the proofs above. ■

Corollary 29.45 Notice the identity

$$\frac{(i_1,i_2,\dots,i_N|R|i'_1,i'_2,\dots,i'_N)}{(i_1,i_2,\dots,i_N|i'_1,i'_2,\dots,i'_N)} = \frac{1}{m!}\sum_{1\le n_1\neq n_2\neq\dots\neq n_m\le \mathrm{d}_\mathcal{H}} \frac{(i_1,i_2,\dots,i_N|R|i'_1,i'_2,\dots,i'_N)}{\langle i_1|i'_1\rangle\langle i_2|i'_2\rangle\cdots\langle i_N|i'_N\rangle} \tag{29.54}$$

Correction note. As written, the right-hand side is not correct: each summand is again the full matrix element divided by the full overlap, i.e. the left-hand side itself, and the sum runs over single-particle states instead of particles. The correct identity [38, Eqs. (1.55b), (1.58b), (1.62)] reads, for $(i|i') = \prod_k \langle i_k|i'_k\rangle \neq 0$,

$$\frac{(i_1,\dots,i_N|R|i'_1,\dots,i'_N)}{(i_1,\dots,i_N|i'_1,\dots,i'_N)} = \frac{1}{m!}\sum_{\substack{a_1,\dots,a_m\in\{1,\dots,N\}\\ \text{pairwise distinct}}} \frac{(i_{a_1},\dots,i_{a_m}|r|i'_{a_1},\dots,i'_{a_m})}{\langle i_{a_1}|i'_{a_1}\rangle\cdots\langle i_{a_m}|i'_{a_m}\rangle}.$$

Hence an m-body-operator is completely determined by its matrix elements in $\mathscr{H}_m$. (For $m=1$: $\sum_a \langle i_a|u|i'_a\rangle/\langle i_a|i'_a\rangle$.)

Proof 29.45

- TBD, cf. Negele, Orland p. 10 .

Proof. Since $r_{a_1\dots a_m}$ acts only on the factors $a_1,\dots,a_m$ and the scalar product of product states factorizes,

$$(i|r_{a_1\dots a_m}|i') = (i_{a_1},\dots,i_{a_m}|r|i'_{a_1},\dots,i'_{a_m}) \prod_{k\notin\{a_1,\dots,a_m\}} \langle i_k|i'_k\rangle.$$

Summing over the tuples with the factor $\frac{1}{m!}$ and dividing by $\prod_k\langle i_k|i'_k\rangle$ gives the claim, cf. [38, Eqs. (1.55a), (1.58a)]. ■

29.2. The Reason why so few People in the DFT-Community use Second Quantization

This is (in my (S.K.) opinion) one of the most important theorems in materials theory. Interestingly, it is (to my knowledge) proven in almost none of the standard-textbooks [38, 4, 6, 32]. I only happened to find a proof in [8] which served as a template for this section.

Notation 29.46 Let $L \in \mathrm{End}(\mathcal{H})$ be a linear operator on the single-particle-Hilbert-space $\mathcal{H}$ with second-quantized version $L^{2\mathrm{Q}}$ acting on the Fock-space $\mathscr{F}_\zeta$ as

$$L^{2\mathrm{Q}} \equiv \sum_{ij}\langle i|L|j\rangle\, c_i^\dagger c_j \quad \in \mathscr{A}_\zeta(\mathcal{H}\oplus\mathcal{H}^*, B_\zeta). \tag{29.55}$$

Notation 29.47 We write for the spectral decomposition of the Hamiltonian

$$H - \mu 1_{\mathcal{H}} = \sum_{n=0}^{\infty} \left(E_n - \mu\right) |n\rangle\langle n| \tag{29.56}$$

Definition 29.48 Finally, we define

$$\rho_{\mathcal{H}} \equiv \mathrm{F}_\beta(H - \mu 1_{\mathcal{H}}) := \sum_{n=0}^{\infty} \mathrm{F}_\beta \left(E_n - \mu\right) |n\rangle\langle n|$$

Theorem 29.49 One finds the identity

$$\mathrm{Tr}_{\mathscr{F}}(\rho_{\mathscr{F}} A^{2\mathrm{Q}}) = \mathrm{Tr}_{\mathcal{H}}(\rho_{\mathcal{H}} A). \tag{29.57}$$

Proof 29.49 We first note that the trace is invariant with respect to the basis used, so we may take the basis as the set of eigenvectors of H for the trace of the single-particle Hilbert space, and we consider the occupation number basis derived from it for the trace of the Fock-space. Then

$$Z = \prod_{n=0}^{\infty} (1 + e^{-\beta(E_n - \mu)}) \tag{29.58}$$

and we can write

$$\mathrm{Tr}_{\mathscr{F}}(\rho_{\mathscr{F}} A^{2\mathrm{Q}}) = \sum_{n_1, n_2, \ldots \in \{0,1\}} \langle \Psi_{n_1, n_2, \ldots}, \rho_{\mathscr{F}} A^{2\mathrm{Q}} \Psi_{n_1, n_2, \ldots} \rangle$$

Since

$$\rho_{\mathscr{F}} \Psi_{n_1, n_2, \ldots} = \frac{1}{Z} e^{-\beta \sum_{j=0}^{\infty} n_j (E_j - \mu)} \Psi_{n_1, n_2, \ldots} = \frac{1}{Z} \prod_{j=0}^{\infty} e^{-\beta n_j (E_j - \mu)} \Psi_{n_1, n_2, \ldots},$$

and

$$\langle \Psi_{n_1, n_2, \ldots}, A^{2\mathrm{Q}} \Psi_{n_1, n_2, \ldots} \rangle = \sum_{k,m} \langle e_k, A e_m \rangle \delta_{n_k, 1} \delta_{n_m, 1} \delta_{k,m},$$

we have

$$\mathrm{Tr}_{\mathscr{F}}(\rho_{\mathscr{F}} A^{2\mathrm{Q}}) = \sum_{k=0}^{\infty} \langle e_k, A e_k \rangle \frac{1}{Z} \sum_{n_1, n_2, \ldots \in \{0,1\}} \prod_{j=0}^{\infty} e^{-\beta n_j (E_j - \mu)} \delta_{n_k, 1}.$$

Note that

$$\sum_{n_1,n_2,\ldots\in\{0,1\}}\prod_{j=0}^{\infty}e^{-\beta n_j(E_j-\mu)}\delta_{n_k,1}=(1+e^{-\beta(E_1-\mu)})(1+e^{-\beta(E_2-\mu)})\cdots e^{-\beta(E_k-\mu)}\cdots(1+e^{-\beta(E_r-\mu)})\cdots,$$

hence

$$\frac{1}{Z}\sum_{n_1,n_2,\ldots\in\{0,1\}}\prod_{j=0}^{\infty}e^{-\beta n_j(E_j-\mu)}\delta_{n_k,1}=\mathrm{F}_\beta(E_k-\mu),$$

and therefore

$$\mathrm{Tr}_{\mathscr{F}}(\rho_{\mathscr{F}}A^{2\mathrm{Q}})=\sum_{k=0}^{\infty}\langle e_k,Ae_k\rangle\,\mathrm{F}_\beta(E_k-\mu)=\mathrm{Tr}_{\mathcal{H}}(\rho_{\mathcal{H}}A),$$

proving the theorem.

29.3. The Zero-Temperature Limit

In this section, we show how one obtains the usual zero-temperature-expressions for Green-functions from the finite-temperature-expressions.

Notation 29.50 We write for the temperature-dependent expectation-value in the natural ensemble

$$\langle \cdots \rangle := \frac{1}{Z} \operatorname{Tr}_{\mathscr{H}} \left(\cdots \mathrm{e}^{-\beta \Xi} \right) \tag{29.59}$$

Case 1: The Non-Degenerate Case

Hypothesis 29.51 We assume, that we can enumerate (neglecting degeneracies) the ground-state, first excited state for the operator $\Xi = H - \eta \mu N$ as

$$|0\rangle, |1\rangle, |2\rangle, \ldots \tag{29.60}$$

with energies

$$E_{|0\rangle} < E_{|1\rangle} < E_{|2\rangle} < \ldots \quad \Longleftrightarrow : \quad E_0 < E_1 < E_2 < \ldots \tag{29.61}$$

We further assume, that these states form an orthonormal basis of the Hilbert-space[1], such that the basis-independence of the trace yields

$$\operatorname{Tr}_{\mathscr{H}} \bullet = \sum_{k=0}^{\infty} \langle\, k \,|\, \bullet \,|\, k \,\rangle \tag{29.62}$$

Corollary 29.52 It holds

$$\lim_{T \to 0} \langle \cdots \rangle = \langle\, 0 \,|\, \cdots \,|\, 0 \,\rangle \tag{29.63}$$

and therefore in particular

$$\lim_{T \to 0} G_{\alpha,\alpha'}(t,t') = -\frac{\mathrm{i}}{\hbar} \langle\, 0 \,|\, \mathrm{T}_t \, a_\alpha(t) \, a^\dagger_{\alpha'}(t') \,|\, 0 \,\rangle \tag{29.64}$$

etc for the other Green-functions / expectation-values.

Proof 29.52 We compute

[1] Notice that this is for example the case for usual Slater-determinants / permanents (in the case of an underlying Fock-space).

$$\begin{aligned}\langle\cdots\rangle &\equiv -\frac{\mathrm{i}}{\hbar}\frac{\mathrm{Tr}_{\mathscr{H}}\left(\cdots \mathrm{e}^{-\beta(H-\eta\mu N)}\right)}{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta(H-\eta\mu N)}}\\ &= -\frac{\mathrm{i}}{\hbar}\frac{\mathrm{e}^{-\beta E_0}\langle\,0\,|\,\cdots\,|\,0\,\rangle + \mathrm{e}^{-\beta E_1}\langle\,1\,|\,\cdots\,|\,1\,\rangle + \mathrm{e}^{-\beta E_2}\langle\,2\,|\,\cdots\,|\,2\,\rangle + \ldots}{\mathrm{e}^{-\beta E_0} + \mathrm{e}^{-\beta E_1} + \mathrm{e}^{-\beta E_2} + \ldots}\\ &= -\frac{\mathrm{i}}{\hbar}\frac{\langle\,0\,|\,\cdots\,|\,0\,\rangle + \mathrm{e}^{-\beta(E_1-E_0)}\langle\,1\,|\,\cdots\,|\,1\,\rangle + \mathrm{e}^{-\beta(E_2-E_0)}\langle\,2\,|\,\cdots\,|\,2\,\rangle + \ldots}{1 + \mathrm{e}^{-\beta(E_1-E_0)} + \mathrm{e}^{-\beta(E_2-E_0)} + \ldots}\end{aligned}$$

Therefore one obtains

$$\lim_{T\to 0}\langle\cdots\rangle = -\frac{\mathrm{i}}{\hbar}\langle\,0\,|\,\cdots\,|\,0\,\rangle$$

This yields then for example for the time-ordered Green-function

$$\begin{aligned}G_{\alpha,\alpha'}(t,t') &\equiv -\frac{\mathrm{i}}{\hbar}\frac{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta(H-\eta\mu N)}\,\mathrm{T}_t\,a_\alpha(t)\,a^\dagger_{\alpha'}(t')}{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta(H-\eta\mu N)}}\\ &= -\frac{\mathrm{i}}{\hbar}\frac{\mathrm{e}^{-\beta E_0}\langle\,0\,|\,\mathrm{T}_t\,a_\alpha(t)\,a^\dagger_{\alpha'}(t')\,|\,0\,\rangle + \mathrm{e}^{-\beta E_1}\langle\,1\,|\,\mathrm{T}_t\,a_\alpha(t)\,a^\dagger_{\alpha'}(t')\,|\,1\,\rangle + \mathrm{e}^{-\beta E_2}\langle\,2\,|\,\mathrm{T}_t\,a_\alpha(t)\,a^\dagger_{\alpha'}(t')\,|\,2\,\rangle + \ldots}{\mathrm{e}^{-\beta E_0} + \mathrm{e}^{-\beta E_1} + \mathrm{e}^{-\beta E_2} + \ldots}\\ &= -\frac{\mathrm{i}}{\hbar}\frac{\langle\,0\,|\,\mathrm{T}_t\,a_\alpha(t)\,a^\dagger_{\alpha'}(t')\,|\,0\,\rangle + \mathrm{e}^{-\beta(E_1-E_0)}\langle\,1\,|\,\mathrm{T}_t\,a_\alpha(t)\,a^\dagger_{\alpha'}(t')\,|\,1\,\rangle + \mathrm{e}^{-\beta(E_2-E_0)}\langle\,2\,|\,\mathrm{T}_t\,a_\alpha(t)\,a^\dagger_{\alpha'}(t')\,|\,2\,\rangle + \ldots}{1 + \mathrm{e}^{-\beta(E_1-E_0)} + \mathrm{e}^{-\beta(E_2-E_0)} + \ldots}\end{aligned}$$

Therefore one obtains

$$\lim_{T\to 0} G_{\alpha,\alpha'}(t,t') = -\frac{\mathrm{i}}{\hbar}\langle\,0\,|\,\mathrm{T}_t\,a_\alpha(t)\,a^\dagger_{\alpha'}(t')\,|\,0\,\rangle$$

Case 2: The Degenerate Case

Corollary 29.53 In the case of degenerate states

$$|0_1\rangle, |0_2\rangle, \ldots |0_{n_0}\rangle,\ |1_1\rangle, |1_2\rangle, \ldots |1_{n_1}\rangle,\ |2_1\rangle, |2_2\rangle, \ldots |2_{n_2}\rangle, \ldots \tag{29.65}$$

with energies

$$E_{|0_1\rangle} = E_{|0_2\rangle} = \ldots = E_{|0_{n_0}\rangle} \quad < \quad E_{|1_1\rangle} = E_{|1_2\rangle} = \ldots = E_{|1_{n_1}\rangle} \quad < \quad E_{|2_1\rangle} = E_{|2_2\rangle} = \ldots = E_{|2_{n_2}\rangle} < \ldots$$

It holds

$$\lim_{T\to 0}\langle\cdots\rangle = \frac{1}{n_0}\sum_{j=1}^{n_0}\langle\, 0_j \mid \cdots \mid 0_j \,\rangle \tag{29.66}$$

and therefore in particular

$$\lim_{T\to 0} G_{\alpha,\alpha'}(t,t') = -\frac{\mathrm{i}}{\hbar}\sum_{j=1}^{n_0}\langle\, 0_j \mid \mathrm{T}_t\, a_\alpha(t)\, a^\dagger_{\alpha'}(t') \mid 0_j \,\rangle \tag{29.67}$$

etc for the other Green-functions / expectation-values.

Proof 29.53 By straightforward generalization of the computation before.

29.4. An Interlude on Thermodynamic Variables in Materials Theory

In materials theory, there is a fundamental dilemma when it comes to the modelling:

On *the one hand* ... the *mathematical apparatus* for crystals (chapters 10 - 23 or, more or less equivalently in the literature [4, 7, 38, 52]) is relatively[2] simple in the natural ensemble (a.k.a. the *grand* canonical ensemble for purely electronic systems), which implies that we need as *input-parameters for predictions*

1. the chemical potential μ	yielding particle number as conjugated variable	$\langle N\rangle(\mu,T,V)$
2. the volume V	yielding pressure as conjugated variable	$\langle P\rangle(\mu,T,V)$
3. the temperature T	yielding entropy as conjugated variable	$\langle S\rangle(\mu,T,V)$

On *the other hand* the *software apparatus* for crystals [18, 54] is relatively simple in the *canonical ensemble*, which implies that we need as *input-parameters for predictions*[3]

1. the particle number N	yielding the chemical potential as conjugated variable	$\langle\mu\rangle(N,T,V)$
2. the volume V	yielding pressure as conjugated variable	$\langle P\rangle(N,T,V)$
3. the temperature T	yielding entropy as conjugated variable	$\langle S\rangle(N,T,V)$

This becomes further complicated by the fact, that many experiments (especially those for heat capacities) are almost always being performed at constant pressure (instead of a constant volume). One often argues, that these corrections are negligible at lower temperatures ([47] p. 89), but at higher temperatures they become very relevant [21].

29.4.1. The Chemical Potential for General Systems

Fact 29.54 Following the literature[4] [32, 38, 9, 22] one *determines* the the chemical potential $\mu \equiv \mu(V,T)$ at a given temperature (and volume) by solving the equation

$$N_{\text{desired}} = \langle N\rangle\,(\mu(T,V),T,V) \tag{29.68}$$

for some desired particle-number $N_{\text{desired}} \geq 0$.

Remark 29.54.1 Notice that the r.h.s. of this equation can be computed with Green-functions by utilizing Equation (14.14).

[2] *Relative* to the other available ensembles! See also [55] page 115 stating
"The thermodynamic functions are easier to calculate explicitly if the constraint of a fixed number N of particles is dropped. It is physically realistic for a system coupled to a reservoir of particles."
or similarly in [16] page 121 stating
"In equilibrium quantum statistical mechanics, the grand canonical ensemble is most useful."

[3] More explicitly: The particle number enters the calculations by setting up a k-grid and therefore determining the size of the crystal. The volume enters the calculations by setting up the lattice-constant and lattice-vectors and basis-vectors.

[4] See, for example, [32] p. 14 or [38] p. 47 and 164, or [22] p. 921, or [9] p. 149.

Remark 29.54.2 For crystalline systems, one usually chooses N_{desired} in such a way, that the total crystal is charge-neutral N_{CN}. This implies that one simply counts the number of electrons that should be in the crystal. This is usually further decomposed into number of electrons per unit-cell times the number of unit-cells as in Equation (27.1).

Fact 29.55 Oftentimes it is so, that one does not have the desire to model a charge neutral crystal:

In cases of ...

- light doping
- external electric fields

one oftentimes *chooses* a value for the chemical potential that is somewhere "close" to the Fermi-energy.

Remark 29.55.1 One also encounters often phenomenological models (tight-binding Hamiltonians and generalizations of that) which simply *set* the chemical potential to "some" value that corresponds to a desired physical situation. In these cases, it is however important to closely monitor the implied the underlying particle number (especially as a function of temperature). One sees, for example in [26] that especially for small models, the temperature-dependence of the chemical potential can be strong. This is also emphasized in [38]:

> *"(...) where the chemical potential for the non-interacting system, (...) need not agree with the chemical potential of the interacting system (...)."*

See [38], p. 164.

29.4.2. The Chemical Potential and the Fermi-Energy of Interacting Electrons in Arbitrary Materials

We simply combine the Fluctuation-Dissipation theorem in Equation (14.14) with the Dyson-Equation 15.13 for electrons (i.e. $\eta = 1 = -\zeta$) to obtain

$$\begin{aligned}\langle N \rangle &= \frac{-1}{\pi} \lim_{\epsilon \to 0} \sum\!\!\!\!\!\!\int_{\substack{\alpha \in \mathscr{A} \\ E \in (-\infty, +\infty)}} \mathrm{F}_\beta(E)\ \mathrm{Im}\ G^{\mathrm{ret}}_{\alpha,\alpha}(E + \mathrm{i}\epsilon) \\ &= \frac{-1}{\pi} \lim_{\epsilon \to 0} \sum\!\!\!\!\!\!\int_{\substack{\alpha \in \mathscr{A} \\ E \in (-\infty, +\infty)}} \mathrm{F}_\beta(E)\ \mathrm{Im} \left(\frac{1}{E + \mathrm{i}\epsilon - (H + \Sigma - \mu)} \right)_{\alpha,\alpha}\end{aligned} \tag{29.69}$$

At this point, the only thing that remains left to do, is choosing the model (i.e. Hamiltonian and implied self-energy) that one wants to work with (cf. for example Section 8.4) and inserting Hamiltonian and self-energies. Notice that this can become increasingly difficult, depending on the level of approximation that one seeks to acquire. A common approximation is, for example, the diagonal bands-approximation (cf. Remark 21.3.1).

29.4.3. The Chemical Potential and the Fermi-Energy of Interacting Electrons in Crystals

Theorem 29.56 We compute the chemical potential, by constraining the number of particles

$$\langle N \rangle = \frac{-1}{\pi} \lim_{\delta \to 0} \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k} \in \mathrm{Q} \\ m \in \{1,\ldots,\infty\} \\ E \in (-\infty,+\infty)}} \mathrm{F}_{\beta}(E)\, \mathrm{Im}\, G^{\mathrm{ret}}_{m,m}(E + \mathrm{i}\delta, \mathbf{k})$$

Proof 29.56

$$\begin{aligned}
\langle N \rangle &= \sum_{\substack{\mathbf{k} \in \mathrm{Q} \\ m \in \{1,2,3,\ldots\}}} \langle c^{\dagger}_{m,\mathbf{k}} c_{m,\mathbf{k}} \rangle \\
&= \frac{\hbar}{\mathrm{i}} \sum_{\substack{\mathbf{k} \in \mathrm{Q} \\ m \in \{1,2,3,\ldots\}}} G^{<}_{\substack{m,m \\ \mathbf{k},\mathbf{k}}}(0) \\
&= \frac{\hbar}{2\pi\mathrm{i}} \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k} \in \mathrm{Q} \\ m \in \{1,2,3,\ldots\} \\ \omega \in (-\infty,\infty)}} G^{<}_{\substack{m,m \\ \mathbf{k},\mathbf{k}}}(\omega) \\
&= \frac{-\hbar}{\pi} \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k} \in \mathrm{Q} \\ m \in \{1,2,3,\ldots\} \\ \omega \in (-\infty,\infty)}} \mathrm{F}_{\hbar\beta}(\omega)\, G^{\mathrm{ret}}_{\substack{m,m \\ \mathbf{k},\mathbf{k}}}(\omega + \mathrm{i}\delta)
\end{aligned}$$

Remark 29.56.1 Recall that the retarded Green-function is given by analytical continuation of the Matsubara-Green-function which is determined by solving the Dyson-equation

$$\mathscr{G}(\mathbf{k}, \mathrm{i}\omega_n) = \frac{1}{\hbar} \frac{1}{\mathrm{i}\omega_n - \left(H_0(\mathbf{k}) + \Sigma(\mathbf{k}, \mathrm{i}\omega_n) - \mu \right)/\hbar} \tag{29.70}$$

with non-interacting band-dispersion-matrix $H_0(\mathbf{k}) \equiv \mathrm{diag}(\epsilon_1(\mathbf{k}), \ldots, \epsilon_J(\mathbf{k}))$, whereas J represents the maximal number of bands that are being considered.

29.4.4. The Chemical Potential and the Fermi-Energy of Non-Interacting Electrons in Crystals

Theorem 29.57 For a non-interacting system

$$H = \sum_{\substack{\mathbf{k} \in \mathrm{Q} \\ m \in \{1,2,3,\ldots\}}} \epsilon_{m,\mathbf{k}}\, c^{\dagger}_{m,\mathbf{k}} c_{m,\mathbf{k}} \tag{29.71}$$

without degeneracies one finds

$$|0\rangle = \prod_{j=1}^{N} c^{\dagger}_{m_j,\mathbf{k}_j}|\text{vac.}\rangle =: \prod_{\substack{\mathbf{k}\in Q \\ m\in\{1,2,3,\dots\} \\ \epsilon_{m,\mathbf{k}}<\epsilon_{\text{Fermi}}}} c^{\dagger}_{m,\mathbf{k}}|\text{vac.}\rangle \tag{29.72}$$

with an (a priori unknown) Fermi-energy ϵ_{Fermi} that yet has to be determined.

Proof 29.57 Non-interacting systems can be diagonalized with standard-techniques from linear algebra, such that one arrives at the diagonal form of the Hamiltonian in second quantization. The orthonormal Slater-determinants span the entire Fock-space. Since there are no degeneracies the ground state is unique. The desired particle number N therefore dictates the Fermi-energy.

Lemma 29.58 It holds in the case of non-interacting electrons in a crystal

$$\lim_{T\to 0} \mu(T) = \epsilon_{\text{Fermi}} \tag{29.73}$$

whereas ϵ_{Fermi} is the highest occupied state in the Slater-determinant $|0\rangle$.

Proof 29.58 We compute the average particle twice.

On the one hand we have

$$\langle N\rangle = \sum_{\substack{\mathbf{k}\in Q \\ m\in\{1,2,3,\dots\}}} \langle c^{\dagger}_{m,\mathbf{k}} c_{m,\mathbf{k}}\rangle = \frac{\hbar}{\mathrm{i}} \sum_{\substack{\mathbf{k}\in Q \\ m\in\{1,2,3,\dots\}}} G^{<}_{\substack{m,m \\ \mathbf{k},\mathbf{k}}}(0) = \sum_{\substack{\mathbf{k}\in Q \\ m\in\{1,2,3,\dots\}}} \mathrm{F}_{\beta}(\epsilon_{m,\mathbf{k}} - \mu) \tag{29.74}$$

on the other hand we have

$$\langle 0|N|0\rangle = \sum_{\substack{\mathbf{k}\in Q \\ m\in\{1,2,3,\dots\}}} \langle 0|c^{\dagger}_{m,\mathbf{k}} c_{m,\mathbf{k}}|0\rangle = \sum_{\substack{\mathbf{k}\in Q \\ m\in\{1,2,3,\dots\}}} \theta(\epsilon_{\text{Fermi}} - \epsilon_{m,\mathbf{k}}) \tag{29.75}$$

This gives in the zero-temperature-limit the equation

$$\sum_{\substack{\mathbf{k}\in Q \\ m\in\{1,2,3,\dots\}}} \theta(\epsilon_{\text{Fermi}} - \epsilon_{m,\mathbf{k}}) = \langle 0|N|0\rangle = \lim_{T\to 0}\langle N\rangle(T) = \sum_{\substack{\mathbf{k}\in Q \\ m\in\{1,2,3,\dots\}}} \theta(\,\mu(T=0) - \epsilon_{m,\mathbf{k}}) \tag{29.76}$$

direct comparison of the two expression yields $\mu(T=0) = \epsilon_{\text{Fermi}}$.

29.5. Specific Heat in the Sommerfeld-Approximation and the Dulong-Petit-Law

29.5.1. Intermezzo: The [C]anonical [E]nsemble

29.5.1.1. Formalism

Notation 29.59 We consider the case in which the above mentioned system has a volume V, and is being treated in the canonical ensemble with temperature T and particle number N and Hilbert-space $\mathscr{H} \equiv \mathscr{H}_N$. This gives us the three natural variables (N, T, V).

Fact 29.60 In the absence of „spontaneous symmetry breaking“[5] expectation-values in the canonical-ensemble are evaluated w.r.t. the state

$$\rho_{\mathrm{CE}} = \frac{\mathrm{e}^{-\beta H}}{\mathrm{Tr}_{\mathscr{H}_N}\, \mathrm{e}^{-\beta H}} \equiv \frac{1}{Z_{\mathrm{CE}}} \mathrm{e}^{-\beta H}, \tag{29.77}$$

whereas we introduced the canonical partition-function $Z_{\mathrm{CE}} \equiv Z_{\mathrm{CE}}(N, T, V)$.

Remark 29.60.1 Note that this is a solution to the stationary von Neumann-equation which represents a stationary-state.

Fact 29.61 Recall, that the thermodynamic potential[6] in the canonical ensemble is given by the so-called grand free energy

$$F \equiv F(N, T, V) = -k_{\mathrm{B}} T \log_{\mathrm{e}} Z_{\mathrm{CE}}(N, T, V) \tag{29.78}$$

from which one can conclude the usual relations for the conjugated variables chemical potential, entropy and pressure

$$\frac{\partial F}{\partial N} = \mu, \qquad \frac{\partial F}{\partial T} = -S, \qquad \frac{\partial F}{\partial V} = -P. \tag{29.79}$$

Fact 29.62 The ionic system of a crystal is usually modelled in the canonical ensemble.

Remark 29.62.1 Looking at the appearing equations, we will realize, that one is tempted (and it is quite usual to do so) to re-interprete the ionic system as a system in the so-called „grand canonical ensemble“ with the additional condition that one sets the chemical potential to zero. However, this is just a mnemonic[7]. A non-zero chemical potential can be defined also in the case of an ionic system.

[5] This subject goes far beyond the scope of this lecture.
[6] Recall that this is a scalar-quantity which is used to represent the thermodynamic state of a system.
[7] See attached excerpts at the end of this chapter.

29.5.1.2. Application to the Ionic System

Preparation:

Before we start calculating and predicting observable quantities for the ionic system, we collect all the things we need.

- Hilbert-space: $\mathscr{H} = \bigotimes_{j=1}^{rd_{\mathbf{x}}N_p} L^2(\mathbb{R}^1) \simeq L^2(\mathbb{R}^{rd_{\mathbf{x}}N_p})$
- Basis: $\mathscr{B} = \left\{ |N\rangle \equiv |n_{\lambda_1}, n_{\lambda_2}, \dots, n_{\lambda_{rd_{\mathbf{x}}N_p}}\rangle \equiv \prod_{j=1}^{rd_{\mathbf{x}}N_p} |n_{\lambda_j}\rangle \,|\, \forall j \in \{1, \dots, rd_{\mathbf{x}}N_p\} : n_{\lambda_j} \in \{0, 1, 2, \dots, \infty\} \right\}$
- Expectation-value: $\langle A\rangle = \frac{\mathrm{Tr}_{\mathscr{H}}\, A\, \mathrm{e}^{-\beta H_{\text{harm.}}}}{\mathrm{Tr}_{\mathscr{H}}\, \mathrm{e}^{-\beta H_{\text{harm.}}}} \equiv \frac{\sum_{N\in\mathscr{B}} \langle\, N \,|\, A\, \mathrm{e}^{-\beta H_{\text{harm.}}} \,|\, N \,\rangle}{\sum_{N\in\mathscr{B}} \langle\, N \,|\, \mathrm{e}^{-\beta H_{\text{harm.}}} \,|\, N \,\rangle}$

(29.80)

whereas A represents an observable (i.e. an hermitian operator, usually written in second quantized form).

Theorem 29.63 One finds for the average occupation-number

$$\langle n_{\nu\mathbf{q}}\rangle = \langle b^\dagger_{\nu\mathbf{q}} b_{\nu\mathbf{q}}\rangle = \mathrm{B}_\beta(\hbar\omega_{\nu\mathbf{q}}) \tag{29.81}$$

Proof 29.63 See Appendix, p. 640.

Corollary 29.64 It follows for the internal energy of the ionic system

$$\langle H_{\text{harm.}}\rangle(N,V,T) = \sum_{\mathbf{q}\in\mathrm{Q}} \sum_{\nu=1}^{rd_{\mathbf{x}}} \hbar\omega_{\nu\mathbf{q}} \left(\left\langle b^\dagger_{\nu\mathbf{q}} b_{\nu\mathbf{q}} \right\rangle + \frac{1}{2} \right) = \sum_{\mathbf{q}\in\mathrm{Q}} \sum_{\nu=1}^{rd_{\mathbf{x}}} \hbar\omega_{\nu\mathbf{q}} \left(\mathrm{B}_\beta(\hbar\omega_{\nu\mathbf{q}}) + \frac{1}{2} \right)$$

Proof 29.64 Follows immediately from the linearity of the expectation-value and Theorem 29.63.

29.5.1.3. The Low-Temperature Limit

Approximation 29.65 We assume that

$$k_{\mathrm{B}}T \ll \hbar\omega_{\text{opt,min}} \wedge k_{\mathrm{B}}T \ll \hbar\omega_{\text{ac,max}} \quad 1 \ll \beta\hbar\omega_{\text{opt,min}} \wedge 1 \ll \beta\hbar\omega_{\text{ac,max}} \tag{29.82}$$

Corollary 29.66 The contribution from the optical branches is negligible.

Proof 29.66 For an optical phonon branch $\nu \in \{d_{\mathbf{x}}+1, \dots, rd_{\mathbf{x}}\}$ we obtain

$$0 \leq \sum_{\mathbf{q}\in \mathrm{Q}} \hbar\omega_{\nu\mathbf{q}}\, \mathrm{B}_{\beta}(\hbar\omega_{\nu\mathbf{q}}) = \sum_{\mathbf{q}\in \mathrm{Q}} \hbar\omega_{\nu\mathbf{q}} \frac{1}{\mathrm{e}^{\beta\hbar\omega_{\nu\mathbf{q}}}-1} \leq \sum_{\mathbf{q}\in \mathrm{Q}} \hbar\omega_{\nu\mathbf{q}} \frac{1}{\mathrm{e}^{\beta\hbar\omega_{\mathrm{opt,min}}}-1} \approx \sum_{\mathbf{q}\in \mathrm{Q}} \hbar\omega_{\nu\mathbf{q}} \mathrm{e}^{-\beta\hbar\omega_{\mathrm{opt,min}}} \overset{T\to 0}{\longrightarrow} 0 \tag{29.83}$$

Approximation 29.67 Recalling that

$$\hbar\omega_{\nu}(\mathbf{q}) \approx c_{\nu} q \quad \text{for } \nu \in \{1, \dots, d_{\mathbf{x}}\} \equiv \{\text{"indices for acoustic phonons"}\} \text{ and } q \approx 0 \tag{29.84}$$

we can also evaluate the contribution from the acoustic branches.

Corollary 29.68 In the low-temperature limit, the internal energy is dominated by the acoustic phonons, i.e.

$$E \overset{T\approx 0}{\equiv} \langle H_{\mathrm{harm.}} \rangle (N, V, T) \approx E_0 + \sum_{\nu=1}^{d_{\mathbf{x}}} \sum_{\mathbf{q}\in \mathrm{Q}} c_{\nu} q \frac{1}{\mathrm{e}^{\beta c_{\nu} q}-1} \tag{29.85}$$

Proof 29.68 ToBeFormulated Cleanly

Theorem 29.69 It follows

$$E - E_0 \approx \frac{\pi^2}{30} \frac{1}{\hbar^3 \overline{c^3}} N_p V_{\mathrm{uc}} k_{\mathrm{B}}^4 T^4 \tag{29.86}$$

Proof 29.69 TBDigitalized; Cf. Bulla Script.

29.5.1.4. The High-Temperature Limit

TBD.

29.5.1.5. Summary

Corollary 29.70 One finds for the internal energy of the system

$$\begin{aligned}\langle H_{\text{harm.}}\rangle(N,V,T) &\equiv E(N,V,T)\\ &= \begin{cases} E_0 + rd_{\mathbf{x}} N_p k_{\text{B}} T & \text{if } \forall \underline{q} \in \Xi : \ k_{\text{B}} T \gg \hbar\omega_{\underline{q}} \\ E_0 + \text{const.} \times V \times T^4 & \text{if both equations are fulfilled } \forall \underline{q} \in \Xi : \ k_{\text{B}} T \ll \hbar\omega_{\underline{q}} \approx \hbar c q. \end{cases}\end{aligned} \tag{29.87}$$

Proof 29.70 See below.

Remark 29.70.1 Notice that one gets for the specific heat capacity per volume

$$\begin{aligned}C_{N,V}(T) &\equiv \partial_T \langle H_{\text{harm.}}\rangle(N,V,T)\\ &\propto \begin{cases} \text{const.} & \text{if } \forall \underline{q} \in \Xi : \ k_{\text{B}} T \gg \hbar\omega_{\underline{q}} \\ \text{const.} T^3 & \text{if both equations are fulfilled } \forall \underline{q} \in \Xi : \ k_{\text{B}} T \ll \hbar\omega_{\underline{q}} \approx \hbar c q. \end{cases}\end{aligned} \tag{29.88}$$

which reproduces the Dulong-Petit-law for high-temperatures and the experimental behaviour advertised in the beginning of the lecture for low-temperatures.

29.5.2. Intermezzo: The [G]rand [C]anonical [E]nsemble

29.5.2.1. Formalism

Notation 29.71 We further restrict our attention to the case in which the above mentioned system has a volume V, and is being treated in the grand canonical ensemble with temperature T and chemical potential μ that is being set such that the average particle number is fixed to be a constant (see below). We further assume the system to be described the Hilbert-space[8] $\mathscr{H}$. This gives us the three natural variables (μ, T, V).

Remark 29.71.1 Notice that, if we are for example treating a crystal, and we count the number of electrons that we would expect to be inside the crystal, then (in general) we have to *numerically* determine the chemical potential.

Fact 29.72 In the absence of „spontaneous symmetry breaking“ expectation-values in the grand-canonical-ensemble are evaluated w.r.t. the state

$$\rho_{\mathrm{GCE}} = \frac{\mathrm{e}^{-\beta(H-\mu N)}}{\mathrm{Tr}_{\mathscr{H}}\, \mathrm{e}^{-\beta(H-\mu N)}} \equiv \frac{1}{Z_{\mathrm{GCE}}} \mathrm{e}^{-\beta(H-\mu N)}, \tag{29.89}$$

whereas we introduced the grand canonical partition-function $Z_{\mathrm{GCE}} \equiv Z_{\mathrm{GCE}}(\mu, T, V)$.

Remark 29.72.1 Recall that the state above represents a solution to the stationary von Neumann equation.

Remark 29.72.2 Although in the case of „spontaneous symmetry breaking“, the evaluation of observables w.r.t. the state above yields incorrect results, one can oftentimes however use the state above, and break the underlying symmetry „by hand“, in order to recover the „correct“ physical state (or, in the case that we will encounter later, the correct physical „field theory“) again.

Fact 29.73 Recall, that the thermodynamic potential in the grand canonical ensemble is given by the so-called grand canonical potential

$$\Omega \equiv \Omega(\mu, T, V) = -\frac{\mathrm{Log}_{\mathrm{e}}\, Z_{\mathrm{GCE}}(\mu, T, V)}{\beta} \tag{29.90}$$

from which one can conclude the usual relations for the conjugated variables particle-number, entropy and pressure

$$\frac{\partial \Omega}{\partial \mu} = -N, \qquad \frac{\partial \Omega}{\partial T} = -S, \qquad \frac{\partial \Omega}{\partial V} = -P. \tag{29.91}$$

[8] For indistinguishable particles, this Hilbert-space will be equal to a Fock-space $\mathscr{H} \equiv \mathscr{F}_{\zeta}$.

29.5.2.2. Application to the Electronic System

We treat the electronic system within the LDA-approximation of Quantum-Espresso[9].

Notation 29.74 We have the electronic density of states in a free electron gas given as obtained through quantum espresso as

$$\rho_{\text{aux}}(E) = \sum_{\substack{\mathbf{k}\in\text{Q} \\ \sigma\in\{\downarrow,\uparrow\} \\ n\in\{1,2,\dots\}}} \delta(E-\epsilon_{n\mathbf{k}}) \tag{29.92}$$

Lemma 29.75 One obtains the formulae

$$\begin{aligned} \langle N\rangle &= \sum_{\substack{\mathbf{k}\in\text{Q} \\ \sigma\in\{\downarrow,\uparrow\} \\ n\in\{1,2,\dots\}}} \text{F}_\beta(\epsilon_{n\mathbf{k}\sigma}-\mu) &&= \int \text{d}E\ \text{F}_\beta(E-\mu)\rho_{\text{aux}}(E) \\ \langle H_{\text{el}}\rangle &= \sum_{\substack{\mathbf{k}\in\text{Q} \\ \sigma\in\{\downarrow,\uparrow\} \\ n\in\{1,2,\dots\}}} \text{F}_\beta(\epsilon_{n\mathbf{k}\sigma}-\mu)\epsilon_{n\mathbf{k}\sigma} &&= \int \text{d}E\ \text{F}_\beta(E-\mu)\rho_{\text{aux}}(E)E \end{aligned} \tag{29.93}$$

Proof 29.75 TBDigitalized.

Remark 29.75.1 Although the discrete formulae look very tempting and beautiful, they are oftentimes quite inconvenient to use in practice as they are difficult to use for reliable calculations. Therefore, it is oftentimes more convenient to instead use the integral formulae after one introduced a smearing in the density of states in Equation (29.92).

Remark 29.75.2 The smearing that one usually introduced can be explained on physical grounds. This becomes clear after we introduced the concept of self-energies for electron-phonon-systems.

Theorem 29.76 One finds for the heat-capacity $C_{V,N}(T)$ the equation

$$C_{V,N}(T) = \frac{\pi^2}{3}\rho_{\text{aux}}(E_{\text{F}})k_{\text{B}}^2 T \equiv \gamma T \tag{29.94}$$

with heat-capacity coefficient $\gamma = \frac{\pi^2}{3}\rho_{\text{aux}}(E_{\text{F}})k_{\text{B}}^2$.

Proof 29.76 TBDigitalized.

[9] The templates ...
- Cf. Schwabl page 186 [47, Sect. 4.3, p. 186]
- Bulla-Skript
- Czycholl-Book.

Corollary 29.77 Combining the results, we obtain an expression for the molar heat capacity

$$\begin{aligned} C_{V,N,\text{molar}}(T) &= \frac{1}{n} \cdot C_{V,N}(T) \\ &= \frac{1}{N_x N_y N_z 1.66 \cdot 10^{-24}\,\text{mol}} \cdot \frac{\pi^2}{3} \rho_{\text{aux}}(0) k_{\text{B}}^2 T \\ &= \frac{\rho_{\text{aux}}(0)}{N_x N_y N_z} \cdot \frac{\pi^2}{3} \frac{k_{\text{B}}^2}{1.66 \cdot 10^{-24}\,\text{mol}} \cdot T \\ &= \rho_{\text{QE}}(E_{\text{F}}) \cdot \frac{\pi^2}{3} \frac{k_{\text{B}}^2}{1.66 \cdot 10^{-24}\,\text{mol}} \cdot T \\ &\equiv \gamma_m \cdot T \end{aligned}$$

with the final expression for γ_m as

$$\gamma_m = \rho_{\text{QE}}(E_{\text{F}}) \cdot \frac{\pi^2}{3} \frac{k_{\text{B}}^2}{1.66 \cdot 10^{-24}\,\text{mol}} \tag{29.95}$$

with ρ_{QE} as in Equation (24.3).

Proof 29.77 Follows from combining Equation (29.94) with Equation (9.58).

29.5.3. Thermodynamics of a Crystal in the Non-Interacting Gases Approximation

$$\begin{aligned} H_{\text{tot}} &\equiv H_{\text{el}} + H_{\text{ph}} + H_{\text{el-ph-int}} \\ &\equiv \sum_{\substack{\mathbf{k}\in \mathrm{Q} \\ \sigma\in\{\downarrow,\uparrow\} \\ n\in\{1,2,\dots\}}} \epsilon_{n\mathbf{k}} c^{\dagger}_{n\sigma\mathbf{k}} c_{n\sigma\mathbf{k}} + \sum_{\substack{\mathbf{k}\in \mathrm{Q} \\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}}} \hbar\omega_{\nu\mathbf{k}} b^{\dagger}_{\nu\mathbf{k}} b_{\nu\mathbf{k}} + 0 \end{aligned}$$

with allowed wave-vectors Q $\subset$ "First Brillouin Zone". Notice that the total Hilbert-space $\mathscr{H}$ of the system is given as tensor-product

$$\mathscr{H} = \mathscr{H}_{\text{F}} \otimes \mathscr{H}_{\text{B}}$$

with basis and scalar-product inherited from the respective many-identical-particle-Hilbert-spaces as usual. Modelling the system as being connected to a heat-reservoir (the environment dictating the temperature), we work in a hybrid ensemble with thermodynamic variables (T, V, μ, N_p), expectation-values are evaluated w.r.t. the stationary solution of the von Neumann equation. Concretely one has for an observable quantity (expressed as a polynomial expression in second quantized operators) A the expectation-value

$$\langle A \rangle \equiv \frac{\mathrm{Tr}_{\mathscr{H}}\, A\, \mathrm{e}^{-\beta\left(H_{\text{el}} - \mu N_{\text{el}} + H_{\text{ph}}\right)}}{\mathrm{Tr}_{\mathscr{H}}\, \mathrm{e}^{-\beta\left(H_{\text{el}} - \mu N_{\text{el}} + H_{\text{ph}}\right)}} \equiv \frac{\mathrm{Tr}_{\mathscr{H}}\, A\, \mathrm{e}^{-\beta\left(H_{\text{el}} - \mu N_{\text{el}} + H_{\text{ph}}\right)}}{Z}. \tag{29.96}$$

Other thermodynamic properties (such as pressure) are determined by derivatives of the hybrid partition-function. Combining the results, we obtain for the heat capacity at low temperatures

$$C_{V,N,\text{molar}}(T) = \frac{1}{n} \cdot C_{V,N}(T) \approx \gamma_m \cdot T + A \cdot T^3$$

in excellent agreement with several experimental results.

The folklore statement that the chemical potential of phonons is zero is correct, if one treats the phononic system in the grand canonical ensmeble. Notice however that in our derivation it became evident that we are *actually* working in the canonical ensemble. There is a possibility to define a chemical potential for the phononic system, which does not neccessarily need to be zero. Treating the phononic system in the grand canonical ensemble and agreeing to set $\mu = 0$ is just a mnemonic, which is quite common in the literature, but it is not a fundamental statement.

Addendum: The Chemical Potential of Bosons.

Here is a (hopefully convincing) selection of excerpts supporting this claim.

als

$$H_{\text{harm}} = \sum_{\boldsymbol{q}} \sum_{j=1}^{dr} \hbar\omega_j(\boldsymbol{q}) \left(b^\dagger_{\boldsymbol{q}j} b_{\boldsymbol{q}j} + \frac{1}{2} \right) . \tag{4.41}$$

Hierbei erfüllen die Oszillator-Auf- und Absteige-Operatoren $b^{(\dagger)}_{\boldsymbol{q}j}$ gemäß (4.15) die Vertauschungsrelation

$$\left[b_{\boldsymbol{q}j}, b^\dagger_{\boldsymbol{q}'j'} \right] = \delta_{\boldsymbol{q}\boldsymbol{q}'}\delta_{jj'} , \quad \left[b^\dagger_{\boldsymbol{q}j}, b^\dagger_{\boldsymbol{q}'j'} \right] = [b_{\boldsymbol{q}j}, b_{\boldsymbol{q}'j'}] = 0 . \tag{4.42}$$

Dies sind die Vertauschungsrelationen für Bose[2]-Erzeugungs- und Vernichtungs-Operatoren. Die Elementaranregungen des Hamilton-Operators in harmonischer Näherung, also die quantisierten Normalschwingungen, verhalten sich also wie die eines Systems **wechselwirkungsfreier Bosonen**. Diese nennt man auch **Phononen**. Phononen sind keine wirklichen Teilchen sondern **Quasiteilchen**. Insbesondere gibt es keine Teilchenzahlerhaltung (und deshalb auch kein chemisches Potential). Auch in dieser Hinsicht verhalten sich Phononen analog wie Photonen (Quanten des elektromagnetischen Feldes). In der Tat weist auch die Thermodynamik der Phononen (quantisierten Gitterwellen) eine enge Analogie zur Thermodynamik des Photonengases (Hohlraum-Strahlung, quantisierte elektromagnetische Wellen) auf.

Figure 29.1.: An excerpt from the book from Czycholl.

particle reservoirs, or a subsystem is considered. The system can exchange particles with the reservoirs which are described by their chemical potentials (assuming in general several particle species present). This feature is simply included by introducing Lagrange multipliers, i.e. tacitly understanding that single-particle energies are measured relative to their chemical potential, $H \to H - \sum_s \mu_s N_s$. In this case, the partition function instead of being a function of the number of particles, is a function of the chemical potentials for the species in question

$$Z_{\text{gr}}(T, \mu_s) = \text{Tr}\, e^{-(\mathcal{H}-\mu_s N_s)/kT} = e^{-\Omega(T,\mu_s)/kT} \tag{2.90}$$

specified by the average number of particles according to

$$\langle N_s \rangle = -\left(\frac{\partial \Omega}{\partial \mu_s} \right)_{T,V} . \tag{2.91}$$

For systems of particles where the total number of *particles* is not conserved, i.e. where the Hamiltonian and the total number operator do not commute, such as for phonons and photons, the chemical potential vanishes, and the grand canonical ensemble is employed. For degenerate fermions, such as electrons in a metal, the

Figure 29.3.: An excerpt from the book from Rammer.

Chemisches Potential: Das chemische Potential des Photongases kann aus der Gibbs-Duhem-Relation $E = TS - PV + \mu N$ berechnet werden, da es sich um ein homogenes System handelt:

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$$\mu = \frac{1}{N}(E - TS + PV) = \frac{1}{N}\left(4 - \frac{16}{3} + \frac{4}{3}\right) \frac{\sigma V T^3}{3c} \equiv 0 . \tag{4.5.22}$$

Das chemische Potential des Photonengases ist für alle Temperaturen identisch 0, da die Zahl der Photonen nicht fest ist, sondern sich an die Temperatur und das Volumen anpaßt. Photonen werden von der umgebenden Materie, den Wänden des Hohlraums, absorbiert und emittiert. Generell verschwindet das chemische Potential von Teilchen und von Quasiteilchen, wie z.B. Phononen, deren Teilchenzahl durch keinen Erhaltungssatz eingeschränkt ist. Betrachten wir nämlich die freie Energie für eine fiktive feste Zahl von Photonen (Phononen etc.) $F(T, V, N_{\text{Ph}})$. Da die Zahl der Photonen (Phononen) nicht eingeschränkt ist, adjustiert sie sich so, daß die freie Energie minimal wird $\left(\frac{\partial F}{\partial N_{\text{Ph}}}\right)_{T,V} = 0$. Das ist aber gerade der Ausdruck für das chemische Potential, welches somit verschwindet: $\mu = 0$. Ebenso hätten wir von der Maximalität der Entropie ausgehen können $\left(\frac{\partial S}{\partial N_{\text{Ph}}}\right)_{E,V} = -\frac{\mu}{T} = 0$.

Figure 29.2.: An excerpt from the book from Schwabl. [47, Sect. 4.5, Eq. (4.5.22), p. 205 f.]

In thermal equilibrium, the average number of particles in a state λ is given by the usual boson occupation factor:

$$\langle n_\lambda \rangle = \frac{1}{e^{\beta(\varepsilon_\lambda - \mu)} - 1} \equiv N_\lambda = n_B(\varepsilon_\lambda - \mu) \tag{1.118}$$

Now there is a chemical potential, μ, which can vary with temperature and concentration. It is absent in the phonon, and photon, cases because these excitations do not conserve particle number. One may make as many phonons or photons as one wishes. Another operator of interest is the density operator:

Figure 29.4.: An excerpt from the book from Mahan.

29.6. The Wave-like / Massless Nature of the Phononic Quantum Field Theory

Theorem 29.78 Going over to the field-integral-description of the problem gives the action

$$S_{\text{ph}}[\phi,\overline{\phi}] = \sum\!\!\!\!\!\!\int_{\substack{\mathbf{q}\in\text{Q}\\ \tau\in(0,\hbar\beta)\\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\}}} \overline{\phi}_{\nu}(\tau,\mathbf{q})\left(\partial_{\tau}+\omega_{\nu}(\mathbf{q})\right)\phi_{\nu}(\tau,\mathbf{q}) \tag{29.97}$$

and switching to the Matsubara-representation yields

$$S_{\text{ph}}[\phi,\overline{\phi}] = \sum\!\!\!\!\!\!\int_{\substack{\mathbf{q}\in\text{Q}\\ \omega_n\in\Omega_{+1}\\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\}}} \overline{\phi}_{\nu}(\text{i}\omega_n,\mathbf{q})\left(-\text{i}\omega_n+\omega_{\nu}(\mathbf{q})\right)\phi_{\nu}(\text{i}\omega_n,\mathbf{q}) \tag{29.98}$$

$$\equiv \sum\!\!\!\!\!\!\int_{\substack{q\in\text{i}\Omega_{+1}\times\text{Q}\\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\}}} \overline{\phi}_{\nu}(q)\left(-\text{i}\omega_n+\omega_{\nu}(\mathbf{q})\right)\phi_{\nu}(q) \tag{29.99}$$

whereas we introduced the four-momentum $q \equiv (\mathbf{q}, \text{i}\omega_n)$

Proof 29.78 Follows from Corollary 20.15.

Lemma 29.79 We introduce now the auxiliary fields

$$A_{\nu}(q) = \phi_{\nu}(q) + \overline{\phi}_{\nu}(-q), \qquad \Pi_{\nu}(q) = \phi_{\nu}(q) - \overline{\phi}_{\nu}(-q)$$

with inverse transformation

$$\phi(q) = \frac{A_{\nu}(q)+\Pi_{\nu}(q)}{2}, \qquad \overline{\phi}(q) = \frac{A_{\nu}(-q)-\Pi_{\nu}(-q)}{2}$$

Proof 29.79 TBD.

Remark 29.79.1 Notice that the fields defined like this are not independent from each other; One finds symmetries

$$A_\nu(q) = \overline{A}_\nu(-q), \qquad \Pi_\nu(q) = -\overline{\Pi}_\nu(-q). \tag{29.100}$$

In order to be able to change coordinates without double-counting, we restrict attention to the variables

$$\left\{A_\nu(q), \Pi_\nu(q)\right\}_{\substack{q \in \mathrm{i}\Omega_{+1} \times \mathrm{Q}/\sim \\ \nu \in \{1,\ldots,rd_{\mathbf{x}}\}}} \quad \text{with} \quad q \sim q' \ :\Longleftrightarrow\ q = -q'. \tag{29.101}$$

Part 1: No External Sources

Theorem 29.80 Changing integration-variables according to Equations (TBD) and integrating out the Π-fields yields the action

$$S_{\mathrm{ph}}[A, \overline{A}] = \sum_{\substack{\nu \in \{1,\ldots,rd_{\mathbf{x}}\} \\ q \in \mathrm{i}\Omega_{+1} \times \mathrm{Q}/\sim}} \overline{A}_\nu(\mathrm{i}\omega_n, \mathbf{q}) \frac{\omega_n^2 + \omega_\nu(\mathbf{q})^2}{2\omega_\nu(\mathbf{q})} A_\nu(\mathrm{i}\omega_n, \mathbf{q}) \tag{29.102}$$

Proof 29.80 See Appendix, Proofs, page 636.

Remark 29.80.1 It will turn out, that all the interacting theories that one encounters in materials theory are independent of the Π-fields, such that integrating them out is a legitimate step.

Corollary 29.81 It follows

$$\mathscr{D}_{\nu\nu'}(\mathrm{i}\omega_n, \mathbf{q}) = -\frac{1}{\hbar} \frac{2\omega_\alpha \delta_{\alpha,\alpha'}}{\omega_n^2 + \omega_\alpha^2} \tag{29.103}$$

from matrix-inversion.

Proof 29.81 Follows from the identity in Theorem TBD.

Remark 29.81.1 Notice that we derived this identity earlier by straight-forward computation of expectation-values, in Theorem TBReferenced.

TBElaborated.

Part 2: Incorporating External Sources

Theorem 29.82 The action in presence of external sources reads

$$S_{\substack{\text{ph}\\[j,\bar{j}]}}[\phi,\overline{\phi}] = \sum\!\!\!\!\!\!\int_{\substack{\mathbf{q}\in\mathrm{Q}\\ \tau\in(0,\hbar\beta)\\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} \overline{\phi}_\nu(\tau,\mathbf{q})\left(\partial_\tau+\omega_\nu(\mathbf{q})\right)\phi_\nu(\tau,\mathbf{q}) \quad + \quad \sum\!\!\!\!\!\!\int_{\substack{\mathbf{q}\in\mathrm{Q}\\ \tau\in(0,\hbar\beta)\\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} \left[\overline{\phi}_\nu(\tau,\mathbf{q})j(\tau,\mathbf{q})+\bar{j}(\tau,\mathbf{q})\phi_\nu(\tau,\mathbf{q})\right] \tag{29.104}$$

and switching to the Matsubara-representation yields

$$S_{\text{ph}}[\phi,\overline{\phi}] = \sum\!\!\!\!\!\!\int_{\substack{q\in\mathrm{i}\Omega_{+1}\times\mathrm{Q}\\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} \overline{\phi}_\nu(q)\left(-\mathrm{i}\omega_n+\omega_\nu(\mathbf{q})\right)\phi_\nu(q) \quad + \quad \sum\!\!\!\!\!\!\int_{\substack{q\in\mathrm{i}\Omega_{+1}\times\mathrm{Q}\\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} \left[\overline{\phi}_\nu(q)j(q)+\bar{j}(q)\phi_\nu(q)\right] \tag{29.105}$$

whereas we introduced the four-momentum $q \equiv (\mathbf{q}, \mathrm{i}\omega_n)$

29.7. The Equation-of-Motion-Technique as double-edged sword

Corollary 29.83 For non-interacting-systems (i.e. quadratic Hamiltonians as in eq. (8.32)) one finds the equation of motion

$$\begin{aligned} & (\omega + \mathrm{i}\delta) \quad G^{\mathrm{ret}}_{\alpha\alpha'}(\omega + \mathrm{i}\delta) && = \delta_{\alpha\alpha'} + \sum_{\beta} \frac{h_{\alpha\beta} - \mu\delta_{\alpha\beta}}{\hbar} G^{\mathrm{ret}}_{\beta\alpha'}(\omega + \mathrm{i}\delta) \\ \iff & (\omega + \mathrm{i}\delta) \quad \mathbf{G}^{\mathrm{ret}}(\omega + \mathrm{i}\delta) && = \mathbb{1} + \frac{\mathbf{H} - \mu\mathbb{1}}{\hbar} \mathbf{G}^{\mathrm{ret}}(\omega + \mathrm{i}\delta) \\ \iff & \qquad\quad \mathbf{G}^{\mathrm{ret}}(\omega + \mathrm{i}\delta) && = \left[\omega + \mathrm{i}\delta - \frac{\mathbf{H} - \mu\mathbb{1}}{\hbar}\right]^{\mathrm{inv}} \end{aligned} \tag{29.106}$$

Proof 29.83 TBD.

Remark 29.83.1 By straight forward calculation, one also sees, that the various Green-functions (retarded, advanced, time-ordered) obey the very same equation of motion as above.

Remark 29.83.2 The fact, that three Green-functions obey the same equation of motion makes me (personally) a little bit uncomfortable; In [Francesco 04] one comments this in the following way (with adapted notation for better understanding)

> *(...) On the other hand, the detailed time-dependence of $G^{ret}(t)$, $G^{adv}(t)$ and $G(t)$ is obviously very different. From the definition of these quantities follows for example that $G^{r}(t < 0) \equiv 0$, while $G^{a}(t > 0) \equiv 0$. Thus, if one wants to determine the correct solution of the equation of motion, one must incorporate those boundary conditions appropriately. This implies that the Fourier-transformation in eq. (...) has to be performed with some care.*

And nonetheless, despite these warnings, one usually determines the retarded- and advanced-Green-functions by the equation-of-motion-technique. Update: It can be proven (from the functional integral formalism) that the equation-of-motion-technique yields the correct result for the retarded- and advanced-Green-functions. But **not** for the time-ordered Green-function.

29.8. The Curious Formalism of Position Eigenstates

In materials theory, it is unfortunately common to invoke the concept of so-called position eigenstates. The author of these notes dislikes them, as they are (in his opinion) only nice to have for aesthetical reasons, without any concrete use. We will elucidate the concept here, and then make comments about their usefulness.

Notation 29.84 We consider the situation in Notation 10.1. Let

$$\mathcal{H} = \mathrm{span}_{\mathbb{C}}\{|\alpha\rangle \quad | \quad \alpha \in \mathscr{A}\} \tag{29.107}$$

be a single-particle Hilbert-space with orthonormal basis. Let $\{c_\alpha, c_\alpha^\dagger\}_{\alpha\in\mathscr{A}}$ denote the corresponding creation- and annihilation-operators obeying the statistical commutation-relations.

Completion (notation and assumptions used throughout this section). We write $x \equiv (\mathbf{x}, s)$ for a combined position- and spin-label, $\oint\!\!\!\!\!\!\sum_x \equiv \sum_s \int \mathrm{d}^3\mathbf{x}$, and $\delta(x - x') \equiv \delta_{ss'}\,\delta^{(3)}(\mathbf{x} - \mathbf{x}')$. The kets $|x\rangle$ are the generalized eigenvectors of the position- and spin-operators. They are *not* elements of $\mathcal{H}$, but satisfy (in the sense of distributions)

$$\langle x|x'\rangle = \delta(x - x'), \qquad \oint\!\!\!\!\!\!\sum_x |x\rangle\langle x| = 1_{\mathcal{H}}.$$

The wave functions of the basis states are $\phi_\alpha(x) := \langle x|\alpha\rangle$, hence $\phi_\alpha^*(x) = \langle \alpha|x\rangle$. Orthonormality and completeness of $\{|\alpha\rangle\}_{\alpha\in\mathscr{A}}$ read in this language

$$\oint\!\!\!\!\!\!\sum_x \phi_\alpha^*(x)\,\phi_\beta(x) = \langle\alpha|\beta\rangle = \delta_{\alpha\beta}, \qquad \sum_{\alpha\in\mathscr{A}} \phi_\alpha(x)\,\phi_\alpha^*(x') = \langle x|\Big(\sum_{\alpha\in\mathscr{A}} |\alpha\rangle\langle\alpha|\Big)|x'\rangle = \delta(x - x').$$

Two caveats, which are used below:

- The second identity requires that $\{|\alpha\rangle\}$ is a basis of the *full* single-particle space $L^2(\mathbb{R}^3) \otimes \mathbb{C}^{2S+1}$. Then $\mathscr{A}$ is infinite, and $\mathcal{H}$ is the closure of the span. For a truncated basis (finitely many bands, Wannier- or tight-binding-orbitals), $\sum_\alpha \phi_\alpha(x)\phi_\alpha^*(x') =: P(x, x')$ is the integral kernel of the orthogonal projector onto the span of the basis, and every $\delta(x - x')$ obtained from completeness below has to be replaced by $P(x, x')$.
- Since $|x\rangle \notin \mathcal{H}$, the objects $\psi(x)$ and $\psi^\dagger(x)$ defined below are operator-valued distributions. Only the smeared versions are operators: for $f \in \mathcal{H}$ with $f(x) := \langle x|f\rangle$,

  $$\oint\!\!\!\!\!\!\sum_x f^*(x)\,\psi(x) = \sum_\alpha \Big(\oint\!\!\!\!\!\!\sum_x \langle f|x\rangle\langle x|\alpha\rangle\Big) c_\alpha = \sum_\alpha \langle f|\alpha\rangle\, c_\alpha = c_f$$

  is the annihilation operator of the state $|f\rangle$ (Theorem 29.34).

Definition 29.85 One introduces the so-called *position eigenstates*

$$\psi(x) = \sum_{\alpha\in\mathscr{A}} \langle\, x \mid \alpha\,\rangle c_\alpha = \sum_{\alpha\in\mathscr{A}} \phi_\alpha(x) c_\alpha,$$
$$\psi^\dagger(x) = \sum_{\alpha\in\mathscr{A}} \langle\, \alpha \mid x\,\rangle c_\alpha^\dagger = \sum_{\alpha\in\mathscr{A}} \phi_\alpha^*(x) c_\alpha^\dagger.$$

Correction note (naming). The operators $\psi(x)$, $\psi^\dagger(x)$ are the *field operators*; they are not position eigenstates. The position eigenstates are the kets $|x\rangle$, and the field operators create them out of the vacuum, $\psi^\dagger(x)|0\rangle = |x\rangle$ (see the completion after the Remark below). The Definition is the special case $|\tilde{\alpha}\rangle = |x\rangle$ of the basis change of Theorem 29.34, i.e. $\psi^\dagger(x) = c_x^\dagger$. The two lines are consistent: $\big(\psi(x)\big)^\dagger = \sum_\alpha \langle x|\alpha\rangle^* c_\alpha^\dagger = \sum_\alpha \langle\alpha|x\rangle c_\alpha^\dagger = \psi^\dagger(x)$.

Remark 29.85.1 The usual interpretation is that these operators create or annihilate a particle in a position-/spin-state x.

Completion. The interpretation is made precise by the following identities ($N \in \mathbb{N}_0$, $|0\rangle$ the vacuum, $\hat{N} = \sum_\alpha c_\alpha^\dagger c_\alpha$):

(a) $\psi(x)|0\rangle = 0$ and $\psi^\dagger(x)|0\rangle = |x\rangle$.

(b) $\psi^\dagger(x_1)\cdots\psi^\dagger(x_N)|0\rangle = |x_1, \ldots, x_N\} = \sqrt{N!}\,\mathrm{P}_\zeta\, |x_1\rangle \otimes \cdots \otimes |x_N\rangle$.

(c) $[\hat{N}, \psi^\dagger(x)] = \psi^\dagger(x)$ and $[\hat{N}, \psi(x)] = -\psi(x)$. Hence $\psi^\dagger(x)$ raises and $\psi(x)$ lowers the particle number by one; equivalently $\hat{N}\psi(x) = \psi(x)(\hat{N} - 1)$.

(d) $\hat{n}(x) := \psi^\dagger(x)\psi(x)$ is the particle-density operator: $\oint\!\!\!\!\!\!\int_x \hat{n}(x) = \hat{N}$.

Proof. (a) $c_\alpha|0\rangle = 0$ for all α, and $\psi^\dagger(x)|0\rangle = \sum_\alpha \langle\alpha|x\rangle\,|\alpha\rangle = \sum_\alpha |\alpha\rangle\langle\alpha|x\rangle = |x\rangle$ by completeness. (b) By multilinearity and $c^\dagger_{\alpha_1}\cdots c^\dagger_{\alpha_N}|0\rangle = |\alpha_1,\dots,\alpha_N\} = \sqrt{N!}\,\mathrm{P}_\zeta\,|\alpha_1\rangle\otimes\cdots\otimes|\alpha_N\rangle$,

$$\psi^\dagger(x_1)\cdots\psi^\dagger(x_N)|0\rangle = \sqrt{N!}\,\mathrm{P}_\zeta \bigotimes_{a=1}^{N}\Big(\sum_{\alpha_a}|\alpha_a\rangle\langle\alpha_a|x_a\rangle\Big) = \sqrt{N!}\,\mathrm{P}_\zeta\;|x_1\rangle\otimes\cdots\otimes|x_N\rangle.$$

(c) For operators A, B, C and $\zeta^2 = 1$ one has $[AB, C] = A[B, C]_\zeta + \zeta[A, C]_\zeta B$ (the right-hand side is $ABC - \zeta ACB + \zeta ACB - \zeta^2 CAB$). Hence $[c^\dagger_\alpha c_\alpha, c^\dagger_\beta] = c^\dagger_\alpha\delta_{\alpha\beta} + \zeta[c^\dagger_\alpha, c^\dagger_\beta]_\zeta c_\alpha = \delta_{\alpha\beta}c^\dagger_\alpha$, so $[\hat{N}, c^\dagger_\beta] = c^\dagger_\beta$. Taking the adjoint gives $[\hat{N}, c_\beta] = -c_\beta$. Linearity in β gives the claims for $\psi^\dagger(x)$ and $\psi(x)$. (d) By orthonormality,

$$\oint\!\!\!\!\!\!\int_x \psi^\dagger(x)\psi(x) = \sum_{\alpha,\beta}\Big(\oint\!\!\!\!\!\!\int_x \phi^*_\alpha(x)\phi_\beta(x)\Big)c^\dagger_\alpha c_\beta = \sum_\alpha c^\dagger_\alpha c_\alpha = \hat{N}. \qquad \blacksquare$$

Lemma 29.86 One finds the commutation-relations

$$[\psi(x),\,\psi(x')]_\zeta = 0 = [\psi^\dagger(x),\,\psi^\dagger(x')]_\zeta, \qquad [\psi(x),\,\psi^\dagger(x')]_\zeta = \delta(x - x') \tag{29.108}$$

Proof 29.86 We compute straightforwardly

$$\begin{aligned}
[\psi(x),\,\psi^\dagger(x')]_\zeta &= \sum_{\alpha,\alpha'\in\mathscr{A}} \phi_\alpha(x)\phi^*_{\alpha'}(x)[c_\alpha, c^\dagger_{\alpha'}]_\zeta \\
&= \sum_{\alpha,\alpha'\in\mathscr{A}} \phi_\alpha(x)\phi^*_{\alpha'}(x)\delta_{\alpha,\alpha'} \\
&= \sum_{\alpha\in\mathscr{A}} \phi_\alpha(x)\phi^*_\alpha(x) \\
&= \langle\, x \,|\, \sum_{\alpha\in\mathscr{A}} |\,\alpha\,\rangle\langle\,\alpha\,|\,|\,x'\,\rangle \\
&= \delta(x - x')
\end{aligned}$$

whereas we used the completeness-relation of the basis.

Correction note. In the first line of the proof, $\phi^*_{\alpha'}(x)$ has to be $\phi^*_{\alpha'}(x')$, and in the third line $\phi^*_\alpha(x)$ has to be $\phi^*_\alpha(x')$; as written, the computation would end with $\delta(0)$. Moreover, the last step needs the completeness of $\{|\alpha\rangle\}$ in the full space $L^2(\mathbb{R}^3)\otimes\mathbb{C}^{2S+1}$. For a truncated basis the result is $[\psi(x), \psi^\dagger(x')]_\zeta = P(x, x')$ (completion after the Notation).

Completion (the other two relations). By bilinearity of $[\cdot,\cdot]_\zeta$ and $[c^\dagger_\alpha, c^\dagger_{\alpha'}]_\zeta = 0$ (Equation (29.31)), together with its adjoint $[c_\alpha, c_{\alpha'}]_\zeta = 0$:

$$[\psi(x), \psi(x')]_\zeta = \sum_{\alpha,\alpha'} \phi_\alpha(x)\phi_{\alpha'}(x')[c_\alpha, c_{\alpha'}]_\zeta = 0, \qquad [\psi^\dagger(x), \psi^\dagger(x')]_\zeta = \sum_{\alpha,\alpha'} \phi^*_\alpha(x)\phi^*_{\alpha'}(x')[c^\dagger_\alpha, c^\dagger_{\alpha'}]_\zeta = 0.$$

For fermions, $x = x'$ gives $\psi(x)^2 = 0 = \psi^\dagger(x)^2$ (Pauli principle). ■

Lemma 29.87 The inverse transformation reads

$$c_\alpha^\dagger = \int_y \phi_\alpha(y)\,\psi^\dagger(y), \qquad c_\alpha = \int_y \phi_\alpha^*(y)\,\psi(y) \tag{29.109}$$

Proof 29.87 We compute straightforwardly

$$\psi^\dagger(x) = \sum_{\alpha\in\mathscr{A}} \phi_\alpha^*(x) c_\alpha^\dagger = \sum_{\alpha\in\mathscr{A}} \int_y \phi_\alpha^*(x)\phi_\alpha(y)\psi^\dagger(y) = \int_y \sum_{\alpha\in\mathscr{A}} \langle y|\alpha\rangle\langle\alpha|x\rangle\psi^\dagger(y) = \int_y \delta(y-x)\psi^\dagger(y) = \psi^\dagger(x)$$

Correction note. The proof is circular. It inserts the claimed formula for $c_\alpha^\dagger$ into the definition of $\psi^\dagger(x)$ and arrives at $\psi^\dagger(x) = \psi^\dagger(x)$. This only shows that the claim is consistent with the definition (and it uses completeness, which is not needed). The formula for c_α is not addressed, and $\int_y$ should read $\oint\!\!\!\!\!\!\int_y$ if y contains a spin label.

Proof (direct). Insert the Definition and use the orthonormality $\oint\!\!\!\!\!\!\int_y \phi_\beta^*(y)\phi_\alpha(y) = \delta_{\alpha\beta}$:

$$\oint\!\!\!\!\!\!\int_y \phi_\alpha(y)\,\psi^\dagger(y) = \sum_{\beta\in\mathscr{A}} \Big(\oint\!\!\!\!\!\!\int_y \phi_\beta^*(y)\,\phi_\alpha(y)\Big) c_\beta^\dagger = \sum_{\beta\in\mathscr{A}} \delta_{\alpha\beta}\, c_\beta^\dagger = c_\alpha^\dagger.$$

Taking the adjoint gives $c_\alpha = \oint\!\!\!\!\!\!\int_y \phi_\alpha^*(y)\,\psi(y)$. Equivalently, this is the basis change of Theorem 29.34 from $\{|y\rangle\}$ back to $\{|\alpha\rangle\}$, $c_\alpha^\dagger = \oint\!\!\!\!\!\!\int_y \langle y|\alpha\rangle\, c_y^\dagger$. Only orthonormality enters, so the formula also holds for a truncated basis. ■

Lemma 29.88 If $x \equiv (\mathbf{x}, s)$ represents a combination of a spatial- and a spin-coordinate, then the kinetic energy operator $T \equiv -\frac{\hbar^2}{2m}\Delta$ and a local one-body potential operator $\mathbf{x} \mapsto U(\mathbf{x})$ and a two-body operator V can be written in second quantization as

- $T = \frac{\hbar^2}{2m} \oint\!\!\!\!\!\!\int_x \big(\nabla\psi^\dagger(x)\big)\,(\nabla\psi(x))$
- $U = \oint\!\!\!\!\!\!\int_x \psi^\dagger(x) U(x) \psi(x)$
- $V = \frac{1}{2} \oint\!\!\!\!\!\!\int_{x,x'} \psi^\dagger(x)\psi^\dagger(x')V(x,x')\psi(x')\psi(x)$

which gives an expression for the total Hamiltonian rewritten w.r.t. field-operators as

$$\begin{aligned} H &= T + U + V \\ &= \frac{\hbar^2}{2m} \oint\!\!\!\!\!\!\int \Big[\big(\nabla\psi^\dagger(x)\big)\,(\nabla\psi(x)) + \psi^\dagger(x)U(x)\psi(x)\Big] \quad + \quad \frac{1}{2} \oint\!\!\!\!\!\!\int_{x,x'} \psi^\dagger(x)\psi^\dagger(x')V(x,x')\psi(x')\psi(x) \end{aligned}$$

Correction note.

- In the formula for H, the prefactor $\frac{\hbar^2}{2m}$ also multiplies the potential term, which is wrong (and the first $\sum\!\!\!\!\!\!\int$ lacks its integration variable). Correct is

$$H = \sum\!\!\!\!\!\!\int_x \left[\frac{\hbar^2}{2m}\big(\nabla\psi^\dagger(x)\big)\cdot\big(\nabla\psi(x)\big) + \psi^\dagger(x)\,U(x)\,\psi(x)\right] + \frac{1}{2}\sum\!\!\!\!\!\!\int_{x,x'} \psi^\dagger(x)\psi^\dagger(x')\,V(x,x')\,\psi(x')\psi(x).$$

- ∇ acts only on the spatial part $\mathbf{x}$ of $x = (\mathbf{x}, s)$. The form $\frac{\hbar^2}{2m}(\nabla\psi^\dagger)\cdot(\nabla\psi)$ arises from $\psi^\dagger(-\frac{\hbar^2}{2m}\Delta)\psi$ by a partial integration. It therefore needs vanishing boundary terms (periodic boundary conditions in a box, or decaying wave functions).
- U has to be *local*, i.e. a multiplication operator, $\langle x|U|x'\rangle = U(x)\,\delta(x-x')$. A spin-dependent local potential $U_{ss'}(\mathbf{x})$ gives $\sum_{s,s'}\int \mathrm{d}^3\mathbf{x}\,\psi_s^\dagger(\mathbf{x})U_{ss'}(\mathbf{x})\psi_{s'}(\mathbf{x})$. Note also that the letter U denotes both the Fock-space operator and the function $U(x)$.
- Likewise, the formula for V only holds for a *local* two-body interaction, i.e. a multiplication operator in the two-particle coordinate space, $(x_1, x_2|v|x_3, x_4) = \delta(x_1 - x_3)\,\delta(x_2 - x_4)\,V(x_1, x_2)$ with $V(x_1, x_2) = V(x_2, x_1)$ (cf. the Definition of local interactions below). A general two-body operator gives

$$V = \frac{1}{2}\sum\!\!\!\!\!\!\int_{x_1,x_2,x_3,x_4} (x_1, x_2|v|x_3, x_4)\,\psi^\dagger(x_1)\psi^\dagger(x_2)\psi(x_4)\psi(x_3),$$

  see the completion of the proof below.

Proof 29.88 This is proven by straight-forward computation. For the kinetic energy operator we obtain

$$T = \sum_{i,j} c_i^\dagger T_{ij} c_j = \sum_{i,j} c_i^\dagger\langle i|-\hbar^2\frac{\Delta}{2m}|j\rangle c_j = \sum_{i,j}\sum\!\!\!\!\!\!\int_x c_i^\dagger\phi_i^*(x)\left(-\hbar^2\frac{\Delta}{2m}\right)\phi_j(x)c_j = \frac{\hbar^2}{2m}\sum\!\!\!\!\!\!\int\big(\nabla\psi^\dagger(x)\big)\,(\nabla\psi(x))$$

therefore we obtain for a one-body operator

$$U = \sum_{i,j} c_i^\dagger U_{ij} c_j = \sum_{i,j} c_i^\dagger\langle i|U|j\rangle c_j = \sum_{i,j}\sum\!\!\!\!\!\!\int_x c_i^\dagger\phi_i^*(x)U(x)\phi_j(x)c_j = \sum\!\!\!\!\!\!\int\psi^\dagger(x)U(x)\psi(x)$$

and for the two-body interaction

$$\begin{aligned} V = \frac{1}{2}\sum_{i,j,k,m} c_i^\dagger c_j^\dagger V_{ijkm} c_m c_k &= \frac{1}{2}\sum_{i,j,k,m} c_i^\dagger c_j^\dagger\langle i,j|V|k,m\rangle c_m c_k \\ &= \frac{1}{2}\sum_{i,j,k,m}\sum\!\!\!\!\!\!\int_{x,x'} c_i^\dagger c_j^\dagger\phi_i^*(x)\phi_j^*(x')V(x,x')\phi_k(x)\phi_m(x')c_m c_k \\ &= \frac{1}{2}\sum\!\!\!\!\!\!\int_{x,x'}\psi^\dagger(x)\psi^\dagger(x')V(x,x')\psi(x')\psi(x) \end{aligned}$$

Completion of the proof. The proof uses the one-body and two-body formulas of the second-quantization section,

$$U = \sum_{i,j}\langle i|u|j\rangle\,c_i^\dagger c_j, \qquad V = \frac{1}{2}\sum_{i,j,k,l}(i,j|v|k,l)\,c_i^\dagger c_j^\dagger c_l c_k,$$

which are proven there with Lemma 29.39 (cf. [38, Eqs. (1.97), (1.107)]). The omitted steps are:

- *Matrix elements.* Inserting $\sum\!\!\!\!\!\!\int_x |x\rangle\langle x| = 1$ twice gives $\langle i|u|j\rangle = \sum\!\!\!\!\!\!\int_{x,x'} \phi_i^*(x)\langle x|u|x'\rangle\phi_j(x')$. For the kinetic energy, $\langle x|T|x'\rangle = -\frac{\hbar^2}{2m}\Delta_{\mathbf{x}}\,\delta(x-x')$ (coordinate representation of $\mathbf{p}^2/2m$, $\mathbf{p} = -\mathrm{i}\hbar\nabla$), so $T_{ij} = \sum\!\!\!\!\!\!\int_x \phi_i^*(x)\big(-\frac{\hbar^2}{2m}\Delta\big)\phi_j(x)$. For a local potential, $U_{ij} = \sum\!\!\!\!\!\!\int_x \phi_i^*(x)U(x)\phi_j(x)$. For the two-body operator,

$$(i,j|v|k,l) = \sum\!\!\!\!\!\!\int_{x_1,\dots,x_4} \phi_i^*(x_1)\phi_j^*(x_2)\,(x_1,x_2|v|x_3,x_4)\,\phi_k(x_3)\phi_l(x_4),$$

  which reduces for a local interaction to $\sum\!\!\!\!\!\!\int_{x,x'} \phi_i^*(x)\phi_j^*(x')V(x,x')\phi_k(x)\phi_l(x')$. This is the matrix element used in the proof, which therefore has to be taken between *unsymmetrized* product states, $\langle i,j|V|k,m\rangle \equiv (i,j|v|k,m)$.

- *Resummation.* Since the c's do not depend on x, sums and integrals may be interchanged, and the differential operator may be moved past c_j:

$$\sum_{i,j} c_i^\dagger T_{ij} c_j = \sum\!\!\!\!\!\!\int_x \Big(\sum_i \phi_i^*(x)c_i^\dagger\Big)\Big(-\frac{\hbar^2}{2m}\Delta\Big)\Big(\sum_j \phi_j(x)c_j\Big) = -\frac{\hbar^2}{2m}\sum\!\!\!\!\!\!\int_x \psi^\dagger(x)\,\Delta\psi(x).$$

  In the same way, $\sum_i \phi_i^*(x)c_i^\dagger = \psi^\dagger(x)$, $\sum_j \phi_j^*(x')c_j^\dagger = \psi^\dagger(x')$, $\sum_m \phi_m(x')c_m = \psi(x')$ and $\sum_k \phi_k(x)c_k = \psi(x)$ give the last lines of the one- and two-body computations. The order $\psi(x')\psi(x)$ is inherited from $c_m c_k$. For a general two-body operator the same resummation gives the general formula of the correction note above.

- *Partial integration.* For each spin component, $\int \mathrm{d}^3\mathbf{x}\,\psi_s^\dagger\Delta\psi_s = -\int \mathrm{d}^3\mathbf{x}\,(\nabla\psi_s^\dagger)\cdot(\nabla\psi_s) + \oint \mathrm{d}\mathbf{S}\cdot\psi_s^\dagger\nabla\psi_s$. The surface term vanishes for periodic boundary conditions (or decaying wave functions), hence $T = \frac{\hbar^2}{2m}\sum\!\!\!\!\!\!\int_x(\nabla\psi^\dagger(x))\cdot(\nabla\psi(x))$. ■

Lemma 29.89 In the momentum-basis the kinetic energy operator acquires the form [Negele Eq. (1.100)].

Completion (statement). Consider a box of volume $\mathcal{V} = L^3$ with periodic boundary conditions and the momentum basis $|\mathbf{k},s\rangle$,

$$\phi_{\mathbf{k}s}(\mathbf{x},s') = \langle \mathbf{x},s'|\mathbf{k},s\rangle = \delta_{ss'}\frac{\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}}{\sqrt{\mathcal{V}}}, \qquad \mathbf{k}\in\frac{2\pi}{L}\mathbb{Z}^3,$$

and write $a_{\mathbf{k}s} \equiv c_{\mathbf{k}s}$. Then $\psi_s(\mathbf{x}) = \mathcal{V}^{-1/2}\sum_{\mathbf{k}} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}a_{\mathbf{k}s}$, $a_{\mathbf{k}s} = \mathcal{V}^{-1/2}\int_{\mathcal{V}} \mathrm{d}^3\mathbf{x}\,\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}\psi_s(\mathbf{x})$, and

$$T = \sum_{\mathbf{k},s}\frac{\hbar^2\mathbf{k}^2}{2m}\,a_{\mathbf{k}s}^\dagger a_{\mathbf{k}s}.$$

In the continuum with δ-normalized momentum eigenstates and the corresponding field operators,

$$\langle\mathbf{x}|\mathbf{p}\rangle = (2\pi\hbar)^{-3/2}\mathrm{e}^{\mathrm{i}\mathbf{p}\cdot\mathbf{x}/\hbar}, \qquad \hat\psi(\mathbf{p}) = \int \mathrm{d}^3\mathbf{x}\,\langle\mathbf{p}|\mathbf{x}\rangle\,\psi(\mathbf{x}),$$

this becomes (spin suppressed)

$$T = \int \mathrm{d}^3\mathbf{p}\,\frac{\mathbf{p}^2}{2m}\,\hat\psi^\dagger(\mathbf{p})\hat\psi(\mathbf{p}),$$

which is [38, Eq. (1.100), p. 18] (there $\hbar = 1$).

Proof 29.89 TBD, or maybe not since it is so useless?

Proof. For $\mathbf{k},\mathbf{k}' \in \frac{2\pi}{L}\mathbb{Z}^3$, $\int_{\mathcal{V}} \mathrm{d}^3\mathbf{x}\,\mathrm{e}^{\mathrm{i}(\mathbf{k}'-\mathbf{k})\cdot\mathbf{x}} = \mathcal{V}\delta_{\mathbf{k}\mathbf{k}'}$ (each factor is $\int_0^L \mathrm{d}x\,\mathrm{e}^{2\pi\mathrm{i}nx/L} = L\delta_{n0}$, $n\in\mathbb{Z}$), so the $\phi_{\mathbf{k}s}$ are orthonormal. They are complete in $L^2([0,L]^3)\otimes\mathbb{C}^{2S+1}$ by the completeness of the Fourier series. The formulas

for ψ_s and $a_{\mathbf{k}s}$ are the Definition and the inverse transformation (Lemma above) with $\phi_{\mathbf{k}s}$. The plane waves are eigenfunctions of T, $-\frac{\hbar^2}{2m}\Delta\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} = \frac{\hbar^2\mathbf{k}^2}{2m}\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}$, hence

$$\langle \mathbf{k}, s|T|\mathbf{k}', s'\rangle = \delta_{ss'}\frac{1}{\mathcal{V}}\int_{\mathcal{V}} \mathrm{d}^3\mathbf{x}\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}\Big(-\frac{\hbar^2}{2m}\Delta\Big)\mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot\mathbf{x}} = \frac{\hbar^2\mathbf{k}^2}{2m}\,\delta_{\mathbf{k}\mathbf{k}'}\delta_{ss'},$$

and the one-body formula $T = \sum_{i,j} c_i^\dagger T_{ij} c_j$ gives the claim. Alternatively, insert

$$\nabla\psi_s(\mathbf{x}) = \mathcal{V}^{-1/2}\sum_{\mathbf{k}} \mathrm{i}\mathbf{k}\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} a_{\mathbf{k}s}$$

into $\frac{\hbar^2}{2m}\sum_s \int (\nabla\psi_s^\dagger)\cdot(\nabla\psi_s)$ and use orthonormality. In the continuum,

$$\langle \mathbf{p}|T|\mathbf{p}'\rangle = \frac{\mathbf{p}^2}{2m}\delta^{(3)}(\mathbf{p}-\mathbf{p}'), \qquad \text{because} \qquad \int \mathrm{d}^3\mathbf{x}\, \mathrm{e}^{\mathrm{i}(\mathbf{p}'-\mathbf{p})\cdot\mathbf{x}/\hbar} = (2\pi\hbar)^3\delta^{(3)}(\mathbf{p}-\mathbf{p}'),$$

and the one-body formula with continuous index gives [38, Eq. (1.100)]. ■

Definition 29.90 A two-body operator V that is diagonal in its position representation as

$$\langle \mathbf{x}_1\mathbf{x}_2|V|\mathbf{x}_3\mathbf{x}_4\rangle = \delta(\mathbf{x}_1-\mathbf{x}_3)\delta(\mathbf{x}_2-\mathbf{x}_4)V(\mathbf{x}_1-\mathbf{x}_2) \tag{29.110}$$

is said to be *local*[10], or *velocity independent*.

Correction note.

(i) As in the two-body Theorem, the kets have to be unsymmetrized product states, $(\mathbf{x}_1,\mathbf{x}_2|v|\mathbf{x}_3,\mathbf{x}_4)$ with $|\mathbf{x}_3,\mathbf{x}_4) = |\mathbf{x}_3\rangle\otimes|\mathbf{x}_4\rangle$. With (anti)symmetrized kets an additional exchange term $\propto \zeta\,\delta(\mathbf{x}_1-\mathbf{x}_4)\delta(\mathbf{x}_2-\mathbf{x}_3)$ appears.

(ii) "Local" alone means

$$(\mathbf{x}_1,\mathbf{x}_2|v|\mathbf{x}_3,\mathbf{x}_4) = \delta(\mathbf{x}_1-\mathbf{x}_3)\delta(\mathbf{x}_2-\mathbf{x}_4)V(\mathbf{x}_1,\mathbf{x}_2),$$

i.e. v is the multiplication operator $V(\hat{\mathbf{x}}_1,\hat{\mathbf{x}}_2)$. The dependence on $\mathbf{x}_1-\mathbf{x}_2$ only is the additional property of translation invariance.

(iii) For identical particles, v has to commute with the exchange of the two particles, and it has to be hermitian, i.e. $V(\mathbf{x}) = V(-\mathbf{x}) \in \mathbb{R}$.

(iv) With spin, a local and spin-independent interaction has the matrix element $\delta_{s_1s_3}\delta_{s_2s_4}\delta(\mathbf{x}_1-\mathbf{x}_3)\delta(\mathbf{x}_2-\mathbf{x}_4)V(\mathbf{x}_1-\mathbf{x}_2)$. "Velocity independent" refers to the fact that $v = V(\hat{\mathbf{x}}_1-\hat{\mathbf{x}}_2)$ contains no momentum operators.

Corollary 29.91 Let V denote a two-body operator which is diagonal in the position-representation. Then, it becomes in second quantized form

$$V = \frac{1}{2}\int \mathrm{d}^3x\mathrm{d}^3y\, V(\mathbf{x}-\mathbf{y})\,\psi^\dagger(\mathbf{x})\psi^\dagger(\mathbf{y})\psi(\mathbf{y})\psi(\mathbf{x}) \tag{29.111}$$

Proof 29.91 TBD

[10] Cf. Marcos Marinos p. 46 ff

Proof. By the general formula for two-body operators in terms of field operators (correction note and completion of the proof of the Lemma on T, U, V above),

$$V = \frac{1}{2}\int \mathrm{d}^3x_1 \cdots \mathrm{d}^3x_4\, (\mathbf{x}_1,\mathbf{x}_2|v|\mathbf{x}_3,\mathbf{x}_4)\, \psi^\dagger(\mathbf{x}_1)\psi^\dagger(\mathbf{x}_2)\psi(\mathbf{x}_4)\psi(\mathbf{x}_3).$$

Inserting the local matrix element, the δ-functions set $\mathbf{x}_3 = \mathbf{x}_1 \equiv \mathbf{x}$ and $\mathbf{x}_4 = \mathbf{x}_2 \equiv \mathbf{y}$, and the c-number $V(\mathbf{x}-\mathbf{y})$ can be moved to the front. This is the claim. With spin and a spin-independent interaction (item (iv) above), the same computation gives

$$V = \frac{1}{2}\sum_{s,s'}\int \mathrm{d}^3x\,\mathrm{d}^3y\, V(\mathbf{x}-\mathbf{y})\, \psi_s^\dagger(\mathbf{x})\psi_{s'}^\dagger(\mathbf{y})\psi_{s'}(\mathbf{y})\psi_s(\mathbf{x}).$$

Hence the Corollary is the special case $V(x,x') = V(\mathbf{x}-\mathbf{x}')$ of the Lemma on T, U, V; the spin sums are suppressed in its statement. In a basis $\{|\alpha\rangle\}$ in which v is diagonal, this is [38, Eq. (1.106)]. ■

Identity for expectation-value of the Hamilton-operator as in Problem 1.6 of Negele.

Lemma 29.92 *([38, Problem 1.6 a), p. 41].)* Let $\zeta = -1$, let $\phi_1,\dots,\phi_N$ be orthonormal single-particle wave functions (completed to an orthonormal basis $\{\phi_\alpha\}$), and let $|\Phi\rangle = c_1^\dagger\cdots c_N^\dagger|0\rangle$ be the corresponding normalized Slater determinant. Let $H = T + V$ with $T = \int\!\!\!\!\!\!\diagup_x \psi^\dagger(x)\Big(-\frac{\hbar^2}{2m}\Delta\Big)\psi(x)$ and a local, spin-independent two-body interaction $V = \frac{1}{2}\int\!\!\!\!\!\!\diagup_{x,y} v(\mathbf{x}-\mathbf{y})\,\psi^\dagger(x)\psi^\dagger(y)\psi(y)\psi(x)$. Then

$$\begin{aligned}\langle\Phi|H|\Phi\rangle = &\sum_{a=1}^{N}\int\!\!\!\!\!\!\diagup_x \phi_a^*(x)\Big(-\frac{\hbar^2}{2m}\Delta\Big)\phi_a(x)\\ &+\frac{1}{2}\sum_{a,b=1}^{N}\int\!\!\!\!\!\!\diagup_{x,y}\phi_a^*(x)\phi_b^*(y)\,v(\mathbf{x}-\mathbf{y})\,\big(\phi_a(x)\phi_b(y)-\phi_a(y)\phi_b(x)\big).\end{aligned}$$

In terms of field operators: with the one-body density matrix $\rho(x,y) := \langle\Phi|\psi^\dagger(y)\psi(x)|\Phi\rangle = \sum_{a=1}^N \phi_a(x)\phi_a^*(y)$,

$$\langle\Phi|\psi^\dagger(x)\psi^\dagger(y)\psi(y)\psi(x)|\Phi\rangle = \rho(x,x)\,\rho(y,y) - |\rho(x,y)|^2.$$

Proof 29.92 Let $n_\alpha = 1$ for $\alpha\in\{1,\dots,N\}$ and $n_\alpha = 0$ otherwise; $|\Phi\rangle$ is the occupation-number state with these occupations. By the (corrected) action of the annihilation operators on occupation-number states in the second-quantization section, $c_\alpha|\Phi\rangle = 0$ if $n_\alpha = 0$, and $c_\alpha|\Phi\rangle = \pm|\Phi_\alpha\rangle$ otherwise, where $|\Phi_\alpha\rangle$ is the normalized occupation-number state with α removed. Likewise, $c_lc_k|\Phi\rangle = \pm|\Phi_{kl}\rangle$ (normalized, k and l removed) if $k\neq l$ are both occupied, and $c_lc_k|\Phi\rangle = 0$ otherwise. Occupation-number states with different occupations are orthogonal.

- One-body part: $\langle\Phi|c_i^\dagger c_j|\Phi\rangle = \langle c_i\Phi|c_j\Phi\rangle = \delta_{ij}n_i$.
- Two-body part: $\langle\Phi|c_i^\dagger c_j^\dagger c_lc_k|\Phi\rangle = \langle c_jc_i\Phi|c_lc_k\Phi\rangle$ vanishes unless $k\neq l$ are occupied and $\{i,j\} = \{k,l\}$. For $(i,j) = (k,l)$ it equals $\|c_lc_k\Phi\|^2 = 1$. For $(i,j) = (l,k)$ we have $c_jc_i = c_kc_l = -c_lc_k$, so it equals -1. Hence

  $$\langle\Phi|c_i^\dagger c_j^\dagger c_lc_k|\Phi\rangle = n_kn_l\big(\delta_{ik}\delta_{jl}-\delta_{il}\delta_{jk}\big),$$

  which also covers $k=l$ (both sides vanish).

With the one- and two-body formulas,

$$\langle\Phi|T|\Phi\rangle = \sum_{a=1}^N T_{aa},\qquad \langle\Phi|V|\Phi\rangle = \frac{1}{2}\sum_{k,l=1}^N\big[(k,l|v|k,l)-(l,k|v|k,l)\big].$$

Insert T_{aa} and $(i,j|v|k,l) = \int\!\!\!\!\!\!\diagup_{x,y} \phi_i^*(x)\phi_j^*(y)v(\mathbf{x}-\mathbf{y})\phi_k(x)\phi_l(y)$ (completion of the proof of the Lemma on T, U, V). Renaming $(k,l)\to(a,b)$ in the direct term and $(l,k)\to(a,b)$ in the exchange term gives the claim. The terms $a=b$ cancel, so the sum may run over $a\neq b$ or over all a,b. For the field-operator form, insert $\psi=\sum_\alpha \phi_\alpha c_\alpha$ and use the two identities above:

$$\langle\Phi|\psi^\dagger(y)\psi(x)|\Phi\rangle = \sum_{i,j}\phi_i^*(y)\phi_j(x)\,\delta_{ij}n_i = \rho(x,y),$$

$$\begin{aligned}\langle\Phi|\psi^\dagger(x)\psi^\dagger(y)\psi(y)\psi(x)|\Phi\rangle &= \sum_{k,l=1}^{N}\left(|\phi_k(x)|^2|\phi_l(y)|^2-\phi_l^*(x)\phi_k^*(y)\phi_l(y)\phi_k(x)\right)\\ &= \rho(x,x)\rho(y,y)-\rho(x,y)\rho(y,x),\end{aligned}$$

and $\rho(y,x)=\rho(x,y)^*$. ■

Remarks. [38] sets $\hbar=1$ and writes $\int \mathrm{d}x$ for $\int\!\!\!\!\!\!\diagup_x$. For spin orbitals $\phi_a(\mathbf{x},s)=\varphi_a(\mathbf{x})\chi_a(s)$ and spin-independent v, the exchange term only couples orbitals with equal spin. Parts b) and c) of the Problem (Hartree-Fock equations, Koopmans' theorem) follow by varying this functional and are not reproduced here.

Definition 29.93 Now we introduce the field operator in the Heisenberg-representation as

$$\psi(\mathbf{x},t)=\mathrm{e}^{\mathrm{i}Ht/\hbar}\psi(\mathbf{x},0)\mathrm{e}^{-\mathrm{i}Ht/\hbar} \tag{29.112}$$

Note. Here the time evolution is generated by H, whereas the Green-function chapters use the ensemble-Heisenberg-representation with $\Xi = H-\mu\hat N$ (Theorem 8.9). If $[H,\hat N]=0$, the two differ only by a phase. From $\hat N\psi=\psi(\hat N-1)$ (item (c) of the completion after the Remark on field operators) one gets

$$\mathrm{e}^{-\mathrm{i}\mu\hat N t/\hbar}\psi(\mathbf{x})\mathrm{e}^{\mathrm{i}\mu\hat N t/\hbar}=\mathrm{e}^{\mathrm{i}\mu t/\hbar}\psi(\mathbf{x}),\qquad\text{hence}\qquad \psi_\Xi(\mathbf{x},t)=\mathrm{e}^{\mathrm{i}\mu t/\hbar}\psi_H(\mathbf{x},t).$$

In the equation of motion below this replaces $U(\mathbf{x})$ by $U(\mathbf{x})-\mu$.

Lemma 29.94 It follows the equation of motion

$$\mathrm{i}\partial_t\psi(\mathbf{x},t)=\left(-\frac{\hbar^2}{2m}\Delta+U(\mathbf{x})\right)\psi(\mathbf{x},t)+\int \mathrm{d}^3x'\psi^\dagger(\mathbf{x}',t)V(\mathbf{x},\mathbf{x}')\psi(\mathbf{x}',t)\psi(\mathbf{x},t) \tag{29.113}$$

Correction note. A factor $\hbar$ is missing on the left-hand side: it has to read $\mathrm{i}\hbar\,\partial_t\psi(\mathbf{x},t)$, cf. [48, Eq. (1.5.15)]. The formula assumes the Hamiltonian of the Lemma on T, U, V with a local interaction that is symmetric, $V(\mathbf{x},\mathbf{x}')=V(\mathbf{x}',\mathbf{x})$. With spin, $\mathbf{x}\to x=(\mathbf{x},s)$ and $\int \mathrm{d}^3x'\to\int\!\!\!\!\!\!\diagup_{x'}$.

Proof 29.94 TBDigitalized from Schwabl p. 24 [48, Sect. 1.5, Eq. (1.5.15), p. 24]

Proof ([48, p. 24], here for both statistics at once). Since H does not depend on time,

$$\frac{\mathrm{d}}{\mathrm{d}t}\psi(\mathbf{x},t)=\frac{\mathrm{i}}{\hbar}\mathrm{e}^{\mathrm{i}Ht/\hbar}[H,\psi(\mathbf{x})]\mathrm{e}^{-\mathrm{i}Ht/\hbar},\qquad\text{i.e.}\qquad \mathrm{i}\hbar\,\partial_t\psi(\mathbf{x},t)=\mathrm{e}^{\mathrm{i}Ht/\hbar}\,[\psi(\mathbf{x}),H]\,\mathrm{e}^{-\mathrm{i}Ht/\hbar}.$$

We need, for operators A,B,C and $\zeta^2=1$,

$$[A,BC]=[A,B]_\zeta\,C+\zeta\,B\,[A,C]_\zeta,\qquad [A,BC]=[A,B]\,C+B\,[A,C]$$

(expand the first one: $ABC-\zeta BAC+\zeta BAC-\zeta^2BCA=ABC-BCA$). Together with $[\psi(\mathbf{x}),\psi^\dagger(\mathbf{y})]_\zeta=\delta(\mathbf{x}-\mathbf{y})$ and $[\psi(\mathbf{x}),\psi(\mathbf{y})]_\zeta=0$ this gives:

- For any linear differential operator or function $\mathcal{D}_{\mathbf{y}}$ acting on $\mathbf{y}$,

$$[\psi(\mathbf{x}), \psi^\dagger(\mathbf{y})\,\mathcal{D}_{\mathbf{y}}\psi(\mathbf{y})] = \delta(\mathbf{x}-\mathbf{y})\,\mathcal{D}_{\mathbf{y}}\psi(\mathbf{y}) + \zeta\psi^\dagger(\mathbf{y})\,\mathcal{D}_{\mathbf{y}}[\psi(\mathbf{x}),\psi(\mathbf{y})]_\zeta = \delta(\mathbf{x}-\mathbf{y})\,\mathcal{D}_{\mathbf{y}}\psi(\mathbf{y}).$$

  With $\mathcal{D} = -\frac{\hbar^2}{2m}\Delta + U$ and $T = \int \mathrm{d}^3y\,\psi^\dagger(-\frac{\hbar^2}{2m}\Delta)\psi$ (the form before the partial integration):

$$[\psi(\mathbf{x}), T+U] = \Big(-\frac{\hbar^2}{2m}\Delta + U(\mathbf{x})\Big)\psi(\mathbf{x}).$$

- $[\psi(\mathbf{x}), \psi(\mathbf{z})\psi(\mathbf{y})] = \psi(\mathbf{x})\psi(\mathbf{z})\psi(\mathbf{y}) - \psi(\mathbf{z})\psi(\mathbf{y})\psi(\mathbf{x}) = (\zeta^2-1)\psi(\mathbf{z})\psi(\mathbf{y})\psi(\mathbf{x}) = 0$, and $[\psi(\mathbf{x}), \psi^\dagger(\mathbf{y})\psi^\dagger(\mathbf{z})] = \delta(\mathbf{x}-\mathbf{y})\psi^\dagger(\mathbf{z}) + \zeta\,\delta(\mathbf{x}-\mathbf{z})\psi^\dagger(\mathbf{y})$. Hence, with the ordinary product rule,

$$\begin{aligned}
[\psi(\mathbf{x}), V] &= \frac{1}{2}\int \mathrm{d}^3y\,\mathrm{d}^3z\,V(\mathbf{y},\mathbf{z})\,[\psi(\mathbf{x}),\psi^\dagger(\mathbf{y})\psi^\dagger(\mathbf{z})]\,\psi(\mathbf{z})\psi(\mathbf{y}) \\
&= \frac{1}{2}\int \mathrm{d}^3z\,V(\mathbf{x},\mathbf{z})\,\psi^\dagger(\mathbf{z})\psi(\mathbf{z})\psi(\mathbf{x}) + \frac{\zeta}{2}\int \mathrm{d}^3y\,V(\mathbf{y},\mathbf{x})\,\psi^\dagger(\mathbf{y})\psi(\mathbf{x})\psi(\mathbf{y}) \\
&= \int \mathrm{d}^3x'\,\psi^\dagger(\mathbf{x}')V(\mathbf{x},\mathbf{x}')\psi(\mathbf{x}')\psi(\mathbf{x}),
\end{aligned}$$

  using $\zeta\psi(\mathbf{x})\psi(\mathbf{y}) = \psi(\mathbf{y})\psi(\mathbf{x})$ and $V(\mathbf{y},\mathbf{x}) = V(\mathbf{x},\mathbf{y})$ in the last step.

Finally, $\mathrm{e}^{\mathrm{i}Ht/\hbar}XYZ\,\mathrm{e}^{-\mathrm{i}Ht/\hbar} = X(t)Y(t)Z(t)$ (insert $1 = \mathrm{e}^{-\mathrm{i}Ht/\hbar}\mathrm{e}^{\mathrm{i}Ht/\hbar}$), and Δ and $U(\mathbf{x})$ commute with the conjugation. Adding the three commutators gives the (corrected) equation of motion. ■

Green-Functions

Definition 29.95 We introduce the Green-function of the field-operators as

$$G_{\sigma,\sigma'}(\mathbf{x}-\mathbf{x}', t-t') = \langle\psi^\dagger_\sigma(\mathbf{x},t)\psi_{\sigma'}(\mathbf{x}',t')\rangle \tag{29.114}$$

Correction note.

(i) This is not the (time-ordered) one-body Green-function of Definition 12.5, but a correlation function. In the notation of that chapter, $\langle\psi^\dagger_\sigma(\mathbf{x},t)\psi_{\sigma'}(\mathbf{x}',t')\rangle = \mathrm{i}\hbar\,\zeta\,G^<_{\psi_{\sigma'}(\mathbf{x}'),\psi^\dagger_\sigma(\mathbf{x})}(t',t)$. At equal times it is the one-body density matrix $\langle\psi^\dagger_\sigma(\mathbf{x})\psi_{\sigma'}(\mathbf{x}')\rangle$, which [48, Eq. (2.1.6)] calls *Einteilchenkorrelationsfunktion*.

(ii) "GW01" is D. Golze, M. Dvorak, P. Rinke, *The GW Compendium*, Front. Chem. **7**, 377 (2019). Its Eq. (6) is the time-ordered function at $T = 0$. In the conventions of Definition 12.5 (GW01 sets $\hbar = 1$ and drops the factor $\frac{1}{\hbar}$) it reads

$$G_{\sigma\sigma'}(\mathbf{x}t,\mathbf{x}'t') := -\frac{\mathrm{i}}{\hbar}\Big\langle\,\mathrm{T}_t\;\psi_\sigma(\mathbf{x},t)\,\psi^\dagger_{\sigma'}(\mathbf{x}',t')\Big\rangle = \sum_{\alpha,\alpha'}\phi_\alpha(\mathbf{x},\sigma)\,G_{\alpha\alpha'}(t,t')\,\phi^*_{\alpha'}(\mathbf{x}',\sigma'),$$

where the second equality follows from the Definition of the field operators. The correlation function above is its equal-time limit, $G_{\sigma'\sigma}(\mathbf{x}'t,\mathbf{x}t^+) = -\frac{\mathrm{i}}{\hbar}\zeta\langle\psi^\dagger_\sigma(\mathbf{x},t)\psi_{\sigma'}(\mathbf{x}',t)\rangle$, $t^+ = t+0^+$. This G is used in the completions below.

(iii) The left-hand side presupposes that only differences enter. This holds only for homogeneous and stationary situations (see the completion after the Remark below).

Remark 29.95.1 From this definition, it is actually quite non-trivial that the defined Green-function only depends on space- and time-differences. The time-difference is proven analog to Lemma TBReferenced. The space-difference can be seen as follows TBDone.

Completion. The "Lemma TBReferenced" is Lemma 12.3. Write $\langle X\rangle = \mathrm{Tr}(\rho X)$ with a statistical operator ρ (e.g. $\rho = \mathrm{e}^{-\beta\Xi}/Z$, or $\rho = |\Psi_0\rangle\langle\Psi_0|$ for a ground state).

Time. If $[\rho, H] = 0$, then by the cyclicity of the trace

$$\begin{aligned}\langle A(t)B(t')\rangle &= \mathrm{Tr}\left(\rho\,\mathrm{e}^{\mathrm{i}Ht/\hbar}A\,\mathrm{e}^{-\mathrm{i}Ht/\hbar}\,\mathrm{e}^{\mathrm{i}Ht'/\hbar}B\,\mathrm{e}^{-\mathrm{i}Ht'/\hbar}\right)\\ &= \mathrm{Tr}\left(\rho\,\mathrm{e}^{\mathrm{i}H(t-t')/\hbar}A\,\mathrm{e}^{-\mathrm{i}H(t-t')/\hbar}B\right) = \langle A(t-t')B(0)\rangle.\end{aligned}$$

Space. Let $\mathbf{P} := \sum\!\!\!\!\!\!\int_x \psi^\dagger(x)(-\mathrm{i}\hbar\nabla)\psi(x)$ be the total momentum. Assume $[\rho, \mathbf{P}] = 0$ and $[H, \mathbf{P}] = 0$. The latter holds if U is constant and $V(\mathbf{x}, \mathbf{x}') = V(\mathbf{x} - \mathbf{x}')$: by step 2 below, $\mathrm{e}^{\mathrm{i}\mathbf{P}\cdot\mathbf{a}/\hbar}H\mathrm{e}^{-\mathrm{i}\mathbf{P}\cdot\mathbf{a}/\hbar}$ is H with all fields shifted by $-\mathbf{a}$, which equals H after the substitution $\mathbf{x} \to \mathbf{x} + \mathbf{a}$ in the integrals; differentiating at $\mathbf{a} = 0$ gives $[\mathbf{P}, H] = 0$. The former is then automatic for $\rho \propto \mathrm{e}^{-\beta\Xi}$; for a ground state it requires a translation-invariant ground state.

1. By the first item of the proof of the equation of motion (with $\mathcal{D} = -\mathrm{i}\hbar\nabla$), $[\psi_s(\mathbf{x}), \mathbf{P}] = -\mathrm{i}\hbar\nabla\psi_s(\mathbf{x})$.
2. For $\mathbf{a} \in \mathbb{R}^3$ let $f(\mathbf{a}) := \mathrm{e}^{\mathrm{i}\mathbf{P}\cdot\mathbf{a}/\hbar}\psi_s(\mathbf{x})\mathrm{e}^{-\mathrm{i}\mathbf{P}\cdot\mathbf{a}/\hbar}$. Then $\partial_{a_j} f(\mathbf{a}) = \frac{\mathrm{i}}{\hbar}\mathrm{e}^{\mathrm{i}\mathbf{P}\cdot\mathbf{a}/\hbar}[P_j, \psi_s(\mathbf{x})]\mathrm{e}^{-\mathrm{i}\mathbf{P}\cdot\mathbf{a}/\hbar} = -\partial_{x_j} f(\mathbf{a})$ and $f(\mathbf{0}) = \psi_s(\mathbf{x})$. The unique solution of this transport equation is $f(\mathbf{a}) = \psi_s(\mathbf{x} - \mathbf{a})$, i.e.

   $$\mathrm{e}^{\mathrm{i}\mathbf{P}\cdot\mathbf{a}/\hbar}\psi_s(\mathbf{x})\,\mathrm{e}^{-\mathrm{i}\mathbf{P}\cdot\mathbf{a}/\hbar} = \psi_s(\mathbf{x} - \mathbf{a}).$$

   The same holds for $\psi_s^\dagger$ (adjoint) and, since $[H, \mathbf{P}] = 0$, for the Heisenberg operators $\psi_s(\mathbf{x}, t)$.
3. With $\rho = \mathrm{e}^{\mathrm{i}\mathbf{P}\cdot\mathbf{a}/\hbar}\rho\,\mathrm{e}^{-\mathrm{i}\mathbf{P}\cdot\mathbf{a}/\hbar}$ and cyclicity,

   $$\langle\psi_\sigma^\dagger(\mathbf{x}, t)\psi_{\sigma'}(\mathbf{x}', t')\rangle = \langle\psi_\sigma^\dagger(\mathbf{x} + \mathbf{a}, t)\psi_{\sigma'}(\mathbf{x}' + \mathbf{a}, t')\rangle \qquad \forall\,\mathbf{a} \in \mathbb{R}^3.$$

   Choosing $\mathbf{a} = -\mathbf{x}'$ shows that the left-hand side depends only on $\mathbf{x} - \mathbf{x}'$. The same argument applies to the time-ordered G. ■

Correction note. In a crystal, $U(\mathbf{x} + \mathbf{R}) = U(\mathbf{x})$ only for lattice vectors $\mathbf{R}$. Then only $G(\mathbf{x} + \mathbf{R}, \mathbf{x}' + \mathbf{R}) = G(\mathbf{x}, \mathbf{x}')$ holds (same proof with the lattice translations), and G is *not* a function of $\mathbf{x}-\mathbf{x}'$ alone. The notation $G_{\sigma\sigma'}(\mathbf{x}-\mathbf{x}', t-t')$ is therefore restricted to homogeneous systems (free electron gas, jellium).

- See Schwabl 2 Eq. (2.1.6), GW01 Eq. (6) [48, Sect. 2.1.2, Eq. (2.1.6), p. 35] for the concrete values at equal times at zero temperature.
- Flensberg (somewhere): real-space version of the green-functions in the non-interacting electron-case.
- Imaginary time Green-function in coordinate space: Henk p. 145.

Completion of the three items.

- The equal-time correlation function of the free electron gas at $T = 0$,

  $$\langle\phi_0|\psi_\sigma^\dagger(\mathbf{x})\psi_\sigma(\mathbf{x}')|\phi_0\rangle = \frac{3n}{2}\frac{\sin(k_F r) - k_F r\cos(k_F r)}{(k_F r)^3}, \qquad r = |\mathbf{x} - \mathbf{x}'|,$$

  is derived in the Example "Non-Interacting Electrons" below.
- *Real-space Green-functions of non-interacting particles.* Let $H = \sum\!\!\!\!\!\!\int_x \psi^\dagger(x)\,h\,\psi(x)$ with a single-particle Hamiltonian $h = \sum_\alpha \varepsilon_\alpha|\alpha\rangle\langle\alpha|$ (time evolution with H). Then, for every state ρ and both statistics,

  $$G^{\mathrm{ret}}(xt, x't') := -\frac{\mathrm{i}}{\hbar}\theta(t - t')\left\langle[\psi(x, t), \psi^\dagger(x', t')]_\zeta\right\rangle = -\frac{\mathrm{i}}{\hbar}\theta(t - t')\,\langle x|\mathrm{e}^{-\mathrm{i}h(t-t')/\hbar}|x'\rangle.$$

For free particles, $h = \frac{\mathbf{p}^2}{2m}$, in infinite volume (diagonal in spin, spin index suppressed), with $\mathbf{r} = \mathbf{x} - \mathbf{x}'$, $r = |\mathbf{r}|$, $G_0^{\mathrm{ret}}(\mathbf{r}, t) \equiv G_0^{\mathrm{ret}}(\mathbf{x}t, \mathbf{x}'0)$:

$$G_0^{\mathrm{ret}}(\mathbf{r}, t) = -\frac{\mathrm{i}}{\hbar}\theta(t)\Big(\frac{m}{2\pi \mathrm{i}\hbar t}\Big)^{3/2} \mathrm{e}^{\mathrm{i}mr^2/(2\hbar t)}, \qquad G_0^{\mathrm{ret}}(\mathbf{r}, \omega) := \int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t} G_0^{\mathrm{ret}}(\mathbf{r}, t) = -\frac{m}{2\pi\hbar^2}\frac{\mathrm{e}^{\mathrm{i}qr}}{r},$$

where $q = \sqrt{2m(\hbar\omega + \mathrm{i}0^+)}/\hbar$ with $\operatorname{Im} q > 0$.

- *Imaginary-time Green-function in coordinate space* ([52, Eq. (7.56), p. 145]). With the conventions of Definition 13.1 and Lemma 1.11, $\mathscr{G}(x\tau, x'\tau') := -\frac{1}{\hbar}\langle \mathrm{T}_\tau\, \psi(x,\tau)\psi^\dagger(x',\tau')\rangle$. For $\Xi = \sum_x \psi^\dagger(h-\mu)\psi$, $\xi_\alpha = \varepsilon_\alpha - \mu$ and $n_\alpha = (\mathrm{e}^{\beta\xi_\alpha} - \zeta)^{-1}$:

$$\begin{aligned}
\mathscr{G}_0(x\tau, x'\tau') &= -\frac{1}{\hbar}\sum_\alpha \phi_\alpha(x)\phi_\alpha^*(x')\,\mathrm{e}^{-\xi_\alpha(\tau-\tau')/\hbar}\big[\theta(\tau-\tau')(1+\zeta n_\alpha) + \zeta\,\theta(\tau'-\tau)\,n_\alpha\big] \\
&= \frac{1}{\hbar\beta}\sum_{\omega_n\in\Omega_\zeta} \mathrm{e}^{-\mathrm{i}\omega_n(\tau-\tau')}\sum_\alpha \frac{\phi_\alpha(x)\phi_\alpha^*(x')}{\mathrm{i}\hbar\omega_n - \xi_\alpha} \\
&= \frac{1}{\hbar\beta}\sum_{\omega_n\in\Omega_\zeta} \mathrm{e}^{-\mathrm{i}\omega_n(\tau-\tau')}\,\langle x|(\mathrm{i}\hbar\omega_n - h + \mu)^{-1}|x'\rangle.
\end{aligned}$$

For the homogeneous gas, $\phi_{\mathbf{k}s}(\mathbf{x}, s') = \delta_{ss'}\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}/\sqrt{\mathcal{V}}$, this is

$$\mathscr{G}_{0,ss'}(\mathbf{x}\tau, \mathbf{x}'\tau') = \delta_{ss'}\frac{1}{\hbar\beta\mathcal{V}}\sum_{\mathbf{k},n}\frac{\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}\mathrm{e}^{-\mathrm{i}\omega_n(\tau-\tau')}}{\mathrm{i}\hbar\omega_n - \varepsilon_{\mathbf{k}} + \mu},$$

which is [52, Eq. (7.56)] up to the factor $\hbar$ (there $G_0 = \hbar\mathscr{G}_0$).

Proof (item 2). In the eigenbasis of h, $H = \sum_\alpha \varepsilon_\alpha c_\alpha^\dagger c_\alpha$ (one-body formula). The identity $[A, BC] = [A, B]_\zeta C + \zeta B[A, C]_\zeta$ from the proof of the equation of motion gives $[c_\alpha, c_\beta^\dagger c_\beta] = \delta_{\alpha\beta}c_\alpha$, hence $[c_\alpha, H] = \varepsilon_\alpha c_\alpha$ and $c_\alpha(t) = \mathrm{e}^{-\mathrm{i}\varepsilon_\alpha t/\hbar}c_\alpha$ (both sides solve $\mathrm{i}\hbar\dot{c}_\alpha = [c_\alpha, H]$ with the same initial value). Therefore

$$[\psi(x,t), \psi^\dagger(x',t')]_\zeta = \sum_{\alpha,\beta}\phi_\alpha(x)\phi_\beta^*(x')\,\mathrm{e}^{-\mathrm{i}(\varepsilon_\alpha t - \varepsilon_\beta t')/\hbar}\,\delta_{\alpha\beta} = \langle x|\mathrm{e}^{-\mathrm{i}h(t-t')/\hbar}|x'\rangle.$$

This is a c-number, so the expectation value is trivial. For $h = \mathbf{p}^2/2m$, $\langle \mathbf{x}|\mathrm{e}^{-\mathrm{i}ht/\hbar}|\mathbf{x}'\rangle = \int \frac{\mathrm{d}^3k}{(2\pi)^3}\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r} - a\mathbf{k}^2}$ with $a = \mathrm{i}\hbar t/2m$ (regularized by $a \to a + 0^+$). The Gaussian integral gives $(4\pi a)^{-3/2}\mathrm{e}^{-r^2/4a}$, which is the stated result. In frequency space, $-\frac{\mathrm{i}}{\hbar}\int_0^\infty \mathrm{d}t\, \mathrm{e}^{\mathrm{i}(\omega+\mathrm{i}0^+)t}\mathrm{e}^{-\mathrm{i}\varepsilon_{\mathbf{k}}t/\hbar} = (\hbar\omega - \varepsilon_{\mathbf{k}} + \mathrm{i}0^+)^{-1}$, so

$$G_0^{\mathrm{ret}}(\mathbf{r}, \omega) = \int \frac{\mathrm{d}^3k}{(2\pi)^3}\frac{\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}}{\hbar\omega - \frac{\hbar^2\mathbf{k}^2}{2m} + \mathrm{i}0^+} = -\frac{2m}{\hbar^2}\int \frac{\mathrm{d}^3k}{(2\pi)^3}\frac{\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}}{\mathbf{k}^2 - q^2} = -\frac{2m}{\hbar^2}\frac{\mathrm{e}^{\mathrm{i}qr}}{4\pi r}.$$

For the last step, the angular integration gives $\frac{1}{2\pi^2 r}\int_0^\infty \mathrm{d}k\, \frac{k\sin(kr)}{k^2-q^2} = \frac{1}{4\pi^2\mathrm{i}r}\int_{-\infty}^\infty \mathrm{d}k\, \frac{k\,\mathrm{e}^{\mathrm{i}kr}}{k^2-q^2}$. Closing the contour in the upper half-plane picks up the pole $k = q$ ($\operatorname{Im} q > 0$) with residue $\frac{1}{2}\mathrm{e}^{\mathrm{i}qr}$.

Proof (item 3). With $\Xi = \sum_\alpha \xi_\alpha c_\alpha^\dagger c_\alpha$ one gets in the same way $c_\alpha(\tau) = \mathrm{e}^{\tau\Xi/\hbar}c_\alpha\mathrm{e}^{-\tau\Xi/\hbar} = \mathrm{e}^{-\xi_\alpha\tau/\hbar}c_\alpha$ and $c_\alpha^\dagger(\tau) = \mathrm{e}^{\xi_\alpha\tau/\hbar}c_\alpha^\dagger$. With $\langle c_\alpha^\dagger c_\beta\rangle = \delta_{\alpha\beta}n_\alpha$ and $\langle c_\alpha c_\beta^\dagger\rangle = \delta_{\alpha\beta}(1+\zeta n_\alpha)$, this gives the first line. For the Matsubara form, use $\mathrm{e}^{\mathrm{i}\omega_n\hbar\beta} = \zeta$ and $(1+\zeta n_\alpha)(1-\zeta\mathrm{e}^{-\beta\xi_\alpha}) = 1$:

$$\int_0^{\hbar\beta}\mathrm{d}\tau\,\mathrm{e}^{\mathrm{i}\omega_n\tau}\Big(-\frac{1}{\hbar}\Big)\mathrm{e}^{-\xi_\alpha\tau/\hbar}(1+\zeta n_\alpha) = -\frac{1}{\hbar}(1+\zeta n_\alpha)\frac{\zeta\mathrm{e}^{-\beta\xi_\alpha}-1}{\mathrm{i}\omega_n - \xi_\alpha/\hbar} = \frac{1}{\mathrm{i}\hbar\omega_n - \xi_\alpha},$$

and Lemma 1.11. ■

Corollary 29.96 The Green-function obeys the equation of motion

$$TBD. \tag{29.115}$$

Completion (statement) (GW01, Eq. (B9), there with $\hbar = 1$). Let $G(xt, x't') = -\frac{\mathrm{i}}{\hbar}\langle \mathrm{T}_t\, \psi(x,t)\psi^\dagger(x',t')\rangle$ be the time-ordered Green-function (correction note after the Definition above), with $x = (\mathbf{x}, s)$, time evolution with $H = T + U + V$ (local, symmetric, spin-independent V), and $h(x) := -\frac{\hbar^2}{2m}\Delta_{\mathbf{x}} + U(\mathbf{x})$. Then

$$\big[\mathrm{i}\hbar\partial_t - h(x)\big]G(xt,x't') = \delta(t-t')\,\delta(x-x') \\ - \frac{\mathrm{i}}{\hbar}\int\!\!\!\!\!\!\sum_{x''} V(\mathbf{x},\mathbf{x}'')\,\Big\langle\, \mathrm{T}_t\,\big[\psi^\dagger(x'',t)\psi(x'',t)\psi(x,t)\big]\psi^\dagger(x',t')\Big\rangle.$$

The time ordering treats the bracket as one (odd) operator at time t, and the expectation value is a two-particle Green-function at equal times (cf. GW01, Eq. (B10), and the Definition of the self-energy below). For $V = 0$ the right-hand side is $\delta(t-t')\delta(x-x')$, i.e. G_0 is a Green-function of the differential operator $\mathrm{i}\hbar\partial_t - h$ in the mathematical sense, which explains the name. With Ξ instead of H, replace h by $h - \mu$.

Proof 29.96 See GW01 Eq. B(9)

Proof. $\psi(x,t)$ and $\dot\psi(x,t)$ have the statistics ζ, and H is even. Lemma 8.21 (with H instead of Ξ) for $X = \psi(x)$, $X' = \psi^\dagger(x')$ gives

$$\partial_t\,\mathrm{T}_t\,\big[\psi(x,t)\psi^\dagger(x',t')\big] = \mathrm{T}_t\,\big[\dot\psi(x,t)\psi^\dagger(x',t')\big] + \delta(t-t')\,[\psi(x),\psi^\dagger(x')]_\zeta(t),$$

and the equal-time commutator is the c-number $\delta(x-x')$. Multiplying by $\mathrm{i}\hbar\cdot(-\frac{\mathrm{i}}{\hbar}) = 1$ and taking the expectation value,

$$\mathrm{i}\hbar\partial_t G(xt,x't') = \delta(t-t')\delta(x-x') - \frac{\mathrm{i}}{\hbar}\Big\langle\, \mathrm{T}_t\,\big[\mathrm{i}\hbar\dot\psi(x,t)\big]\psi^\dagger(x',t')\Big\rangle.$$

Insert the (corrected) equation of motion of the field operator,

$$\mathrm{i}\hbar\dot\psi(x,t) = h(x)\psi(x,t) + \int\!\!\!\!\!\!\sum_{x''} V(\mathbf{x},\mathbf{x}'')\psi^\dagger(x'',t)\psi(x'',t)\psi(x,t).$$

Since $h(x)$ acts on x only, it can be taken out of T_t and $\langle\cdot\rangle$, and $-\frac{\mathrm{i}}{\hbar}\langle \mathrm{T}_t\,\psi(x,t)\psi^\dagger(x',t')\rangle = G$. ■

Lemma 29.97 The Green-function of the field-operators has the Lehmann-representation

See GW01 Eq. (7)

Completion (statement) (GW01, Eqs. (4), (5), (7)). Let $\zeta = -1$, $T = 0$, and let $|N\rangle$ be the non-degenerate N-particle ground state, $H|N\rangle = E(N)|N\rangle$. Let $\{|N\pm1, s\rangle\}_s$ be orthonormal eigenbases of H in the $(N\pm1)$-particle sectors, with energies $E(N\pm1, s)$. Define the excitation energies and amplitudes

$$\begin{aligned} \varepsilon_s &= E(N+1,s) - E(N), & \psi_s(x) &= \langle N|\psi(x)|N+1,s\rangle & &\text{(addition, } s\in\text{add.)},\\ \varepsilon_s &= E(N) - E(N-1,s), & \psi_s(x) &= \langle N-1,s|\psi(x)|N\rangle & &\text{(removal, } s\in\text{rem.)}. \end{aligned}$$

Then, with time evolution generated by H, $G(x,x';\omega) := \int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t} G(xt, x'0)$ is

$$G(x,x';\omega) = \sum_{s\in\text{add.}} \frac{\psi_s(x)\psi_s^*(x')}{\hbar\omega - \varepsilon_s + \mathrm{i}0^+} + \sum_{s\in\text{rem.}} \frac{\psi_s(x)\psi_s^*(x')}{\hbar\omega - \varepsilon_s - \mathrm{i}0^+}.$$

Always $\varepsilon_{\text{rem}} \le \mu_- := E(N) - E(N-1)$ and $\varepsilon_{\text{add}} \ge \mu_+ := E(N+1) - E(N)$, with the ground-state energies $E(N \pm 1)$. If $E(N)$ is convex in N, i.e. $\mu_- \le \mu_+$, then for $\mu \in (\mu_-, \mu_+)$ both sums combine to $\sum_s \frac{\psi_s(x)\psi_s^*(x')}{\hbar\omega - \varepsilon_s + \mathrm{i}0^+ \operatorname{sgn}(\varepsilon_s - \mu)}$. This is GW01, Eq. (7), with $\hbar = 1$, $\mu = E_{\text{F}}$, Θ-functions instead of the sign, and an additional spin sum. With Ξ instead of H, $\varepsilon_s \to \varepsilon_s - \mu$. For bosons the removal term has the opposite sign.

Proof 29.97 $\psi^\dagger(x')|N\rangle$ lies in the $(N+1)$-particle sector (item (c) of the completion after the Remark on field operators). For $t > 0$ insert $1 = \sum_s |N+1, s\rangle\langle N+1, s|$ there and use $\mathrm{e}^{-\mathrm{i}Ht/\hbar}|N+1, s\rangle = \mathrm{e}^{-\mathrm{i}E(N+1,s)t/\hbar}|N+1, s\rangle$:

$$G(xt, x'0) = -\frac{\mathrm{i}}{\hbar}\langle N|\mathrm{e}^{\mathrm{i}Ht/\hbar}\psi(x)\mathrm{e}^{-\mathrm{i}Ht/\hbar}\psi^\dagger(x')|N\rangle = -\frac{\mathrm{i}}{\hbar}\sum_{s\in\text{add.}} \psi_s(x)\psi_s^*(x')\,\mathrm{e}^{-\mathrm{i}\varepsilon_s t/\hbar}.$$

For $t < 0$, analogously with $1 = \sum_s |N-1, s\rangle\langle N-1, s|$:

$$G(xt, x'0) = -\frac{\mathrm{i}}{\hbar}\zeta\langle N|\psi^\dagger(x')\mathrm{e}^{\mathrm{i}Ht/\hbar}\psi(x)\mathrm{e}^{-\mathrm{i}Ht/\hbar}|N\rangle = -\frac{\mathrm{i}}{\hbar}\zeta\sum_{s\in\text{rem.}} \psi_s(x)\psi_s^*(x')\,\mathrm{e}^{-\mathrm{i}\varepsilon_s t/\hbar}.$$

The Fourier integrals converge after the regularization $\omega \to \omega + \mathrm{i}0^+$ for $t > 0$ and $\omega \to \omega - \mathrm{i}0^+$ for $t < 0$:

$$-\frac{\mathrm{i}}{\hbar}\int_0^\infty \mathrm{d}t\,\mathrm{e}^{\mathrm{i}(\omega-\varepsilon_s/\hbar+\mathrm{i}0^+)t} = \frac{1}{\hbar\omega - \varepsilon_s + \mathrm{i}0^+}, \qquad -\frac{\mathrm{i}}{\hbar}\zeta\int_{-\infty}^0 \mathrm{d}t\,\mathrm{e}^{\mathrm{i}(\omega-\varepsilon_s/\hbar-\mathrm{i}0^+)t} = \frac{-\zeta}{\hbar\omega - \varepsilon_s - \mathrm{i}0^+},$$

and $-\zeta = 1$ for fermions. The bounds on ε_s follow from $E(N \pm 1, s) \ge E(N \pm 1)$. ■

Self-Energy

TBDigitalized from GW01 Eq. (81), (82).

Completion (GW01, Eqs. (13), (81), (82), (B10)–(B14)). From here on: fermions ($\zeta = -1$), $\hbar = 1$ (so that $G = -\mathrm{i}\langle \mathrm{T}\,\psi\psi^\dagger\rangle$ agrees with GW01), and the abbreviations $1 \equiv (x_1, t_1)$, $\int \mathrm{d}1 \equiv \int\!\!\!\!\!\!\int_{x_1} \mathrm{d}t_1$, $\delta(1,2) \equiv \delta(x_1 - x_2)\delta(t_1 - t_2)$, $v(1,2) \equiv V(\mathbf{x}_1, \mathbf{x}_2)\,\delta(t_1 - t_2)$, $1^+ \equiv (x_1, t_1 + 0^+)$. Integral kernels are multiplied like matrices, $(AB)(1,2) = \int \mathrm{d}3\, A(1,3)B(3,2)$, and G^{-1} denotes the inverse kernel (assumed to exist).

Definition 29.98 Let G_0 be the Green-function of the non-interacting system ($V = 0$), i.e. $[\mathrm{i}\partial_{t_1} - h(1)]G_0(1,2) = \delta(1,2)$ with time-ordered boundary conditions. The *self-energy* $\bar{\Sigma}$ is defined by *Dyson's equation*

$$G(1,2) = G_0(1,2) + \int \mathrm{d}(3,4)\, G_0(1,3)\bar{\Sigma}(3,4)G(4,2), \qquad \text{i.e.} \qquad \bar{\Sigma} = G_0^{-1} - G^{-1}.$$

Equivalently, $\int \mathrm{d}3\,\bar{\Sigma}(1,3)G(3,2) = -\mathrm{i}\int \mathrm{d}3\, v(1,3)\,G_2(1,3;2,3^+)$ (GW01, Eq. (B10)) with the two-particle Green-function

$$G_2(1,2;1',2') := (-\mathrm{i})^2\langle \mathrm{T}\,\psi(1)\psi(2)\psi^\dagger(2')\psi^\dagger(1')\rangle.$$

One splits off the Hartree potential $v_{\text{H}}(1) := \int \mathrm{d}3\, v(1,3)\langle\hat{n}(3)\rangle = -\mathrm{i}\int \mathrm{d}3\, v(1,3)G(3,3^+)$ (GW01, Eqs. (B11), (B12)): $\bar{\Sigma}(1,2) = v_{\text{H}}(1)\delta(1,2) + \Sigma(1,2)$.

Proof of the equivalence. By the Corollary on the equation of motion,

$$(G_0^{-1}G)(1,2) = [\mathrm{i}\partial_{t_1} - h(1)]G(1,2) = \delta(1,2) - \mathrm{i}\int \mathrm{d}3\, v(1,3)\big\langle\, \mathrm{T}[\psi^\dagger(3)\psi(3)\psi(1)]\psi^\dagger(2)\big\rangle\Big|_{t_3=t_1}.$$

Inside T, write $\psi^\dagger(3) \to \psi^\dagger(3^+)$ (this keeps it to the left of $\psi(3)$ and $\psi(1)$). Then reorder $(\psi^\dagger(3^+), \psi(3), \psi(1)) \to (\psi(1), \psi(3), \psi^\dagger(3^+))$; this is a transposition of two odd operators, with sign -1 (Lemma 8.18). With $(-\mathrm{i})^{-2} =$

-1 the expectation value is exactly $G_2(1,3;2,3^+)$. Hence $G_0^{-1}G = 1 + \bar{\Sigma}G$, which is Dyson's equation after multiplication with G_0 from the left. Finally, $\langle \hat{n}(3)\rangle = \langle \psi^\dagger(3)\psi(3)\rangle = -\langle \mathrm{T}\,\psi(3)\psi^\dagger(3^+)\rangle = -\mathrm{i}G(3,3^+)$. ■

Remark (GW01, Eqs. (81), (82)). Iterating Dyson's equation gives $G = G_0 + G_0\bar{\Sigma}G_0 + G_0\bar{\Sigma}G_0\bar{\Sigma}G_0 + \ldots$, the sum of all diagrams with an arbitrary number of self-energy insertions. If $\bar{\Sigma}$ is replaced by a fixed approximation Σ_0 (e.g. G_0W_0, evaluated with G_0), the solution G_1 of $G_1 = G_0 + G_0\Sigma_0 G_1$ (Eq. (82)) resums all these reducible diagrams with Σ_0-insertions, while Σ_0 itself is not updated. This is why one works with the irreducible self-energy.

Theorem 29.99 The Green-function can be obtained from Hedins-equations

$$TBD. \tag{29.116}$$

Completion (statement) (Hedin 1965; GW01, Eqs. (B14), (B17)–(B26)). With the total potential V_{tot}, the vertex Γ, the irreducible polarizability P and the screened interaction W defined in the proof, G and the self-energy Σ of Definition 29.98 satisfy the closed set of equations

$$\begin{aligned}
G(1,2) &= G_{\mathrm{H}}(1,2) + \int \mathrm{d}(3,4)\, G_{\mathrm{H}}(1,3)\Sigma(3,4)G(4,2),\\
\Sigma(1,2) &= \mathrm{i}\int \mathrm{d}(3,4)\, G(1,4)\, W(1^+,3)\,\Gamma(4,2;3),\\
W(1,2) &= v(1,2) + \int \mathrm{d}(3,4)\, v(1,3)P(3,4)W(4,2),\\
P(1,2) &= -\mathrm{i}\int \mathrm{d}(3,4)\, G(1,3)\,\Gamma(3,4;2)\, G(4,1^+),\\
\Gamma(1,2;3) &= \delta(1,2)\delta(1,3) + \int \mathrm{d}(4,5,6,7)\,\frac{\delta\Sigma(1,2)}{\delta G(4,5)}\, G(4,6)\,\Gamma(6,7;3)\, G(7,5).
\end{aligned}$$

Here G_{H} is the Hartree Green-function, $[\mathrm{i}\partial_{t_1} - h(1) - v_{\mathrm{H}}(1)]G_{\mathrm{H}}(1,2) = \delta(1,2)$. Setting $\Gamma(1,2;3) \approx \delta(1,2)\delta(1,3)$ gives the *GW approximation* $\Sigma(1,2) = \mathrm{i}G(1,2)W(1^+,2)$, $P(1,2) = -\mathrm{i}G(1,2)G(2,1^+)$.

Proof 29.99 See GW01 Appendix.

Proof (Schwinger's functional-derivative technique, GW01, Appendix B.2). The derivation is formal: functional derivatives and inverse kernels are assumed to exist. At $T = 0$ the expectation values are ground-state expectation values (Gell-Mann–Low). The same steps hold verbatim on the imaginary-time axis.

Step 1 (auxiliary field). Add a time-dependent external potential φ, $H \to H + \sum\!\!\!\!\!\!\int_x \varphi(x,t)\hat{n}(x)$. With $S := \mathrm{T}\exp\big(-\mathrm{i}\int \mathrm{d}3\,\varphi(3)\hat{n}(3)\big)$ and Heisenberg operators w.r.t. H (cf. the S-matrix expansion, Corollary 15.8), define

$$G(1,2) := -\mathrm{i}\frac{\langle \mathrm{T}[S\,\psi(1)\psi^\dagger(2)]\rangle}{\langle \mathrm{T}\,S\rangle}, \qquad G_2(1,2;1',2') := (-\mathrm{i})^2\frac{\langle \mathrm{T}[S\,\psi(1)\psi(2)\psi^\dagger(2')\psi^\dagger(1')]\rangle}{\langle \mathrm{T}\,S\rangle},$$

and $\langle \hat{n}(1)\rangle_\varphi := \langle \mathrm{T}[S\,\hat{n}(1)]\rangle/\langle \mathrm{T}\,S\rangle = -\mathrm{i}G(1,1^+)$. For $\varphi = 0$ these are the previous quantities. The equation of motion acquires the term $\varphi(1)G(1,2)$:

$$[\mathrm{i}\partial_{t_1} - h(1) - \varphi(1)]G(1,2) = \delta(1,2) - \mathrm{i}\int \mathrm{d}3\, v(1,3)\, G_2(1,3;2,3^+).$$

Step 2 (Schwinger's identity, GW01, Eq. (B15)). Since $\hat{n}$ is even, $\frac{\delta}{\delta\varphi(3)}\,\mathrm{T}[S\,X] = -\mathrm{i}\,\mathrm{T}[S\,\hat{n}(3)X]$. With the quotient rule and $\frac{\langle \mathrm{T}[S\psi(1)\psi^\dagger(2)]\rangle}{\langle \mathrm{T}\,S\rangle} = \mathrm{i}G(1,2)$,

$$\frac{\delta G(1,2)}{\delta\varphi(3)} = -\frac{\langle \mathrm{T}[S\,\hat{n}(3)\psi(1)\psi^\dagger(2)]\rangle}{\langle \mathrm{T}\,S\rangle} + \mathrm{i}\,G(1,2)\,\langle \hat{n}(3)\rangle_\varphi = -G_2(1,3;2,3^+) + G(1,2)\,G(3,3^+).$$

Here $\hat{n}(3) = \psi^\dagger(3^+)\psi(3)$ was reordered inside T to $\psi(1)\psi(3)\psi^\dagger(3^+)\psi^\dagger(2)$ (sign -1, as in the proof of the equivalence after Definition 29.98), and $(-\mathrm{i})^{-2} = -1$ was used.

Step 3 (self-energy, GW01, Eq. (B16)). Insert Step 2 into Step 1. The product term gives the Hartree potential, $-\mathrm{i}\int \mathrm{d}3\, v(1,3)G(3,3^+)G(1,2) = v_{\mathrm{H}}(1)G(1,2)$. With the total potential $V_{\mathrm{tot}}(1) := \varphi(1)+v_{\mathrm{H}}(1)$ (GW01, Eq. (B17)):

$$[\mathrm{i}\partial_{t_1} - h(1) - V_{\mathrm{tot}}(1)]G(1,2) = \delta(1,2) + \mathrm{i}\int \mathrm{d}3\, v(1,3)\frac{\delta G(1,2)}{\delta\varphi(3)} =: \delta(1,2) + \int \mathrm{d}4\, \Sigma(1,4)G(4,2).$$

Differentiating $GG^{-1} = 1$ gives $\frac{\delta G}{\delta\varphi(3)} = -G\frac{\delta G^{-1}}{\delta\varphi(3)}G$. Multiplying with G^{-1} from the right,

$$\Sigma(1,2) = -\mathrm{i}\int \mathrm{d}(3,4)\, v(1,3)\, G(1,4)\, \frac{\delta G^{-1}(4,2)}{\delta\varphi(3)}.$$

In operator notation, $G^{-1} = G_{\mathrm{H}}^{-1} - \Sigma$ with $G_{\mathrm{H}}^{-1}(1,2) = [\mathrm{i}\partial_{t_1} - h(1) - V_{\mathrm{tot}}(1)]\delta(1,2)$. At $\varphi = 0$ this is the Dyson equation of the statement, and $\bar{\Sigma} = v_{\mathrm{H}}\delta + \Sigma$ agrees with Definition 29.98.

Step 4 (vertex and screened interaction). By the chain rule through V_{tot},

$$\frac{\delta G^{-1}(4,2)}{\delta\varphi(3)} = \int \mathrm{d}5\, \frac{\delta G^{-1}(4,2)}{\delta V_{\mathrm{tot}}(5)}\frac{\delta V_{\mathrm{tot}}(5)}{\delta\varphi(3)} =: -\int \mathrm{d}5\, \Gamma(4,2;5)\,\varepsilon^{-1}(5,3),$$

which defines the vertex $\Gamma(1,2;3) := -\delta G^{-1}(1,2)/\delta V_{\mathrm{tot}}(3)$ and the inverse dielectric function $\varepsilon^{-1}(1,2) := \delta V_{\mathrm{tot}}(1)/\delta\varphi(2)$ (GW01, Eqs. (B18), (B19)). With $W(1,2) := \int \mathrm{d}3\, \varepsilon^{-1}(1,3)v(3,2)$ (Eq. (B20)) and $v(1,3) = v(3,1)$,

$$\Sigma(1,2) = \mathrm{i}\int \mathrm{d}(4,5)\, G(1,4)\,\Gamma(4,2;5)\Big[\int \mathrm{d}3\, \varepsilon^{-1}(5,3)v(3,1)\Big] = \mathrm{i}\int \mathrm{d}(3,4)\, G(1,4)\, W(3,1)\,\Gamma(4,2;3),$$

and $W(3,1) = W(1,3)$ (Step 5). The time argument 1^+ in $W(1^+,3)$ records that the equal-time (exchange) part stems from $\hat{n}(3) = \psi^\dagger(3^+)\psi(3)$. For example, the lowest order $\Gamma = \delta\delta$, $W = v$ gives the Fock term $\Sigma_{\mathrm{x}}(1,2) = \mathrm{i}\, v(1,2)G(1,2^+) = -V(\mathbf{x}_1,\mathbf{x}_2)\langle\psi^\dagger(x_2)\psi(x_1)\rangle\delta(t_1 - t_2)$.

Step 5 (polarizability and screening). Define $P(1,2) := \delta\langle\hat{n}(1)\rangle_\varphi/\delta V_{\mathrm{tot}}(2)$ and $\chi(1,2) := \delta\langle\hat{n}(1)\rangle_\varphi/\delta\varphi(2)$ (GW01, Eqs. (B21), (B22)). From $V_{\mathrm{tot}}(1) = \varphi(1) + \int \mathrm{d}3\, v(1,3)\langle\hat{n}(3)\rangle_\varphi$ and the chain rule,

$$\varepsilon^{-1}(1,2) = \delta(1,2) + \int \mathrm{d}3\, v(1,3)\chi(3,2) = \delta(1,2) + \int \mathrm{d}(3,4)\, v(1,3)P(3,4)\varepsilon^{-1}(4,2).$$

Multiplying the second form by v from the right gives $W = v + vPW$ (Eq. (B24)); the first form gives $W = v + v\chi v$. As in Step 2, $\chi(1,2) = -\mathrm{i}\langle\mathrm{T}\,\delta\hat{n}(1)\,\delta\hat{n}(2)\rangle_\varphi$ with $\delta\hat{n} = \hat{n} - \langle\hat{n}\rangle_\varphi$ (GW01, Eq. (B29), there without the factor $-\mathrm{i}$). It is symmetric because $\hat{n}$ is even, and therefore W is symmetric. Finally, $\langle\hat{n}(1)\rangle_\varphi = -\mathrm{i}G(1,1^+)$ and $\frac{\delta G}{\delta V_{\mathrm{tot}}(3)} = -G\frac{\delta G^{-1}}{\delta V_{\mathrm{tot}}(3)}G$ give

$$P(1,2) = -\mathrm{i}\frac{\delta G(1,1^+)}{\delta V_{\mathrm{tot}}(2)} = -\mathrm{i}\int \mathrm{d}(3,4)\, G(1,3)\,\Gamma(3,4;2)\, G(4,1^+).$$

GW01, Eq. (B23), writes the transposed form; P is symmetric as well, since $\chi = P\varepsilon^{-1} = P + Pv\chi$ gives $P = \chi(1+v\chi)^{-1}$.

Step 6 (vertex equation). From $G^{-1} = G_{\mathrm{H}}^{-1} - \Sigma$ and $\delta G_{\mathrm{H}}^{-1}(1,2)/\delta V_{\mathrm{tot}}(3) = -\delta(1,2)\delta(1,3)$ one gets $\Gamma(1,2;3) = \delta(1,2)\delta(1,3) + \delta\Sigma(1,2)/\delta V_{\mathrm{tot}}(3)$. Regard Σ as a functional of G (skeleton expansion). Then the chain rule and $\frac{\delta G(4,5)}{\delta V_{\mathrm{tot}}(3)} = \int \mathrm{d}(6,7)\, G(4,6)\Gamma(6,7;3)G(7,5)$ give the vertex equation. Setting $\varphi = 0$ completes the proof. ■

Notice that the differential equation for the finite temperature Green-function now has the form of a heat-equation

$$TBD. \tag{29.117}$$

Completion. Restore $\hbar$. Let $\mathscr{G}(x\tau, x'\tau') = -\frac{1}{\hbar}\langle \mathrm{T}_\tau\, \psi(x,\tau)\psi^\dagger(x',\tau')\rangle$ be the imaginary-time Green-function (Definition 13.1), with $\psi(x,\tau) = \mathrm{e}^{\tau\Xi/\hbar}\psi(x)\mathrm{e}^{-\tau\Xi/\hbar}$ and $\Xi = H - \mu\hat{N}$. The same steps as in the proof of the Corollary on the equation of motion give

$$\big[-\hbar\partial_\tau - h(x) + \mu\big]\mathscr{G}(x\tau, x'\tau') = \delta(\tau-\tau')\,\delta(x-x') \\ - \frac{1}{\hbar}\sum\!\!\!\!\!\!\int_{x''} V(\mathbf{x},\mathbf{x}'')\Big\langle \mathrm{T}_\tau\,\big[\psi^\dagger(x'',\tau)\psi(x'',\tau)\psi(x,\tau)\big]\psi^\dagger(x',\tau')\Big\rangle.$$

For free particles ($U = 0$, $V = 0$) and $\tau \neq \tau'$ this reads

$$\partial_\tau \mathscr{G}_0 = \frac{\hbar}{2m}\Delta\mathscr{G}_0 + \frac{\mu}{\hbar}\mathscr{G}_0.$$

After the substitution $\mathscr{G}_0 = \mathrm{e}^{\mu\tau/\hbar}g$ this is the heat equation $\partial_\tau g = D\Delta g$ with "diffusion constant" $D = \hbar/2m$. It is the Schrödinger equation $\mathrm{i}\hbar\partial_t G_0 = -\frac{\hbar^2}{2m}\Delta G_0$ after the Wick rotation $t = -\mathrm{i}\tau$. Accordingly, for $0 < \tau - \tau' < \hbar\beta$ and in the non-degenerate limit $n_{\mathbf{k}} \ll 1$, $\mathscr{G}_0$ is $-\frac{1}{\hbar}\mathrm{e}^{\mu(\tau-\tau')/\hbar}$ times the Gaussian heat kernel $\big(\frac{m}{2\pi\hbar(\tau-\tau')}\big)^{3/2}\mathrm{e}^{-mr^2/(2\hbar(\tau-\tau'))}$. This follows from the first line of the imaginary-time item above and the Gaussian integral of the real-time item.

Proof. By Theorem 8.24, $\hbar\partial_\tau\psi(x,\tau) = -[\psi(x),\Xi](\tau) = -[\psi(x),H](\tau) + \mu[\psi(x),\hat{N}](\tau)$. Here $[\psi,H]$ was computed in the proof of the equation of motion of the field operator, and $[\psi,\hat{N}] = \psi$. Hence

$$-\hbar\partial_\tau\psi(x,\tau) = \big(h(x)-\mu\big)\psi(x,\tau) + \sum\!\!\!\!\!\!\int_{x''} V(\mathbf{x},\mathbf{x}'')\psi^\dagger(x'',\tau)\psi(x'',\tau)\psi(x,\tau).$$

The imaginary-time version of Lemma 8.21 gives

$$\partial_\tau\langle \mathrm{T}_\tau\,\psi(x,\tau)\psi^\dagger(x',\tau')\rangle = \delta(\tau-\tau')\delta(x-x') + \langle \mathrm{T}_\tau\,\partial_\tau\psi(x,\tau)\,\psi^\dagger(x',\tau')\rangle.$$

Since $-\hbar\partial_\tau\mathscr{G} = \partial_\tau\langle \mathrm{T}_\tau\,\psi\psi^\dagger\rangle$, inserting $\partial_\tau\psi$ gives the claim. ■

Example: Non-Interacting Electrons

Marcos Marinos QFT-notes p. 46f: Two-Body-Interactions in real and momentum-space

TBDigitalized from Schwabl p. 35. [48, Sect. 2.1, p. 35]

Note. Mariño's notes (p. 46 f.) treat two-body interactions in real and momentum space; this is completed in the next subsection.

Completion ([48, Sect. 2.1, Eqs. (2.1.6)–(2.1.8), p. 35]). Consider N free electrons ($\zeta = -1$, spin $\sigma = \pm\frac{1}{2}$) in the box of volume $\mathcal{V}$ with periodic boundary conditions, $H_0 = \sum_{\mathbf{k},\sigma}\varepsilon_{\mathbf{k}}a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma}$, $\varepsilon_{\mathbf{k}} = \frac{\hbar^2\mathbf{k}^2}{2m}$ (momentum-basis Lemma above).

- *Ground state.* $|\phi_0\rangle = \prod_{|\mathbf{k}|<k_F,\sigma} a^\dagger_{\mathbf{k}\sigma}|0\rangle$ (Fermi sphere; the order of the factors only fixes the overall sign). It is the Slater determinant of the plane waves with $|\mathbf{k}| < k_F$, so $\langle\phi_0|a^\dagger_{\mathbf{p}\sigma}a_{\mathbf{p}'\sigma'}|\phi_0\rangle = \delta_{\mathbf{p}\mathbf{p}'}\delta_{\sigma\sigma'}n_{\mathbf{p}\sigma}$ with $n_{\mathbf{p}\sigma} = \theta(k_F - p)$ (proof of Lemma 29.92, first item). In the thermodynamic limit, $\frac{1}{\mathcal{V}}\sum_{\mathbf{k}} \to \int\frac{\mathrm{d}^3k}{(2\pi)^3}$, and the density is

$$n = \frac{N}{\mathcal{V}} = 2\int_{|\mathbf{k}|<k_F}\frac{\mathrm{d}^3k}{(2\pi)^3} = \frac{k_F^3}{3\pi^2}.$$

- *One-particle correlation function.* With $\psi_\sigma(\mathbf{x}) = \mathcal{V}^{-1/2}\sum_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{x}} a_{\mathbf{p}\sigma}$ and $r = |\mathbf{x}-\mathbf{x}'|$:

$$\begin{aligned} G_\sigma(\mathbf{x}-\mathbf{x}') &:= \langle\phi_0|\psi_\sigma^\dagger(\mathbf{x})\psi_\sigma(\mathbf{x}')|\phi_0\rangle = \frac{1}{\mathcal{V}}\sum_{\mathbf{p}} e^{-i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')} n_{\mathbf{p}\sigma} \to \int_{p<k_F} \frac{d^3p}{(2\pi)^3} e^{-i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')} \\ &= \frac{1}{(2\pi)^2}\int_0^{k_F} dp\, p^2 \int_{-1}^{1} d\eta\, e^{ipr\eta} = \frac{1}{2\pi^2 r}\int_0^{k_F} dp\, p\sin(pr) = \frac{\sin(k_F r) - k_F r\cos(k_F r)}{2\pi^2 r^3} \\ &= \frac{3n}{2}\frac{\sin(k_F r) - k_F r\cos(k_F r)}{(k_F r)^3}. \end{aligned}$$

  Steps: spherical coordinates with the polar axis along $-(\mathbf{x}-\mathbf{x}')$ and $\eta = \cos\theta$; $\int_{-1}^{1} d\eta\, e^{ipr\eta} = \frac{2\sin(pr)}{pr}$; $\int_0^k dp\, p\sin(pr) = \frac{\sin(kr)-kr\cos(kr)}{r^2}$ (partial integration); and $\frac{1}{2\pi^2} = \frac{3n}{2k_F^3}$.

- *Properties.* Since $\frac{\sin y - y\cos y}{y^3} = \frac{1}{3} - \frac{y^2}{30} + \mathcal{O}(y^4)$, $G_\sigma(0) = \frac{n}{2}$, the density per spin direction. For $r \to \infty$, $G_\sigma \simeq -\frac{3n}{2}\frac{\cos(k_F r)}{(k_F r)^2} \to 0$, i.e. it decays while oscillating with period $2\pi/k_F$ in r. Its zeros are the solutions $y = k_F r > 0$ of $\tan y = y$; for large y they approach $(l+\frac{1}{2})\pi$, $l \in \mathbb{N}$, from below.
- *Relation to the Green-functions above.* G_σ is the equal-time limit of the time-ordered Green-function, $G_{\sigma\sigma}(\mathbf{x}'t, \mathbf{x}t^+) = \frac{i}{\hbar}G_\sigma(\mathbf{x}-\mathbf{x}')$ (correction note after the Definition of the Green-function, $\zeta = -1$).

Example: Free Electrons with Two-Body-Interactions

Now one can also introduce the Fourier-transform of these operators as in [Negele, page 18]. This is the so-called momentum-basis. Cf. Schwabl p. 25 onwards [48, Sect. 1.6, p. 25 ff.]. See also Schwabl p. 46 for the Coulomb-interaction in second quantization. ([48, Sect. 2.2.1, Eq. (2.2.1), p. 41]; in this 5th edition, p. 46 shows the Hartree-Fock energy of the electron gas.)

Completion. "[Negele, page 18]" is [38, Eq. (1.100), p. 18]; see the momentum-basis Lemma above. The following computation is contained in [48, Sect. 1.6, Eqs. (1.6.4)–(1.6.6)] and in Mariño's QFT notes (p. 46 f., Eqs. (2.93)–(2.103)).

Lemma 29.100 Work in the momentum basis of the box $\mathcal{V}$ (momentum-basis Lemma above), and let

$$U_{\mathbf{q}} := \int_{\mathcal{V}} d^3x\, e^{-i\mathbf{q}\cdot\mathbf{x}} U(\mathbf{x}), \qquad V_{\mathbf{q}} := \int_{\mathcal{V}} d^3x\, e^{-i\mathbf{q}\cdot\mathbf{x}} V(\mathbf{x}), \qquad V(\mathbf{x}) = \frac{1}{\mathcal{V}}\sum_{\mathbf{q}} V_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{x}}$$

(V periodically continued). Then $H = T + U + V$ with a local, spin-independent interaction $V(\mathbf{x}-\mathbf{x}')$ reads

$$\begin{aligned} H = &\sum_{\mathbf{k},s} \frac{\hbar^2\mathbf{k}^2}{2m} a_{\mathbf{k}s}^\dagger a_{\mathbf{k}s} + \frac{1}{\mathcal{V}}\sum_{\mathbf{k},\mathbf{k}',s} U_{\mathbf{k}'-\mathbf{k}}\, a_{\mathbf{k}'s}^\dagger a_{\mathbf{k}s} \\ &+ \frac{1}{2\mathcal{V}}\sum_{\mathbf{q},\mathbf{k},\mathbf{k}'}\sum_{s,s'} V_{\mathbf{q}}\, a_{\mathbf{k}+\mathbf{q},s}^\dagger a_{\mathbf{k}'-\mathbf{q},s'}^\dagger a_{\mathbf{k}'s'} a_{\mathbf{k}s}. \end{aligned}$$

The interaction transfers the momentum $\hbar\mathbf{q}$ from one particle to the other and conserves the total momentum.

Proof 29.100 The kinetic term is the momentum-basis Lemma. Inserting $\psi_s(\mathbf{x}) = \mathcal{V}^{-1/2}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} a_{\mathbf{k}s}$ into $U = \sum_s \int d^3x\, U(\mathbf{x})\psi_s^\dagger\psi_s$ gives $\frac{1}{\mathcal{V}}\sum_{\mathbf{k}_1,\mathbf{k}_2}\int d^3x\, e^{-i(\mathbf{k}_1-\mathbf{k}_2)\cdot\mathbf{x}} U(\mathbf{x})\, a_{\mathbf{k}_1 s}^\dagger a_{\mathbf{k}_2 s} = \frac{1}{\mathcal{V}}\sum U_{\mathbf{k}_1-\mathbf{k}_2} a_{\mathbf{k}_1 s}^\dagger a_{\mathbf{k}_2 s}$. For the interaction (Corol-

lary on local two-body operators, with spin) insert also the Fourier series of V:

$$V = \frac{1}{2\mathcal{V}^2}\sum_{s,s'}\sum_{\mathbf{k}_1,\dots,\mathbf{k}_4}\int \mathrm{d}^3x\,\mathrm{d}^3y\,V(\mathbf{x}-\mathbf{y})\,\mathrm{e}^{\mathrm{i}(\mathbf{k}_4-\mathbf{k}_1)\cdot\mathbf{x}}\,\mathrm{e}^{\mathrm{i}(\mathbf{k}_3-\mathbf{k}_2)\cdot\mathbf{y}}\,a^\dagger_{\mathbf{k}_1 s}a^\dagger_{\mathbf{k}_2 s'}a_{\mathbf{k}_3 s'}a_{\mathbf{k}_4 s}$$
$$= \frac{1}{2\mathcal{V}^3}\sum_{s,s'}\sum_{\mathbf{q},\mathbf{k}_1,\dots,\mathbf{k}_4} V_{\mathbf{q}}\Big(\int \mathrm{d}^3x\,\mathrm{e}^{\mathrm{i}(\mathbf{q}-\mathbf{k}_1+\mathbf{k}_4)\cdot\mathbf{x}}\Big)\Big(\int \mathrm{d}^3y\,\mathrm{e}^{\mathrm{i}(-\mathbf{q}-\mathbf{k}_2+\mathbf{k}_3)\cdot\mathbf{y}}\Big)\,a^\dagger_{\mathbf{k}_1 s}a^\dagger_{\mathbf{k}_2 s'}a_{\mathbf{k}_3 s'}a_{\mathbf{k}_4 s}.$$

The two integrals are $\mathcal{V}\delta_{\mathbf{k}_1,\mathbf{k}_4+\mathbf{q}}$ and $\mathcal{V}\delta_{\mathbf{k}_2,\mathbf{k}_3-\mathbf{q}}$; with $\mathbf{k} := \mathbf{k}_4$, $\mathbf{k}' := \mathbf{k}_3$ the claim follows. Each interaction term changes the total momentum $\mathbf{P} = \sum_{\mathbf{k},s}\hbar\mathbf{k}\,a^\dagger_{\mathbf{k}s}a_{\mathbf{k}s}$ by $\hbar[(\mathbf{k}+\mathbf{q})+(\mathbf{k}'-\mathbf{q})-\mathbf{k}'-\mathbf{k}] = 0$. ∎

Corollary 29.101 *(Coulomb interaction, jellium; [48, Eq. (2.2.1), p. 41].)* For $V(\mathbf{x}) = \frac{e^2}{|\mathbf{x}|}$ (Gaussian units; $e^2 \to \frac{e^2}{4\pi\varepsilon_0}$ in SI units) one has $V_{\mathbf{q}} = \frac{4\pi e^2}{\mathbf{q}^2}$ for $\mathbf{q}\neq 0$ (for $\mathcal{V}\to\infty$). For electrons in a homogeneous positive background of the same density (jellium), the $\mathbf{q}=0$ term cancels against the background, and in the thermodynamic limit

$$H = \sum_{\mathbf{k},s}\frac{\hbar^2\mathbf{k}^2}{2m}a^\dagger_{\mathbf{k}s}a_{\mathbf{k}s} + \frac{e^2}{2\mathcal{V}}\sum_{\mathbf{q}\neq 0}\sum_{\mathbf{k},\mathbf{k}',s,s'}\frac{4\pi}{\mathbf{q}^2}\,a^\dagger_{\mathbf{k}+\mathbf{q},s}a^\dagger_{\mathbf{k}'-\mathbf{q},s'}a_{\mathbf{k}'s'}a_{\mathbf{k}s}.$$

Proof 29.101 Regularize with the Yukawa potential $V_\lambda(\mathbf{x}) = e^2\mathrm{e}^{-\lambda|\mathbf{x}|}/|\mathbf{x}|$, $\lambda>0$ (Mariño, Example 2.9). In spherical coordinates with the polar axis along $\mathbf{q}$, $\eta=\cos\theta$:

$$V_{\lambda,\mathbf{q}} = 2\pi e^2\int_0^\infty \mathrm{d}r\,r\,\mathrm{e}^{-\lambda r}\int_{-1}^{1}\mathrm{d}\eta\,\mathrm{e}^{-\mathrm{i}qr\eta} = \frac{4\pi e^2}{q}\int_0^\infty \mathrm{d}r\,\mathrm{e}^{-\lambda r}\sin(qr) = \frac{4\pi e^2}{q^2+\lambda^2}.$$

This tends to $\frac{4\pi e^2}{q^2}$ for $\lambda\to 0$, $q\neq 0$, while $V_{\lambda,\mathbf{0}} = 4\pi e^2/\lambda^2$ diverges. The background has the charge density en, $n = N/\mathcal{V}$. Neglecting surface effects, $\int \mathrm{d}^3y\,V_\lambda(\mathbf{x}-\mathbf{y}) = V_{\lambda,\mathbf{0}}$ for $\mathbf{x}$ in the bulk. On the N-particle space:

- background-background: $\frac{1}{2}\int \mathrm{d}^3x\,\mathrm{d}^3y\,n^2\,V_\lambda(\mathbf{x}-\mathbf{y}) = \frac{N^2}{2\mathcal{V}}V_{\lambda,\mathbf{0}}$;
- electron-background: $-\sum_{i=1}^N\int \mathrm{d}^3y\,n\,V_\lambda(\mathbf{x}_i-\mathbf{y}) = -\frac{N^2}{\mathcal{V}}V_{\lambda,\mathbf{0}}$;
- the $\mathbf{q}=0$ term of the electron-electron interaction: $\frac{V_{\lambda,\mathbf{0}}}{2\mathcal{V}}\sum a^\dagger_{\mathbf{k}s}a^\dagger_{\mathbf{k}'s'}a_{\mathbf{k}'s'}a_{\mathbf{k}s} = \frac{V_{\lambda,\mathbf{0}}}{2\mathcal{V}}(\hat N^2-\hat N)$. Here $a_i^\dagger a_j^\dagger a_j a_i = \hat n_i\hat n_j - \delta_{ij}\hat n_i$, which follows from $\hat n_i\hat n_j = a_i^\dagger(\delta_{ij}+\zeta a_j^\dagger a_i)a_j$ and $\zeta^2=1$.

The sum of the three is $-\frac{N}{2\mathcal{V}}V_{\lambda,\mathbf{0}} = -\frac{2\pi e^2 n}{\lambda^2}$, i.e. $-\frac{2\pi e^2}{\lambda^2\mathcal{V}}$ per particle. This vanishes in the thermodynamic limit $\mathcal{V}\to\infty$ at fixed λ and n. Afterwards, $\lambda\to 0$ in the terms with $\mathbf{q}\neq 0$. The order of the two limits is essential. ∎

29.9. Generalized Matrices

As we will shortly see, we can catch two birds with one stone by introducing the following abbreviations.

Notation 29.102 We introduce a multi-index with a time-argument

$$A \equiv (\alpha, \tau) \quad \in \quad \mathscr{A} \times (0, +\hbar\beta) \equiv I_\tau$$

and consider generalized matrices with indices

$$\begin{aligned} \mathscr{G} :\ & I_\tau \times I_\tau \longrightarrow \mathbb{C} \\ & (A, A') \mapsto \mathscr{G}(A, A') \equiv \mathscr{G}_{\alpha,\alpha'}(\tau, \tau'). \end{aligned}$$

Definition 29.103 Completely analogous to usual matrices, one defines a generalized trace and generalized matrix-multiplication[11] as

$$\left(\mathscr{G} \cdot \mathscr{G}'\right)(A, A') \equiv \int\!\!\!\!\!\!\sum_{B \in I_\tau} \mathscr{G}(A, B)\, \mathscr{G}'(B, A')$$

Remark 29.103.1 Note that the inversion-relation now reads

$$\left(\mathscr{G} \cdot \mathscr{G}^{-1}\right)(A, A') = \delta_{\alpha,\alpha'}\, \delta(\tau - \tau') \equiv \mathrm{Id}$$

Definition 29.104 We call a generalized matrix a *propagator in thermal equilibrium with statistics* ζ, if there exists a periodic standard-continuation (denoted by the same symbol) on the temporal-axis

$$\mathbb{R} \ni \tau \mapsto \mathscr{G}_{\alpha,\alpha'}(\tau) \in \mathbb{C}$$

s.t. the following equations holds

$$\forall (\tau, \tau') \in \mathbb{R}^2 :\ \mathscr{G}_{\alpha,\alpha'}(\tau, \tau') = \mathscr{G}_{\alpha,\alpha'}(\tau - \tau') = \zeta \mathscr{G}_{\alpha,\alpha'}(\tau - \tau' + \hbar\beta)$$

Remark 29.104.1 We denote the set of all [P]ropagators [I]n [T]hermal [E]quilibrium with statistics ζ as PITE_ζ.

Remark 29.104.2 Note that the analytic standard-continuation of a PITE_ζ can be expanded with Matsubara-frequencies according to Lemma 1.11.

[11] This is a combination of ordinary matrix-multiplication for the α in the multi-index, and a convolution for the time-argument τ.

Theorem 29.105 Let $\mathscr{G}, \mathscr{G}' \in \mathrm{PITE}_\zeta$. Then it follows $\mathscr{G} \cdot \mathscr{G}' \in \mathrm{PITE}_\zeta$.

Proof 29.105 One finds by immediate calculation

$$\begin{aligned}\left(\mathscr{G} \cdot \mathscr{G}'\right)(\tau_1, \tau_2) &= +\int_0^{+\hbar\beta} \mathrm{d}\tau\, \mathscr{G}(\tau_1 - \tau)\mathscr{G}'(\tau - \tau_2) \\ &= +\int_0^{+\hbar\beta} \mathrm{d}\tau\, \mathscr{G}(\tau_1 - \tau)\mathscr{G}'(\tau_1 - \tau_2 - (\tau_1 - \tau)) \\ &= -\int_{\tau_1}^{\tau_1 - \hbar\beta} \mathrm{d}\tau' \mathscr{G}(\tau')\mathscr{G}'(\tau_1 - \tau_2 - \tau') \\ &= +\int_0^{+\hbar\beta} \mathrm{d}\tau' \mathscr{G}(\tau')\mathscr{G}'(\tau_1 - \tau_2 - \tau')\end{aligned} \tag{29.118}$$

where we used the substitution $\tau' = \tau_1 - \tau$ in the second last step and we used Waste-Folder 1, Digital Waste-Folder 1 with Useful Links, topic 4 in the last step. Now it is clear, that the product depends only on the time-difference and that it obeys the same periodicity as the respective Green-function. Therefore there will be a periodic standard-continuation with the desired properties.

Corollary 29.106 It follows for the Matsubara-component of the product

$$\left(\mathscr{G} \cdot \mathscr{G}'\right)(\mathrm{i}\omega_n) = \mathscr{G}(\mathrm{i}\omega_n) \cdot \mathscr{G}'(\mathrm{i}\omega_n). \tag{29.119}$$

Proof 29.106 By definition (1.12) of the Matsubara-component, together with the result of the preceding Theorem that $\mathscr{G} \cdot \mathscr{G}' \in \mathrm{PITE}_\zeta$, we may write

$$\left(\mathscr{G} \cdot \mathscr{G}'\right)(\mathrm{i}\omega_n) = \int_0^{\hbar\beta} \mathrm{d}\tau_1\, \mathrm{e}^{\mathrm{i}\omega_n\tau_1} \left(\mathscr{G} \cdot \mathscr{G}'\right)(\tau_1) = \int_0^{\hbar\beta} \mathrm{d}\tau_1\, \mathrm{e}^{\mathrm{i}\omega_n\tau_1} \int_0^{\hbar\beta} \mathrm{d}\tau\, \mathscr{G}(\tau)\mathscr{G}'(\tau_1 - \tau), \tag{29.120}$$

where we used Definition 29.103 for the convolution appearing under the last integral. Inserting the Matsubara-expansion of Lemma 1.11 for $\mathscr{G}'$,

$$\mathscr{G}'(\tau_1 - \tau) = \frac{1}{\hbar\beta} \sum_{\omega_m \in \Omega_\zeta} \mathscr{G}'(\mathrm{i}\omega_m)\, \mathrm{e}^{-\mathrm{i}\omega_m(\tau_1 - \tau)}, \tag{29.121}$$

we obtain

$$\begin{aligned}\left(\mathscr{G} \cdot \mathscr{G}'\right)(\mathrm{i}\omega_n) &= \frac{1}{\hbar\beta} \sum_{\omega_m \in \Omega_\zeta} \mathscr{G}'(\mathrm{i}\omega_m) \int_0^{\hbar\beta} \mathrm{d}\tau\, \mathscr{G}(\tau)\, \mathrm{e}^{\mathrm{i}\omega_m\tau} \int_0^{\hbar\beta} \mathrm{d}\tau_1\, \mathrm{e}^{\mathrm{i}(\omega_n - \omega_m)\tau_1} \\ &= \frac{1}{\hbar\beta} \sum_{\omega_m \in \Omega_\zeta} \mathscr{G}'(\mathrm{i}\omega_m)\, \mathscr{G}(\mathrm{i}\omega_m)\, \delta_{\omega_m, \omega_n}\, \hbar\beta,\end{aligned} \tag{29.122}$$

where the τ-integral was identified as $\mathscr{G}(\mathrm{i}\omega_m)$ via (1.12), and the τ_1-integral was evaluated using Corollary 1.12 (noting $\omega_n - \omega_m \in \Omega_{+1}$, since the difference of two frequencies of the same statistics ζ is always bosonic). Carrying out the sum over ω_m against the Kronecker-delta yields

$$\left(\mathscr{G}\cdot\mathscr{G}'\right)(\mathrm{i}\omega_n) = \mathscr{G}(\mathrm{i}\omega_n)\,\mathscr{G}'(\mathrm{i}\omega_n), \tag{29.123}$$

which proves the claim.

Remark 29.106.1 This theorem will turn out as a central result for our later discussions with the Dyson-equation of interacting systems; It implies that even if we take only a finite number of contributions from the infinite series in the Dyson-equation, we will still end up with a physically reasonable propagator.

Theorem 29.107 Under the assumption, that the Dyson-equation holds

$$\mathscr{G}(\mathrm{i}\omega_n) = \mathscr{G}_0(\mathrm{i}\omega_n) + \left(\mathscr{G}_0\cdot\Sigma\cdot\mathscr{G}\right)(\mathrm{i}\omega_n),$$

we obtain a corresponding equation with generalized matrix-product for the imaginary-time-version of the propagators, namely

$$\mathscr{G}(\tau,\tau') = \mathscr{G}_0(\tau,\tau') + \left(\mathscr{G}_0\cdot\Sigma\cdot\mathscr{G}\right)(\tau,\tau'). \tag{29.124}$$

Proof 29.107 We perform the straight-forward calculation

$$\begin{aligned}
\mathscr{G}(\tau,\tau') &= \frac{1}{\hbar\beta}\sum_{\omega_n\in\Omega_\zeta}\left(\mathscr{G}_0(\mathrm{i}\omega_n) + \mathscr{G}_0(\mathrm{i}\omega_n)\Sigma(\mathrm{i}\omega_n)\mathscr{G}(\mathrm{i}\omega_n)\right)\mathrm{e}^{-\mathrm{i}\omega_n(\tau-\tau')} \\
&= \mathscr{G}_0(\tau,\tau') + \frac{1}{\hbar\beta}\sum_{\omega_n\in\Omega_\zeta}\int_0^{+\hbar\beta}\mathrm{d}\tau_1\mathscr{G}_0(\tau_1)\,\mathrm{e}^{\mathrm{i}\omega_n\tau_1}\Sigma(\mathrm{i}\omega_n)\int_0^{+\hbar\beta}\mathrm{d}\tau_3\mathscr{G}(\tau_3)\,\mathrm{e}^{\mathrm{i}\omega_n\tau_3}\,\mathrm{e}^{-\mathrm{i}\omega_n(\tau-\tau')} \\
&= \mathscr{G}_0(\tau,\tau') + \frac{1}{\hbar\beta}\sum_{\omega_n\in\Omega_\zeta}\int_\tau^{\tau+\hbar\beta}\mathrm{d}\tilde{\tau}_1\mathscr{G}_0(\tau-\tilde{\tau}_1)\,\mathrm{e}^{\mathrm{i}\omega_n(\tau-\tilde{\tau}_1)}\Sigma(\mathrm{i}\omega_n)\int_0^{+\hbar\beta}\mathrm{d}\tau_3\mathscr{G}(\tau_3)\,\mathrm{e}^{\mathrm{i}\omega_n(\tau_3-\tau+\tau')} = \ldots
\end{aligned}$$

whereas we used the substitution $\tau_1 = \tau - \tilde{\tau}_1$ in the last step. We now use the substitution $\tau_3 = \tilde{\tau}_3 - \tau'$ for the second integral and subsequently Waste-Folder 1, UL, topic 4 which yields

$$\begin{aligned}
\ldots &= \mathscr{G}_0(\tau,\tau') + \frac{1}{\hbar\beta}\sum_{\omega_n\in\Omega_\zeta}\int_\tau^{\tau+\hbar\beta}\mathrm{d}\tilde{\tau}_1\mathscr{G}_0(\tau-\tilde{\tau}_1)\,\mathrm{e}^{\mathrm{i}\omega_n(\tau-\tilde{\tau}_1)}\Sigma(\mathrm{i}\omega_n)\int_{\tau'}^{+\hbar\beta+\tau'}\mathrm{d}\tilde{\tau}_3\mathscr{G}(\tilde{\tau}_3-\tau')\,\mathrm{e}^{\mathrm{i}\omega_n(\tilde{\tau}_3-\tau'-\tau+\tau')} \\
&= \mathscr{G}_0(\tau,\tau') + \int_0^{+\hbar\beta}\mathrm{d}\tilde{\tau}_1\mathscr{G}_0(\tau-\tilde{\tau}_1)\,\frac{1}{\hbar\beta}\sum_{\omega_n\in\Omega_\zeta}\Sigma(\mathrm{i}\omega_n)\mathrm{e}^{-\mathrm{i}\omega_n(\tilde{\tau}_1-\tilde{\tau}_3)}\int_0^{+\hbar\beta}\mathrm{d}\tilde{\tau}_3\mathscr{G}(\tilde{\tau}_3-\tau') \\
&\equiv \mathscr{G}_0(\tau,\tau') + \int_0^{+\hbar\beta}\int_0^{+\hbar\beta}\mathrm{d}\tau_1\mathrm{d}\tau_2\mathscr{G}_0(\tau,\tau_1)\,\Sigma(\tau_1,\tau_2)\mathscr{G}(\tau_2,\tau')
\end{aligned}$$

29.10. The ("Holy") Trinity of Electronic Basis Sets in Materials Theory

Fact 29.108 There are three different levels of description for electrons in materials, which are all related to each other by a mere basis-change:

- *The Continuum-basis* (cf. TBReferenced[12])
- *"The" Bloch-basis* (cf. TBReferenced[13])
- *"The" Wannier-basis* (cf. TBReferenced[14])

29.10.1. Continuum-Basis

TBD

29.10.2. Bloch-Basis

TBD

29.10.3. Wannier-Basis

TBD

[12] Chapter about position eigenstates
[13] LDA-approximation, EPW-system, chapter about thermal QFT
[14] Cf. comment in the Green-function identities and the specifications for real materials

29.11. The Pedestrian Way to Compute Spin-$\frac{1}{2}$-Green-Functions

Corollary 29.109 It follows for the time-evolution

$$
\begin{aligned}
c_\uparrow(t) &= \cos\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\xi_\uparrow t/\hbar}c_{\uparrow_n} + \sin\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\xi_\downarrow t/\hbar}c_{\downarrow_n}\\
c_\downarrow(t) &= \sin\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\phi}\mathrm{e}^{-\mathrm{i}\xi_\uparrow t/\hbar}c_{\uparrow_n} - \cos\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\phi}\mathrm{e}^{-\mathrm{i}\xi_\downarrow t/\hbar}c_{\downarrow_n}\\
c_\uparrow^\dagger(t) &= \cos\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\xi_\uparrow t/\hbar}c_{\uparrow_n}^\dagger + \sin\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\xi_\downarrow t/\hbar}c_{\downarrow_n}^\dagger\\
c_\downarrow^\dagger(t) &= \sin\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\phi}\mathrm{e}^{\mathrm{i}\xi_\uparrow t/\hbar}c_{\uparrow_n}^\dagger - \cos\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\phi}\mathrm{e}^{\mathrm{i}\xi_\downarrow t/\hbar}c_{\downarrow_n}^\dagger
\end{aligned}
$$

Proof 29.109 See Appendix, Proofs, page 469.

Proof 29.109 of Corollary 29.109 Follows by straightforward application fo the time-evolution operator and Remark 12.16.4.

Lemma 29.110 It holds

$$
\begin{aligned}
\langle c_{\uparrow_n}^\dagger c_{\uparrow_n}\rangle &= \frac{\mathrm{e}^{-\beta\xi_\uparrow} + \mathrm{e}^{2\mu\beta}}{1 + \mathrm{e}^{-\beta\xi_\uparrow} + \mathrm{e}^{-\beta\xi_\downarrow} + \mathrm{e}^{2\mu\beta}}, \quad \langle c_{\uparrow_n} c_{\uparrow_n}^\dagger\rangle = 1 - \langle c_{\uparrow_n}^\dagger c_{\uparrow_n}\rangle,\\
\langle c_{\downarrow_n}^\dagger c_{\downarrow_n}\rangle &= \frac{\mathrm{e}^{-\beta\xi_\downarrow} + \mathrm{e}^{2\mu\beta}}{1 + \mathrm{e}^{-\beta\xi_\uparrow} + \mathrm{e}^{-\beta\xi_\downarrow} + \mathrm{e}^{2\mu\beta}}, \quad \langle c_{\downarrow_n} c_{\downarrow_n}^\dagger\rangle = 1 - \langle c_{\downarrow_n}^\dagger c_{\downarrow_n}\rangle,\\
\langle c_{\uparrow_n}^\dagger c_{\downarrow_n}\rangle &= 0, \qquad \langle c_{\downarrow_n} c_{\uparrow_n}^\dagger\rangle = 0,\\
\langle c_{\downarrow_n}^\dagger c_{\uparrow_n}\rangle &= 0, \qquad \langle c_{\uparrow_n} c_{\downarrow_n}^\dagger\rangle = 0.
\end{aligned}
$$

Proof 29.110 See Appendix, Proofs, page 469.

Proof 29.110 of Lemma 29.110. We compute

$$
\langle c_{\uparrow_n}^\dagger c_{\uparrow_n}\rangle = \frac{1}{Z}\sum_{\psi\in\mathbb{B}}\langle\psi|\mathrm{e}^{-\beta(H-\mu N)}c_{\uparrow_n}^\dagger c_{\uparrow_n}|\psi\rangle = \frac{\mathrm{e}^{-\beta(E_\uparrow-\mu)} + \mathrm{e}^{-\beta(-2\mu)}}{1 + \mathrm{e}^{-\beta(E_\uparrow-\mu)} + \mathrm{e}^{-\beta(E_\downarrow-\mu)} + \mathrm{e}^{2\beta\mu}}
$$

$$
\langle c_{\downarrow_n}^\dagger c_{\downarrow_n}\rangle = \frac{1}{Z}\sum_{\psi\in\mathbb{B}}\langle\psi|\mathrm{e}^{-\beta(H-\mu N)}c_{\downarrow_n}^\dagger c_{\downarrow_n}|\psi\rangle = \frac{\mathrm{e}^{-\beta(E_\downarrow-\mu)} + \mathrm{e}^{-\beta(-2\mu)}}{1 + \mathrm{e}^{-\beta(E_\uparrow-\mu)} + \mathrm{e}^{-\beta(E_\downarrow-\mu)} + \mathrm{e}^{2\beta\mu}}
$$

$$\langle c^\dagger_{\uparrow_n} c_{\downarrow_n}\rangle = \langle c^\dagger_{\downarrow_n} c_{\uparrow_n}\rangle = 0$$

and the other identities follow from the CCR.

Remark 29.110.1 Notice that the expectation values in Lemma 12.17 can be rewritten as Fermi-functions in the usual way. Assuming that $E_\uparrow + E_\downarrow = 0$, we have

$$\xi_\uparrow + \xi_\downarrow = (E_\uparrow - \mu) + (E_\downarrow - \mu) = -2\mu,$$

and therefore

$$e^{2\beta\mu} = e^{-\beta(\xi_\uparrow + \xi_\downarrow)} = e^{-\beta\xi_\uparrow} e^{-\beta\xi_\downarrow}.$$

Consequently,

$$\langle c^\dagger_{\uparrow_n} c_{\uparrow_n}\rangle = \frac{e^{-\beta\xi_\uparrow} + e^{2\beta\mu}}{1 + e^{-\beta\xi_\uparrow} + e^{-\beta\xi_\downarrow} + e^{2\beta\mu}} = \frac{e^{-\beta\xi_\uparrow}\left(1 + e^{-\beta\xi_\downarrow}\right)}{\left(1 + e^{-\beta\xi_\uparrow}\right)\left(1 + e^{-\beta\xi_\downarrow}\right)} = \frac{e^{-\beta\xi_\uparrow}}{1 + e^{-\beta\xi_\uparrow}} = \frac{1}{e^{\beta\xi_\uparrow} + 1} = \mathrm{F}_\beta(\xi_\uparrow).$$

Similarly,

$$\langle c^\dagger_{\downarrow_n} c_{\downarrow_n}\rangle = \frac{1}{e^{\beta\xi_\downarrow} + 1}.$$

Thus, the occupation-number expectation values are precisely the Fermi-functions

$$\langle d^\dagger_\sigma d_\sigma\rangle = f_\beta(\xi_\sigma) = \frac{1}{e^{\beta\xi_\sigma} + 1}, \qquad \sigma \in \{\uparrow, \downarrow\}.$$

Lemma 29.111 It follows

$$\begin{aligned}
G^<_{\uparrow\uparrow}(t) &= \frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}\xi_\uparrow t/\hbar}\cos^2\frac{\theta}{2}\langle c^\dagger_{\uparrow_n} c_{\uparrow_n}\rangle &&+ \frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}\xi_\downarrow t/\hbar}\sin^2\frac{\theta}{2}\langle c^\dagger_{\downarrow_n} c_{\downarrow_n}\rangle \\
G^<_{\uparrow\downarrow}(t) &= \frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}\xi_\uparrow t/\hbar}\frac{\sin\theta}{2}\mathrm{e}^{-\mathrm{i}\phi}\langle c^\dagger_{\uparrow_n} c_{\uparrow_n}\rangle &&- \frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}\xi_\downarrow t/\hbar}\frac{\sin\theta}{2}\mathrm{e}^{-\mathrm{i}\phi}\langle c^\dagger_{\downarrow_n} c_{\downarrow_n}\rangle \\
G^<_{\downarrow\uparrow}(t) &= \frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}\xi_\uparrow t/\hbar}\frac{\sin\theta}{2}\mathrm{e}^{\mathrm{i}\phi}\langle c^\dagger_{\uparrow_n} c_{\uparrow_n}\rangle &&- \frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}\xi_\downarrow t/\hbar}\frac{\sin\theta}{2}\mathrm{e}^{\mathrm{i}\phi}\langle c^\dagger_{\downarrow_n} c_{\downarrow_n}\rangle \\
G^<_{\downarrow\downarrow}(t) &= \frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}\xi_\uparrow t/\hbar}\sin^2\frac{\theta}{2}\langle c^\dagger_{\uparrow_n} c_{\uparrow_n}\rangle &&+ \frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}\xi_\downarrow t/\hbar}\cos^2\frac{\theta}{2}\langle c^\dagger_{\downarrow_n} c_{\downarrow_n}\rangle
\end{aligned} \tag{29.125}$$

Proof 29.111 See Appendix, Proofs, page 470.

Proof 29.111 of Lemma 29.111 We compute straightforwardly

$$
\begin{aligned}
G^<_{\uparrow\uparrow}(t) &= \frac{\mathrm{i}}{\hbar}\langle c^\dagger_\uparrow c_\uparrow(t)\rangle \\
&= \frac{\mathrm{i}}{\hbar}\left\langle \left(\cos\frac{\theta}{2}c^\dagger_{\uparrow_n} + \sin\frac{\theta}{2}c^\dagger_{\downarrow_n}\right)\left(\cos\frac{\theta}{2}c_{\uparrow_n}(t) + \sin\frac{\theta}{2}c_{\downarrow_n}(t)\right)\right\rangle \\
&= \cos^2\frac{\theta}{2}\frac{\mathrm{i}}{\hbar}\left\langle c^\dagger_{\uparrow_n}c_{\uparrow_n}(t)\right\rangle + \sin^2\frac{\theta}{2}\frac{\mathrm{i}}{\hbar}\left\langle c^\dagger_{\downarrow_n}c_{\downarrow_n}(t)\right\rangle \\
&= \frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}\xi_\uparrow t/\hbar}\cos^2\frac{\theta}{2}\left\langle c^\dagger_{\uparrow_n}c_{\uparrow_n}\right\rangle + \frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}\xi_\downarrow t/\hbar}\sin^2\frac{\theta}{2}\left\langle c^\dagger_{\downarrow_n}c_{\downarrow_n}\right\rangle
\end{aligned}
$$

proving the first identity.

$$
\begin{aligned}
G^<_{\downarrow\downarrow}(t) &= \frac{\mathrm{i}}{\hbar}\left\langle c^\dagger_\downarrow c_\downarrow(t)\right\rangle \\
&= \frac{\mathrm{i}}{\hbar}\left\langle \left(\sin\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\phi}c^\dagger_{\uparrow_n} - \cos\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\phi}c^\dagger_{\downarrow_n}\right)\left(\sin\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\phi}c_{\uparrow_n}(t) - \cos\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\phi}c_{\downarrow_n}(t)\right)\right\rangle \\
&= \frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}\xi_\uparrow t/\hbar}\sin^2\frac{\theta}{2}\left\langle c^\dagger_{\uparrow_n}c_{\uparrow_n}\right\rangle + \frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}\xi_\downarrow t/\hbar}\cos^2\frac{\theta}{2}\left\langle c^\dagger_{\downarrow_n}c_{\downarrow_n}\right\rangle
\end{aligned}
$$

Proving the fourth identity. For the other identities we obtain

$$
\begin{aligned}
G^<_{\uparrow\downarrow}(t) &= \frac{\mathrm{i}}{\hbar}\left\langle c^\dagger_\downarrow c_\uparrow(t)\right\rangle \\
&= \frac{\mathrm{i}}{\hbar}\left\langle \left(\sin\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\phi}c^\dagger_{\uparrow_n} - \cos\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\phi}c^\dagger_{\downarrow_n}\right)\left(\cos\frac{\theta}{2}c_{\uparrow_n}(t) + \sin\frac{\theta}{2}c_{\downarrow_n}(t)\right)\right\rangle \\
&= \frac{\mathrm{i}}{\hbar}\sin\frac{\theta}{2}\cos\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\phi}\left\langle c^\dagger_{\uparrow_n}c_{\uparrow_n}(t)\right\rangle - \frac{\mathrm{i}}{\hbar}\sin\frac{\theta}{2}\cos\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\phi}\left\langle c^\dagger_{\downarrow_n}c_{\downarrow_n}(t)\right\rangle
\end{aligned}
$$

proving the second identity. For the last identity we obtain

$$
\begin{aligned}
G^<_{\downarrow\uparrow}(t) &= \frac{\mathrm{i}}{\hbar}\left\langle c^\dagger_\uparrow c_\downarrow(t)\right\rangle \\
&= \frac{\mathrm{i}}{\hbar}\left\langle \left(\cos\frac{\theta}{2}c^\dagger_{\uparrow_n} + \sin\frac{\theta}{2}c^\dagger_{\downarrow_n}\right)\left(\sin\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\phi}c_{\uparrow_n}(t) - \cos\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\phi}c_{\downarrow_n}(t)\right)\right\rangle \\
&= \sin\frac{\theta}{2}\cos\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\phi}\frac{\mathrm{i}}{\hbar}\left\langle c^\dagger_{\uparrow_n}c_{\uparrow_n}(t)\right\rangle - \sin\frac{\theta}{2}\cos\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\phi}\frac{\mathrm{i}}{\hbar}\left\langle c^\dagger_{\downarrow_n}c_{\downarrow_n}(t)\right\rangle
\end{aligned}
$$

proving the last identity.

Lemma 29.112 It follows

$$
\begin{aligned}
G^>_{\uparrow\uparrow}(t) &= \frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\xi_\uparrow t/\hbar}\cos^2\frac{\theta}{2}\left(\langle c^\dagger_{\uparrow_n}c_{\uparrow_n}\rangle - 1\right) + \frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}\xi_\downarrow t/\hbar}\sin^2\frac{\theta}{2}\left(\langle c^\dagger_{\downarrow_n}c_{\downarrow_n}\rangle - 1\right) \\
G^>_{\uparrow\downarrow}(t) &= \frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}\xi_\uparrow t/\hbar}\frac{\sin\theta}{2}\mathrm{e}^{-\mathrm{i}\phi}\left(\langle c^\dagger_{\uparrow_n}c_{\uparrow_n}\rangle - 1\right) - \frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}\xi_\downarrow t/\hbar}\frac{\sin\theta}{2}\mathrm{e}^{-\mathrm{i}\phi}\left(\langle c^\dagger_{\downarrow_n}c_{\downarrow_n}\rangle - 1\right) \\
G^>_{\downarrow\uparrow}(t) &= \frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}\xi_\uparrow t/\hbar}\frac{\sin\theta}{2}\mathrm{e}^{\mathrm{i}\phi}\left(\langle c^\dagger_{\uparrow_n}c_{\uparrow_n}\rangle - 1\right) - \frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}\xi_\downarrow t/\hbar}\frac{\sin\theta}{2}\mathrm{e}^{\mathrm{i}\phi}\left(\langle c^\dagger_{\downarrow_n}c_{\downarrow_n}\rangle - 1\right) \\
G^>_{\downarrow\downarrow}(t) &= \frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}\xi_\uparrow t/\hbar}\sin^2\frac{\theta}{2}\left(\langle c^\dagger_{\uparrow_n}c_{\uparrow_n}\rangle - 1\right) + \frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}\xi_\downarrow t/\hbar}\cos^2\frac{\theta}{2}\left(\langle c^\dagger_{\downarrow_n}c_{\downarrow_n}\rangle - 1\right)
\end{aligned}
$$

Proof 29.112 See Appendix, Proofs, page 472.

Proof 29.112 of Lemma 29.112 We compute

$$\begin{aligned} G^{>}_{\uparrow\uparrow}(t) &= -\frac{\mathrm{i}}{\hbar}\langle c_{\uparrow}(t)c^{\dagger}_{\uparrow}\rangle \\ &= -\frac{\mathrm{i}}{\hbar}\langle(\cos\frac{\theta}{2}c_{\uparrow_n}(t)+\sin\frac{\theta}{2}c_{\downarrow_n}(t))(\cos\frac{\theta}{2}c^{\dagger}_{\uparrow_n}+\sin\frac{\theta}{2}c^{\dagger}_{\downarrow_n})\rangle \\ &= -\frac{\mathrm{i}}{\hbar}\cos^2\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\xi_{\uparrow}t/\hbar}\langle c_{\uparrow_n}c^{\dagger}_{\uparrow_n}\rangle - \frac{\mathrm{i}}{\hbar}\sin^2\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\xi_{\downarrow}t/\hbar}\langle c_{\downarrow_n}c^{\dagger}_{\downarrow_n}\rangle \end{aligned} \tag{29.126}$$

proving the first identity. For the second identity we find

$$\begin{aligned} G^{>}_{\downarrow\downarrow}(t) &= -\frac{\mathrm{i}}{\hbar}\langle c_{\downarrow}(t)c^{\dagger}_{\downarrow}\rangle \\ &= -\frac{\mathrm{i}}{\hbar}\left\langle\left(\sin\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\phi}c_{\uparrow_n}(t)-\cos\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\phi}c_{\downarrow_n}(t)\right)\left(\sin\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\phi}c^{\dagger}_{\uparrow_n}-\cos\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\phi}c^{\dagger}_{\downarrow_n}\right)\right\rangle \\ &= -\frac{\mathrm{i}}{\hbar}\sin^2\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\xi_{\uparrow}t/\hbar}\langle c_{\uparrow_n}c^{\dagger}_{\uparrow_n}\rangle - \frac{\mathrm{i}}{\hbar}\cos^2\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\xi_{\downarrow}t/\hbar}\langle c_{\downarrow_n}c^{\dagger}_{\downarrow_n}\rangle \end{aligned} \tag{29.127}$$

proving the fourth identity.

$$\begin{aligned} G^{>}_{\uparrow\downarrow}(t) &= -\frac{\mathrm{i}}{\hbar}\langle c_{\uparrow}(t)c^{\dagger}_{\downarrow}\rangle \\ &= -\frac{\mathrm{i}}{\hbar}\left\langle\left(\cos\frac{\theta}{2}c_{\uparrow_n}(t)+\sin\frac{\theta}{2}c_{\downarrow_n}(t)\right)\left(\sin\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\phi}c^{\dagger}_{\uparrow_n}-\cos\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\phi}c^{\dagger}_{\downarrow_n}\right)\right\rangle \\ &= -\frac{\mathrm{i}}{\hbar}\cos\frac{\theta}{2}\sin\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\phi}\mathrm{e}^{-\xi_{\uparrow}t/\hbar}\langle c_{\uparrow_n}c^{\dagger}_{\uparrow_n}\rangle + \frac{\mathrm{i}}{\hbar}\cos\frac{\theta}{2}\sin\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\phi}\mathrm{e}^{-\xi_{\downarrow}t/\hbar}\langle c_{\downarrow_n}c^{\dagger}_{\downarrow_n}\rangle \end{aligned}$$

For the last identity we find

$$\begin{aligned} G^{<}_{\downarrow\uparrow}(t) &= -\frac{\mathrm{i}}{\hbar}\langle c_{\downarrow}(t)c^{\dagger}_{\uparrow}\rangle \\ &= -\frac{\mathrm{i}}{\hbar}\left\langle\left(\sin\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\phi}c_{\uparrow_n}(t)-\cos\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\phi}c_{\downarrow_n}(t)\right)\left(\cos\frac{\theta}{2}c^{\dagger}_{\uparrow_n}+\sin\frac{\theta}{2}c^{\dagger}_{\downarrow_n}\right)\right\rangle \\ &= -\frac{\mathrm{i}}{\hbar}\sin\frac{\theta}{2}\cos\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\phi}\left(\mathrm{e}^{\mathrm{i}\xi_{\uparrow}t/\hbar}\langle c_{\uparrow_n}c^{\dagger}_{\uparrow_n}\rangle - \mathrm{e}^{\mathrm{i}\xi_{\downarrow}t/\hbar}\langle c_{\downarrow_n}c^{\dagger}_{\downarrow_n}\rangle\right) \end{aligned}$$

proving the last identity after using $\sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\theta}{2}\right)=\frac{1}{2}\sin(\theta)$.

Corollary 29.113 Recalling Lemma 12.4

$$G(t)=\theta(t)\,G^{>}(t)+\theta(-t)\,G^{<}(t) \tag{29.128}$$

we have determined the time-ordered-Green-function, although we do not want to write it down at this moment.

Proof 29.113 See Appendix, Proofs, page 473.

Proof 29.113 of Corollary ?? We compute straightforwardly ...

Corollary 29.114 Recalling another identity from Lemma 12.4, $G^{\text{ret}}(t) = \theta(t) \cdot (G^{>}(t) - G^{<}(t))$, we obtain the retarded Green-function as a function of time:

$$\begin{aligned}
G^{\text{r}}_{\uparrow\uparrow}(t) &= -\frac{\text{i}}{\hbar}\theta(t)\text{e}^{-\text{i}\xi_\uparrow t/\hbar}\cos^2\frac{\theta}{2} &&- \frac{\text{i}}{\hbar}\theta(t)\text{e}^{-\text{i}\xi_\downarrow t/\hbar}\sin^2\frac{\theta}{2} \\
G^{\text{r}}_{\uparrow\downarrow}(t) &= -\frac{\text{i}}{\hbar}\theta(t)\text{e}^{-\text{i}\xi_\uparrow t/\hbar}\frac{\sin\theta}{2}\text{e}^{-\text{i}\phi} &&+ \frac{\text{i}}{\hbar}\theta(t)\text{e}^{-\text{i}\xi_\downarrow t/\hbar}\frac{\sin\theta}{2}\text{e}^{-\text{i}\phi} \\
G^{\text{r}}_{\downarrow\uparrow}(t) &= -\frac{\text{i}}{\hbar}\theta(t)\text{e}^{-\text{i}\xi_\uparrow t/\hbar}\frac{\sin\theta}{2}\text{e}^{\text{i}\phi} &&+ \frac{\text{i}}{\hbar}\theta(t)\text{e}^{-\text{i}\xi_\downarrow t/\hbar}\frac{\sin\theta}{2}\text{e}^{\text{i}\phi} \\
G^{\text{r}}_{\downarrow\downarrow}(t) &= -\frac{\text{i}}{\hbar}\theta(t)\text{e}^{-\text{i}\xi_\uparrow t/\hbar}\sin^2\frac{\theta}{2} &&- \frac{\text{i}}{\hbar}\theta(t)\text{e}^{-\text{i}\xi_\downarrow t/\hbar}\cos^2\frac{\theta}{2}
\end{aligned}$$

Proof 29.114 Follows immediately by insertion.

Corollary 29.115 With the Fourier-transformation we obtain the retarded Green-function as a function of frequency:

$$\begin{aligned}
G^{\text{ret}}_{\uparrow\uparrow}(\omega + \text{i}\eta) &= \frac{1}{\hbar}\frac{1}{\omega + \text{i}\eta - \xi_\uparrow/\hbar}\cos^2\frac{\theta}{2} &&+ \frac{1}{\hbar}\frac{1}{\omega + \text{i}\eta - \xi_\downarrow/\hbar}\sin^2\frac{\theta}{2} \\
G^{\text{ret}}_{\uparrow\downarrow}(\omega + \text{i}\eta) &= \frac{1}{\hbar}\frac{1}{\omega + \text{i}\eta - \xi_\uparrow/\hbar}\frac{\sin\theta}{2}\text{e}^{-\text{i}\phi} &&- \frac{1}{\hbar}\frac{1}{\omega + \text{i}\eta - \xi_\downarrow/\hbar}\frac{\sin\theta}{2}\text{e}^{-\text{i}\phi} \\
G^{\text{ret}}_{\downarrow\uparrow}(\omega + \text{i}\eta) &= \frac{1}{\hbar}\frac{1}{\omega + \text{i}\eta - \xi_\uparrow/\hbar}\frac{\sin\theta}{2}\text{e}^{\text{i}\phi} &&- \frac{1}{\hbar}\frac{1}{\omega + \text{i}\eta - \xi_\downarrow/\hbar}\frac{\sin\theta}{2}\text{e}^{\text{i}\phi} \\
G^{\text{ret}}_{\downarrow\downarrow}(\omega + \text{i}\eta) &= \frac{1}{\hbar}\frac{1}{\omega + \text{i}\eta - \xi_\uparrow/\hbar}\sin^2\frac{\theta}{2} &&+ \frac{1}{\hbar}\frac{1}{\omega + \text{i}\eta - \xi_\downarrow/\hbar}\cos^2\frac{\theta}{2}
\end{aligned} \tag{29.129}$$

Proof 29.115 See Appendix, Proofs, page 527.

Proof 29.115 of Theorem 29.116 Follows immediately by insertion.

Theorem 29.116 It follows

$$G^{\text{ret}}(\omega + \text{i}\eta) = \frac{1}{\hbar}\frac{\left(\omega + \text{i}\eta - \frac{\epsilon_0 - \mu}{\hbar}\right)\sigma_0 + \left(\frac{\vec{\epsilon}_1}{\hbar}\right)\cdot\vec{\sigma}}{\left(\omega + \text{i}\eta - \frac{\epsilon_0 - \mu}{\hbar}\right)^2 - \left(\frac{\vec{\epsilon}_1}{\hbar}\right)^2} \tag{29.130}$$

Proof 29.116 See Appendix, Proofs, page 473.

Remark 29.116.1 Note that the same result can be obtained by matrix-inversion and analytic continuation, as will be elaborated below.

30. Appendix - Applications to Toy Models

30.1. The Free Electron Gas

Possible / reasonable topics:

- fermi-energy and DOS as a function of density
- Sommerfeld-approximation for the free electron-gas and comparison with experiment.
- Band-structure and reduced zone-scheme.

30.2. Superconductivity from BCS-Theory

30.2.1. BCS-Hamiltonian in First Quantization

Notation 30.1 We consider a single electron obeying the time-independent free Schroedinger-equation

$$H_0|\psi\rangle = -\hbar^2 \frac{\Delta}{2m}|\psi\rangle = E|\psi\rangle$$

subject to periodic boundary conditions in a volume $[0, L]^{d_x}/\sim$.

Lemma 30.2 With the inclusion of spin, this gives us a basis for the single-particle Hilbert-space

$$\mathrm{span}_{\mathbb{C}} \left\{\psi_{\mathbf{k}\sigma}\right\}_{\substack{\mathbf{k}\in 2\pi\mathbb{Z}^{d_x}/L \\ \sigma\in\{\downarrow,\uparrow\}}} = \mathrm{span}_{\mathbb{C}} \left\{\psi_{\mathbf{kn}\sigma}\right\}_{\substack{\mathbf{k}\in Q \\ \mathbf{n}\in\mathbb{Z}^{d_x} \\ \sigma\in\{\downarrow,\uparrow\}}} = \mathcal{H} = L^2([0, L]^{d_x}/\sim) \otimes \mathbb{C}^2. \tag{30.1}$$

Proof 30.2 See [Kaul, Fischer] and [Bulla lecture notes].

Remark 30.2.1 Notice that one has to conclude from the context "which" **k** one is referring to.

Definition 30.3 We now consider an *attractive, local BCS-toy-model-interaction potential* V, which acts as a linear operator on the two-body Hilbert-space as

$$\begin{aligned} V : \mathcal{H} \otimes \mathcal{H} &\to \mathcal{H} \otimes \mathcal{H} \\ \psi \otimes \chi &\mapsto V(\psi \otimes \chi) \end{aligned}$$

with

$$V(\psi \otimes \chi)(x, x') := -|g| \delta_{\sigma \neq \sigma'} \delta(\mathbf{r} - \mathbf{r}') \psi(x) \chi(x').$$

for all $x, x' \in [0, L]^3 \times \{\downarrow, \uparrow\}$ with $x \equiv (\mathbf{r}, \sigma)$ etc.

Remark 30.3.1 Usually one refers to V simply as *BCS-interaction*.

Remark 30.3.2 Notice that the Bra-Ket-Notation gives us the integral kernel

$$\begin{aligned} -|g| \delta_{\sigma \neq \sigma'} \delta(\mathbf{r} - \mathbf{r}') \psi(x_1) \chi(x_2) &= \left\langle x_1, x_2 \middle| V \middle| \psi, \chi \right\rangle \\ &= \sum\!\!\!\!\!\!\int_{x_3, x_4 \in [0,L]^3 \times \{\downarrow,\uparrow\}} \left\langle x_1, x_2 \middle| V \middle| x_3, x_4 \right\rangle \left\langle x_3, x_4 \middle| \psi, \chi \right\rangle \\ &= \sum\!\!\!\!\!\!\int_{x_3, x_4 \in [0,L]^3 \times \{\downarrow,\uparrow\}} \left\langle x_1, x_2 \middle| V \middle| x_3, x_4 \right\rangle \psi(x_3) \chi(x_4) \end{aligned}$$

thus one can conclude that the integral kernel reads

$$\langle x_1, x_2 | V | x_3, x_4 \rangle = -|g| \delta_{\sigma_1 \neq \sigma_2} \delta(\mathbf{r}_1 - \mathbf{r}_2) \cdot \delta_{\sigma_1, \sigma_3} \delta(\mathbf{r}_1 - \mathbf{r}_3) \delta_{\sigma_2, \sigma_4} \delta(\mathbf{r}_2 - \mathbf{r}_4) \tag{30.2}$$

Remark 30.3.3 Notice that this is a special case of a "local two-body interaction" a.k.a. "velocity independent"[1].

We will now continue the many body problem defined by the single particle Hamiltonian H_0 above, combined with the many-particle interactions V.

30.2.2. BCS-Hamiltonian in Second Quantization

Lemma 30.4 One computes the matrix-elements of the BCS-interaction w.r.t. the basis in Equation (30.1) to be

$$\langle \mathbf{k}_1 \sigma_1, \mathbf{k}_2 \sigma_2 | V | \mathbf{k}_3 \sigma_3, \mathbf{k}_4 \sigma_4 \rangle = -\frac{|g|}{L^{d_{\mathbf{x}}}} \delta_{\sigma_3 \neq \sigma_4} \delta_{\sigma_1, \sigma_3} \delta_{\sigma_2, \sigma_4} \delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3 + \mathbf{k}_4} \tag{30.3}$$

Proof 30.4 See Appendix, Proofs, page 641.

[1] Cf. MarcosMarino p. 46, Negele Orland page 10.

Theorem 30.5 Using the plane basis in Equation (30.1), one can write the Hamiltonian in second quantization as

$$H_{\mathrm{BCS}} = \sum_{\substack{\mathbf{k}\in 2\pi\mathbb{Z}^{d_{\mathbf{x}}}/L \\ \sigma\in\{\downarrow,\uparrow\}}} \epsilon(\mathbf{k}) c_\sigma^\dagger(\mathbf{k}) c_\sigma(\mathbf{k}) - \frac{g}{L^{d_{\mathbf{x}}}} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}\in 2\pi\mathbb{Z}^{d_{\mathbf{x}}}/L} c_\uparrow^\dagger(\mathbf{k}+\mathbf{q}) c_\downarrow^\dagger(-\mathbf{k}) c_\downarrow(-\mathbf{k}'+\mathbf{q}) c_\uparrow(\mathbf{k}') \tag{30.4}$$

with fermionic creation- and annihilation-operators as usual.

Proof 30.5 See Appendix, Proofs, page 642.

Remark 30.5.1 Notice that this expression is in harmony with the literature[2].

Notation 30.6 Using the basis introduced above, and notating $V \equiv L^{d_{\mathbf{x}}}$, we introduce the field-operators

$$c_\sigma(\mathbf{r}) = \frac{1}{\sqrt{L^{d_{\mathbf{x}}}}} \sum_{\mathbf{k}\in 2\pi\mathbb{Z}^{d_{\mathbf{x}}}/L} \mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{r}} c_\sigma(\mathbf{k}), \qquad c_\sigma^\dagger(\mathbf{r}) = \frac{1}{\sqrt{L^{d_{\mathbf{x}}}}} \sum_{\mathbf{k}\in 2\pi\mathbb{Z}^{d_{\mathbf{x}}}/L} \mathrm{e}^{-\mathrm{i}\mathbf{k}\mathbf{r}} c_\sigma^\dagger(\mathbf{k}) \tag{30.5}$$

Lemma 30.7 Note that these field-operators obey the commutation-relations

$$\left\{c_\sigma(\mathbf{r}),\, c_{\sigma'}^\dagger(\mathbf{r}')\right\} = \delta_{\sigma,\sigma'}\delta(\mathbf{r}-\mathbf{r}'), \qquad \left\{c_\sigma'(\mathbf{r}),\, c_{\sigma'}^\dagger(\mathbf{r}')\right\} = \left\{c_\sigma(\mathbf{r}),\, c_{\sigma'}(\mathbf{r}')\right\} = 0 \tag{30.6}$$

whereas one has to conclude from the context, whether the symbol ψ denotes the single particle wavefunction or the many particle field-operator.

Proof 30.7 See Appendix, Proofs, page 643.

Corollary 30.8 The BCS-Hamiltonian can be rewritten with the field-operators as

$$\begin{aligned} H_{\mathrm{BCS}} &= \sum\!\!\!\!\!\!\int c_\sigma^\dagger(\mathbf{r}) \left(-\hbar^2\frac{\Delta}{2m} - \mu\right) c_\sigma(\mathbf{r}) \quad - \quad g\int \mathrm{d}\mathbf{r}\, c_\uparrow^\dagger(\mathbf{r}) c_\downarrow^\dagger(\mathbf{r}) c_\downarrow(\mathbf{r}) c_\uparrow(\mathbf{r}) \\ &= \sum\!\!\!\!\!\!\int c_\sigma^\dagger(\mathbf{r}) \left(-\hbar^2\frac{\Delta}{2m} - \mu\right) c_\sigma(\mathbf{r}) \quad - \quad \frac{g}{2}\int \mathrm{d}\mathbf{r} : \left[\begin{pmatrix} c_\uparrow^\dagger & c_\downarrow^\dagger \end{pmatrix} \cdot \begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix}\right]^2 (\mathbf{r}) : \end{aligned}$$

Proof 30.8 See Appendix, Proofs, page 643.

[2] Cf. Altland pages 267, 346, Flensberg page 321, Rickayzen page 209.

30.2.3. BCS-Action in the Field Integral Formalism

Fact 30.9 The action of the system reads

$$S_{\mathrm{BCS}}[\psi,\overline{\psi}] = \sum\!\!\!\!\!\!\int_{\substack{\sigma\in\{\downarrow,\uparrow\}\\ \tau\in(0,\hbar\beta)\\ \mathbf{k}\in 2\pi\mathbb{Z}^{d_{\mathbf{x}}}/L}} \left[\overline{\psi}_\sigma(\tau,\mathbf{k})\left(\partial_\tau+\epsilon_\sigma(\mathbf{k})-\mu\right)\psi_\sigma(\tau,\mathbf{k}) - \frac{g}{L^{d_{\mathbf{x}}}}\sum\!\!\!\!\!\!\int_{\substack{\tau\in(0,\hbar\beta)\\ \mathbf{k},\mathbf{k}',\mathbf{q}\in 2\pi\mathbb{Z}^{d_{\mathbf{x}}}/L}} \left(\overline{\psi}_{\mathbf{k}+\mathbf{q}\uparrow}\overline{\psi}_{-\mathbf{k}\downarrow}\psi_{-\mathbf{k}'+\mathbf{q}\downarrow}\psi_{\mathbf{k}'\uparrow}\right)(\tau)\right]$$

Proof 30.9 See [Draft Summary].

Notation 30.10 Recalling the shorthand-notation[3] $x\equiv(\tau,\mathbf{r})$, we introduce the Fourier-transformed integration-variables as

$$\psi_\sigma(\tau,\mathbf{r}) = \frac{1}{\sqrt{\hbar\beta V}}\sum_{\substack{\omega_n\in\Omega_{-1}\\ \mathbf{k}\in 2\pi\mathbb{Z}^{d_{\mathbf{x}}}/L}} \mathrm{e}^{\mathrm{i}(\mathbf{kr}-\omega_n\tau)}\psi_\sigma(\mathrm{i}\omega_n,\mathbf{k}), \qquad \overline{\psi}_\sigma(\tau,\mathbf{r}) = \frac{1}{\sqrt{\hbar\beta V}}\sum_{\substack{\omega_n\in\Omega_{-1}\\ \mathbf{k}\in 2\pi\mathbb{Z}^{d_{\mathbf{x}}}/L}} \mathrm{e}^{-\mathrm{i}(\mathbf{kr}-\omega_n\tau)}\overline{\psi}_\sigma(\mathrm{i}\omega_n,\mathbf{k}). \tag{30.7}$$

and analogously (but with bosonic Matsubara-frequencies) later on for the auxiliary fields Δ and $\overline{\Delta}$.

Fact 30.11 The corresponding action of the real-space-representation in the functional integral formalism reads[4]

$$\begin{aligned} S_{\mathrm{BCS}}[\psi,\overline{\psi}] &= \int \mathrm{d}x\left[\sum_{\sigma\in\{\downarrow,\uparrow\}}\overline{\psi}_\sigma(\mathrm{x})\left(\partial_\tau-\hbar^2\frac{\Delta}{2m}-\mu\right)\psi_\sigma(\mathrm{x}) - g\left(\overline{\psi}_\uparrow\overline{\psi}_\downarrow\psi_\downarrow\psi_\uparrow\right)(\mathrm{x})\right] \\ &= \sum\!\!\!\!\!\!\int_{\mathrm{x},\sigma}\overline{\psi}_\sigma(\mathrm{x})\left(\partial_\tau-\hbar^2\frac{\Delta}{2m}-\mu\right)\psi_\sigma(\mathrm{x}) - g\left(\overline{\psi}_\uparrow\overline{\psi}_\downarrow\psi_\downarrow\psi_\uparrow\right)(\mathrm{x}) \end{aligned}$$

Proof 30.11 By combining the expansions in TBReferenced with Corollary TBReferenced.

Corollary 30.12 For future reference we note the representation of the action using the momentum-eigenstates

$$\begin{aligned} S_{\mathrm{BCS}}[\psi,\overline{\psi}] = &\sum_{\substack{\sigma\in\{\downarrow,\uparrow\}\\ k\in\mathrm{i}\Omega_{-1}\times 2\pi\mathbb{Z}^{d_{\mathbf{x}}}/L}}\overline{\psi}_\sigma(k)\left(-\mathrm{i}\omega_k+\epsilon_\sigma(\mathbf{k})-\mu\right)\psi_\sigma(k) \\ &-\frac{g}{\hbar\beta L^{d_{\mathbf{x}}}}\sum_{k,k',q\in\mathrm{i}\Omega_{-1}\times 2\pi\mathbb{Z}^{d_{\mathbf{x}}}/L}\overline{\psi}_\uparrow(k+q)\overline{\psi}_\downarrow(-k)\psi_\downarrow(-k'+q)\psi_\uparrow(k') \end{aligned}$$

[3] Shit... This is in conflict to earlier where this denoted space and spin-coordinate.

[4] Cf. this to Henk page 275.

Proof 30.12 See Appendix, Proofs, page 644.

Notation 30.13 We implement Graßmann-valued external sources into the partition-function as

$$Z \mapsto Z[j,\bar{j}] = \int \mathscr{D}_{-1}(\overline{\psi},\psi) \exp\left(-S_{\mathrm{BCS}} + \sum\!\!\!\!\!\!\int \bar{j}\psi + \overline{\psi} j\right) \tag{30.8}$$

30.2.4. Hubbard-Stratonovich-Transformation

Lemma 30.14 A Hubbard-Stratonovich-transformation reads

$$\begin{aligned}\exp - S_{\mathrm{int}}[\overline{\psi},\psi] &= \exp g \int \mathrm{d}\,\mathrm{x}\ \left(\overline{\psi}_\uparrow \overline{\psi}_\downarrow \psi_\downarrow \psi_\uparrow\right)(\mathrm{x}) \\ &= \int \mathscr{D}_{+1}(\Delta,\overline{\Delta}) \exp - \int \mathrm{d}\,\mathrm{x}\ \left[\frac{|\Delta|^2(\mathrm{x})}{g} - \left(\overline{\Delta}\psi_\downarrow\psi_\uparrow + \Delta\overline{\psi}_\uparrow\overline{\psi}_\downarrow\right)(\mathrm{x})\right]\end{aligned}$$

with complex integration-variables $\Delta, \overline{\Delta}$.

Proof 30.14 See Appendix, Proofs, page 644.

Fact 30.15 After decoupling the quartic contributions we obtain the following partition-function in presence of external sources

$$Z[j,\bar{j}] = \iint \mathscr{D}_{-1}(\overline{\psi},\psi)\mathscr{D}_{+1}(\Delta,\overline{\Delta}) \exp\left(-\widetilde{S}_{\mathrm{BCS}} + \sum\!\!\!\!\!\!\int \bar{j}\psi + \overline{\psi} j\right).$$

and with the new BCS-action

$$\widetilde{S}_{\mathrm{BCS}} = \sum\!\!\!\!\!\!\int_{\mathrm{x},\sigma} \overline{\psi}_\sigma(\mathrm{x})\left(\partial_\tau - \hbar^2\frac{\Delta}{2m} - \mu\right)\psi_\sigma(\mathrm{x}) + \int \mathrm{d}\,\mathrm{x}\ \left[\frac{|\Delta|^2(\mathrm{x})}{g} - \left(\overline{\Delta}\psi_\downarrow\psi_\uparrow + \Delta\overline{\psi}_\uparrow\overline{\psi}_\downarrow\right)(\mathrm{x})\right] \tag{30.9}$$

Proof 30.15 Follows by combining the previous results.

Lemma 30.16 Switching to the Fourier-representation of the action, we obtain for the individual terms

- $\sum\!\!\!\!\!\!\int_{\mathrm{x},\sigma} \overline{\psi}_\sigma(\mathrm{x})\left(\partial_\tau - \hbar^2\frac{\Delta}{2m} - \mu\right)\psi_\sigma(\mathrm{x}) = \sum_{\substack{\sigma\in\{\downarrow,\uparrow\} \\ k\in \mathrm{i}\Omega_{-1}\times 2\pi\mathbb{Z}^{d_{\mathrm{x}}}/L}} \overline{\psi}_\sigma(k)\left(-\mathrm{i}\omega_k + \epsilon_\sigma(\mathbf{k}) - \mu\right)\psi_\sigma(k)$

- $\int \mathrm{d}\,\mathrm{x}\ \frac{|\Delta|^2(\mathrm{x})}{g} = \sum_{k \in \mathrm{i}\Omega_{-1} \times 2\pi\mathbb{Z}^{d_{\mathbf{x}}}/L} \frac{|\Delta|^2(k)}{g}$
- $\int \mathrm{d}\,\mathrm{x}\ -\left(\overline{\Delta}\psi_{\downarrow}\psi_{\uparrow} + \Delta\overline{\psi}_{\uparrow}\overline{\psi}_{\downarrow}\right)(\mathrm{x}) = \frac{1}{\sqrt{\hbar\beta L^{d_{\mathbf{x}}}}} \sum_{k,k' \in \mathrm{i}\Omega_{-1} \times 2\pi\mathbb{Z}^{d_{\mathbf{x}}}/L} -\left(\overline{\Delta}(k+k')\psi_{\downarrow}(k)\psi_{\uparrow}(k') + \Delta(k+k')\overline{\psi}_{\uparrow}(k)\overline{\psi}_{\downarrow}(k')\right)$

Proof 30.16 See the path-integral-description of BCS-theory-document, pdf-page 10.

Notation 30.17 We further introduce the *Nambu-spinors*

$$\overline{\Psi}_{\mathrm{Nambu}}(\mathrm{i}\omega_n, \mathbf{k}) = \left(\overline{\psi}_{\uparrow}(\mathrm{i}\omega_n, \mathbf{k}),\quad \psi_{\downarrow}(-\mathrm{i}\omega_n, -\mathbf{k})\right), \qquad \Psi_{\mathrm{Nambu}}(\mathrm{i}\omega_n, \mathbf{k}) = \begin{pmatrix} \psi_{\uparrow}(\mathrm{i}\omega_n, \mathbf{k}) \\ \overline{\psi}_{\downarrow}(-\mathrm{i}\omega_n, -\mathbf{k}) \end{pmatrix} \tag{30.10}$$

Lemma 30.18 Changing the integration-variables[5] gives the momentum-representation of the partition-function

$$Z[j, \overline{j}] = \iint \mathscr{D}_{-1}(\overline{\psi}, \psi)\mathscr{D}_{+1}(\overline{\Delta}, \Delta) \exp -\widetilde{S}_{\mathrm{BCS}} \tag{30.11}$$

with

$$\begin{aligned}\widetilde{S}_{\mathrm{BCS}}[\Delta, \overline{\Delta}, \psi, \overline{\psi}, j, \overline{j}] = &- \sum_{\substack{\mathbf{q} \in 2\pi\mathbb{Z}^{d_{\mathbf{x}}}/L \\ \omega_m \in \Omega_{+1}}} \frac{|\Delta(\mathrm{i}\omega_m, \mathbf{q})|^2}{g} \\ &+ \sum_{\substack{\mathbf{k}', \mathbf{k}'' \in 2\pi\mathbb{Z}^{d_{\mathbf{x}}}/L \\ \omega_{n'}, \omega_{n''} \in \Omega_{-1}}} \overline{\Psi}_{\mathrm{Nambu}}(\mathrm{i}\omega_{n'}, \mathbf{k}') \left\langle \mathrm{i}\omega_{n'}, \mathbf{k}' \right| - \frac{1}{\hbar}\mathscr{G}^{-1}_{\mathrm{Gorkov}} \left| \mathrm{i}\omega_{n''}, \mathbf{k}'' \right\rangle \Psi_{\mathrm{Nambu}}(\mathrm{i}\omega_{n''}, \mathbf{k}'') \\ &- \left(\overline{j}\psi + \overline{j}\psi\right)\end{aligned}$$

and Gorkov-Green-function

$$\begin{aligned}\langle \mathrm{i}\omega_n, \mathbf{k}| - \frac{1}{\hbar}\mathscr{G}^{-1}_{\mathrm{Gorkov}} |\mathrm{i}\omega_{n'}, \mathbf{k}'\rangle = \langle \mathrm{i}\omega_n, \mathbf{k}|\mathrm{i}\omega_{n'}, \mathbf{k}'\rangle &\begin{pmatrix} -\mathrm{i}\omega_n + \left(\frac{\hbar^2 k^2}{2m} - \mu\right) & 0 \\ 0 & +\mathrm{i}\omega_n - \left(\frac{\hbar^2 k^2}{2m} - \mu\right) \end{pmatrix} \\ &+ \frac{1}{\sqrt{\hbar\beta V}} \begin{pmatrix} 0 & -\Delta_{n+n', \mathbf{k}+\mathbf{k}'} \\ \overline{\Delta}_{n+n', \mathbf{k}+\mathbf{k}'} & 0 \end{pmatrix}\end{aligned}$$

Proof 30.18 See Appendix, Proofs, page 644.

[5] The unphysical, diverging normalization-factor is irrelevant, when we determine observables later on, as it will cancel out.

Corollary 30.19 Integrating out the fermionic fields gives the partition-function

$$Z[j,\overline{j}] = \int \mathscr{D}_{+1}(\overline{\Delta},\Delta)\exp - S_{\mathrm{BCS}}[\Delta,\overline{\Delta},j,\overline{j}] \tag{30.12}$$

with

$$\begin{aligned} S_{\mathrm{BCS}}[\Delta,\overline{\Delta},j,\overline{j}] = &- \sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ \omega_m\in\Omega_{+1}}} \frac{|\Delta(\mathrm{i}\omega_m,\mathbf{q})|^2}{g} \\ &- \mathrm{Tr}\,\mathrm{Log} - \frac{1}{\hbar}\mathscr{G}^{-1}_{\mathrm{Gorkov}}[\Delta,\overline{\Delta}] \\ &\mp \left(\overline{j}_\uparrow, \quad -j_\downarrow\right)\cdot\left(-\hbar\mathscr{G}_{\mathrm{Gorkov}}[\Delta,\overline{\Delta}]\right)\cdot\begin{pmatrix} j_\uparrow \\ -\overline{j}_\downarrow\end{pmatrix} \end{aligned}$$

Proof 30.19 We first rewrite the source-terms as linear terms in the Nambu-spinor-fields as

$$\begin{aligned} \oint \overline{j}\psi + \overline{\psi}j &= \oint_x \left(\overline{j}_\uparrow\psi_\uparrow + \overline{j}_\downarrow\psi_\downarrow + \overline{\psi}_\uparrow j_\uparrow + \overline{\psi}_\downarrow j_\downarrow\right) \\ &= \sum_k \left(\left(\overline{\psi}_\uparrow, \quad \psi_\downarrow\right)\cdot\begin{pmatrix} j_\uparrow \\ -\overline{j}_\downarrow\end{pmatrix} + \left(\overline{j}_\uparrow, \quad -j_\downarrow\right)\cdot\begin{pmatrix}\psi_\uparrow \\ \overline{\psi}_\downarrow\end{pmatrix}\right) \\ &= \sum_k \left(\overline{\Psi}_{\mathrm{Nambu}}\cdot\begin{pmatrix} j_\uparrow \\ -\overline{j}_\downarrow\end{pmatrix} + \left(\overline{j}_\uparrow, \quad -j_\downarrow\right)\cdot\Psi_{\mathrm{Nambu}}\right) \end{aligned}$$

Now performing the integral in the fermionic variables with the usual identities and using $\mathrm{Log}\,\mathrm{Det}(\bullet) = \mathrm{Tr}\,\mathrm{Log}(\bullet)$ gives the desired result.

30.2.5. Spontaneous Symmetry Breaking

We now perform a mean-field-approximation and subsequently a saddle-point-approximation, and break the U(1)-symmetry by hand[6], in order to identify and determine the (superconducting-)order-parameter.

Corollary 30.20 The BCS-action is invariant under the unitary transformation

$$\Delta \mapsto \Delta \mathrm{e}^{\mathrm{i}\theta} \quad \text{with } \theta\in[0,2\pi). \tag{30.13}$$

Hypothesis 30.21 We make the ansatz for a mean-field-configuration as

[6] Cf. also Metsch 2020 Exercise Sheet 5 for the classical analogon.

$$\Delta(\mathrm{i}\omega_m, \mathbf{q}) \approx \sqrt{\hbar\beta V}\,\delta_{\mathbf{q},0}\delta_{\omega_m,0}\Delta$$
$$\overline{\Delta}(\mathrm{i}\omega_m, \mathbf{q}) \approx \sqrt{\hbar\beta V}\,\delta_{\mathbf{q},0}\delta_{\omega_m,0}\overline{\Delta}$$

Remark 30.21.1 Note that this ansatz assumes, that the mean-field-configuration of the order-parameter is dominated by a single contribution which is constant in the momenta.

Corollary 30.22 Using this ansatz and minimizing the action w.r.t. this configuration in the absence of external sources yields the gap-equation

$$\frac{1}{g} = \frac{1}{\hbar\beta L^{d_{\mathbf{x}}}} \sum_{k \in \mathrm{i}\Omega_{-1}\times 2\pi\mathbb{Z}^{d_{\mathbf{x}}}/L} \frac{1}{\omega_k^2 + \xi_{\mathbf{k}}^2 + |\Delta|^2} \tag{30.14}$$

with $\xi_k \equiv \frac{\hbar^2 k^2}{2m} - \mu$.

Proof 30.22 Varying the action w.r.t. Δ gives

$$\left(\frac{\delta}{\delta\Delta} S\right)[\Delta, \overline{\Delta}] = \frac{\overline{\Delta}}{g} \mp \mathrm{Tr}\left(\mathscr{G}\frac{\delta}{\delta\Delta}\mathscr{G}^{-1}\right) \tag{30.15}$$

The rest is algebra [TBDone and TBDigitalized].

Notation 30.23 One can expand the action w.r.t. a reference-field Δ as

$$\begin{aligned} S_{\mathrm{BCS}}[\Delta + \delta\Delta, \overline{\Delta} + \delta\overline{\Delta}] \equiv \quad & S_{\mathrm{BCS}}[\Delta, \overline{\Delta}] \\ & + \quad \sum \left(\frac{\delta}{\delta\Delta} S_{\mathrm{BCS}}[\Delta, \overline{\Delta}], \frac{\delta}{\delta\overline{\Delta}} S_{\mathrm{BCS}}[\Delta, \overline{\Delta}]\right) \cdot \begin{pmatrix} \delta\Delta \\ \delta\overline{\Delta} \end{pmatrix} \\ & + \frac{1}{2!} \sum \sum \begin{pmatrix} \delta\Delta \\ \delta\overline{\Delta} \end{pmatrix}^{\mathrm{T}} \cdot \begin{pmatrix} \frac{\delta^2}{\delta\Delta\,\delta\Delta} S_{\mathrm{BCS}}[\Delta, \overline{\Delta}] & \frac{\delta^2}{\delta\Delta\,\delta\overline{\Delta}} S_{\mathrm{BCS}}[\Delta, \overline{\Delta}] \\ \frac{\delta^2}{\delta\overline{\Delta}\,\delta\Delta} S_{\mathrm{BCS}}[\Delta, \overline{\Delta}] & \frac{\delta^2}{\delta\overline{\Delta}\,\delta\overline{\Delta}} S_{\mathrm{BCS}}[\Delta, \overline{\Delta}] \end{pmatrix} \cdot \begin{pmatrix} \delta\Delta \\ \delta\overline{\Delta} \end{pmatrix} \\ & + \mathcal{O}\left(\delta\Delta^3, \delta\Delta^2\delta\overline{\Delta}^1, \delta\Delta^1\delta\overline{\Delta}^2, \delta\overline{\Delta}^3\right). \end{aligned}$$

Expanding the action w.r.t. to one of the (infinitely many! cf. Corollary 30.20) fields that fulfills the gap-equation, the contribution that is linear in $\delta\Delta$ vanishes.

Hypothesis 30.24 We perform a saddle-point-approximation and compute the partition-function as sum over mean-field-configurations with different phases of the order parameter.

$$Z[j, \bar{j}] \approx \sum_{\theta \in [0, 2\pi)} Z_\theta[j, \bar{j}] \tag{30.16}$$

with

$$Z_\theta[j,\overline{j}] = \int \mathscr{D}(\delta\Delta,\delta\overline{\Delta})\ \exp -S_{\mathrm{BCS}}[\Delta+\delta\Delta,\overline{\Delta}+\delta\overline{\Delta},j,\overline{j}]. \tag{30.17}$$

Our hypothesis is now, that in the superconducting state, not all of these (infinitely many) summands contribute "matter", but only a single one. We therefore replace the partition-function, which contains all the information about the system, as

$$Z[j,\overline{j}] \mapsto Z_\theta[j,\overline{j}] \tag{30.18}$$

We are therefore left with the computation of a single functional integral again.

Remark 30.24.1 Note that this also implies that the expectation-values to determine the Green-functions have to be taken w.r.t. this new partition-function.

Lemma 30.25 In the mean-field-approximation we evaluate the partition-function as

$$Z_\theta[j,\overline{j}] \approx \exp -S_{\mathrm{BCS}}[\Delta,\overline{\Delta},j,\overline{j}]. \tag{30.19}$$

whereas Δ solves the gap-equation.

Proof 30.25 TBD.

Lemma 30.26 One obtains the following decomposition of the action in the one-loop-approximation. Surpressing the dependence on the external sources, this yields

$$S_{\mathrm{BCS}}[\Delta+\delta\Delta,\overline{\Delta}+\delta\overline{\Delta}] \approx S_{\mathrm{BCS}}[\Delta,\overline{\Delta}] \quad + \quad \frac{1}{2!}\oint\sum\oint\sum \begin{pmatrix}\delta\Delta\\ \delta\overline{\Delta}\end{pmatrix}^{\mathrm{T}} \cdot \begin{pmatrix} \frac{\delta^2}{\delta\Delta\,\delta\Delta}S_{\mathrm{BCS}}[\Delta,\overline{\Delta}] & \frac{\delta^2}{\delta\Delta\,\delta\overline{\Delta}}S_{\mathrm{BCS}}[\Delta,\overline{\Delta}] \\ \frac{\delta^2}{\delta\overline{\Delta}\,\delta\Delta}S_{\mathrm{BCS}}[\Delta,\overline{\Delta}] & \frac{\delta^2}{\delta\overline{\Delta}\,\delta\overline{\Delta}}S_{\mathrm{BCS}}[\Delta,\overline{\Delta}] \end{pmatrix} \cdot \begin{pmatrix}\delta\Delta\\ \delta\overline{\Delta}\end{pmatrix}.$$

Proof 30.26 The one-loop-approximation relies on the expansion Now since Δ solves the gap-equation, the first contribution vanishes. The higher orders are being neglected within the saddle-point-approximation.

Theorem 30.27 One can also compute observables beyond the one-loop-approximation. Then one expands the action w.r.t. its interaction.

30.2.6. Landaus Free Energy Model

We finally want to illustrate where the usual Landau-model for the free-energy comes from.

Notation 30.28 We write the Gorkov-Green-function as

$$\mathscr{G}^{-1}_{\text{Gorkov}} \equiv \mathscr{G}^{-1}_{\substack{0\\ \text{Gorkov}}} + V \equiv \mathscr{G}^{-1}_{\substack{0\\ \text{Gorkov}}} \left(1 + \mathscr{G}_{\substack{0\\ \text{Gorkov}}} V\right) \tag{30.20}$$

with

$$\mathscr{G}^{-1}_{\substack{0\\ \text{Gorkov}}} \equiv \mathscr{G}^{-1}_{\text{Gorkov}}[\Delta = \overline{\Delta} = 0]. \tag{30.21}$$

Lemma 30.29 It holds

$$\operatorname{Tr} \operatorname{Log} \mathscr{G}^{-1}_{\text{Gorkov}} \equiv \text{const.} \quad + \quad \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k} \operatorname{Tr} \left(\mathscr{G}_{\substack{0\\ \text{Gorkov}}} V\right)^k \tag{30.22}$$

Proof 30.29 See Appendix, Proofs, page 645.

Theorem 30.30 Expanding the expansion up to fourth order in the field Δ gives the action

$$\begin{aligned} S_{\text{BCS}}[\Delta, \overline{\Delta}, j, \bar{j}] \approx & - \sum_{\substack{\mathbf{q} \in \mathrm{Q} \\ \omega_m \in \Omega_{+1}}} \frac{|\Delta(\mathrm{i}\omega_m, \mathbf{q})|^2}{g} \\ & + TBD_1 |\Delta|^2 \\ & + TBD_2 |\Delta|^4 \\ & \mp (\bar{j}_\uparrow, \quad -j_\downarrow) \cdot \left(-\frac{1}{\hbar} \mathscr{G}_{\text{Gorkov}}[\Delta, \overline{\Delta}]\right) \cdot \begin{pmatrix} j_\uparrow \\ -\bar{j}_\downarrow \end{pmatrix} \end{aligned}$$

Proof 30.30 See Appendix, Proofs, page 645.

31. Appendix - Crystal Structure Determination with the Debye-Scherrer Method

Motivation and Overview

After this part of the notes you will understand ...

- how one determines the crystal structure of a material by evaluating so-called x-ray diffraction patterns like in Figure 31.1.

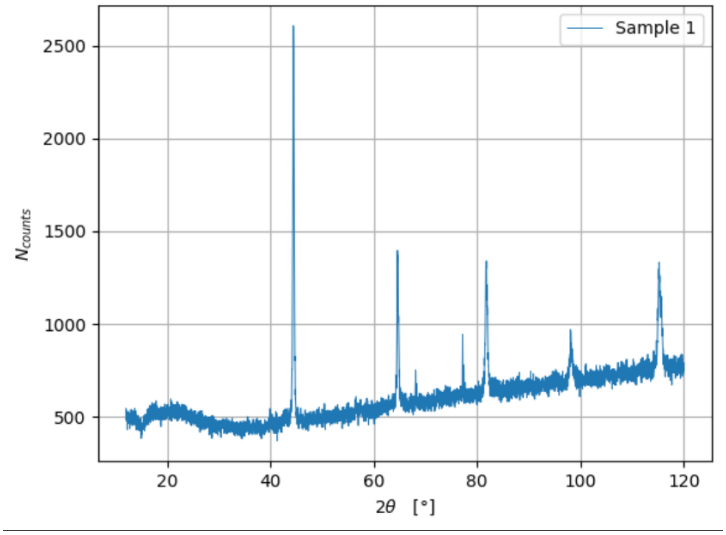


Figure 31.1.: X-Ray Diffraction Pattern of a sample that will be examined / identified in the laboratory-part of the course.

31.1. Preparation: The Miller-Indices

Notation 31.1 For the discussion of the „Miller-indices“ (to be introduced below) it is advantageous to have conventional lattice-vectors. We therefore consider a crystal with conventional lattice-vectors $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$ in this subsection.

Definition 31.2 A *lattice plane* is defined by at least three grid points that do not lie on a straight line.

Lemma 31.3 Each lattice-plane has intersection-points $\vec{S}_i \equiv m_i \mathbf{a}_i$ (whereas $m_i \in \mathbb{Q} \cup \{\infty\}$) with the axes that are asssociated to the primitive basis-vectors, whereas $\vec{S}_i \equiv \infty \cdot \vec{a}_i$ is defined for planes that never intersect an axis (i.e. are parallel to it).

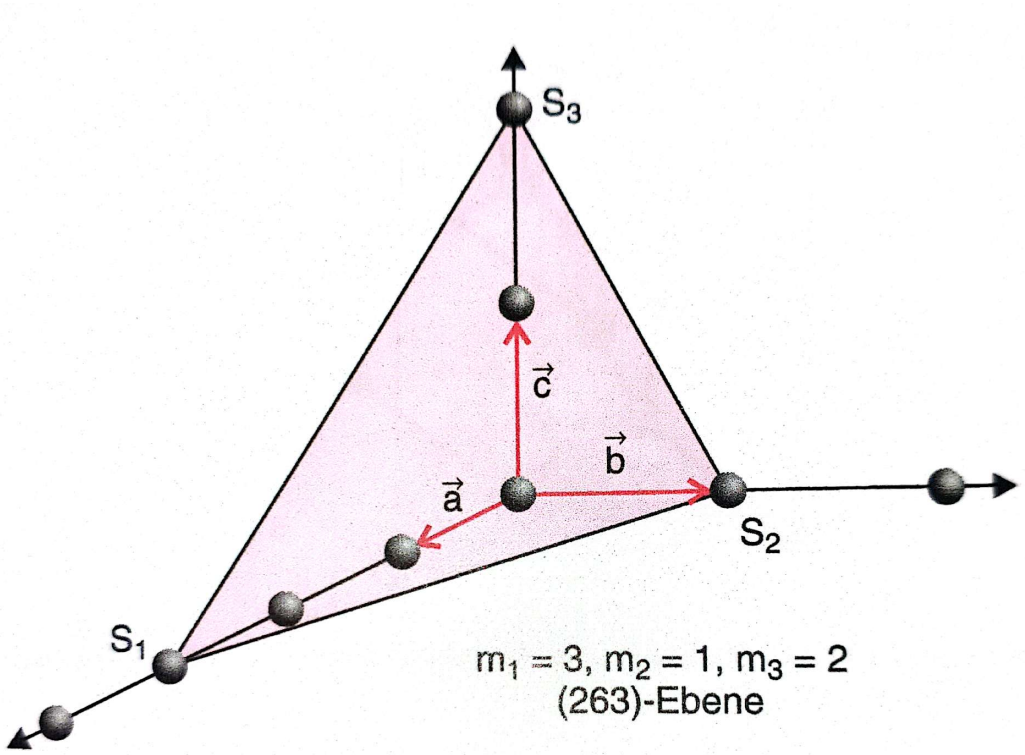


Figure 31.2.: Excerpt from Wolfang Demtröders Experimentalphysik 3.

Proof 31.3 By taking two non-identical vectors that span the plane and simultaneously represents differences between lattice-points, we can form linear combinations such that $m_i \in \mathbb{Q}$.

Definition 31.4 Let $p \in \mathbb{N}_{>0}$ denote the smallest positive natural number s.t.

$$h = \frac{p}{m_1} \qquad k = \frac{p}{m_2} \qquad l = \frac{p}{m_3} \tag{31.1}$$

are three (non-partial) integers. This triple (hkl) is called the Miller's indices associated to the lattice-plane above.

Remark 31.4.1 If one considers the lattice-plane, that has the intersection-points $\vec{S}_i \equiv nm_i\mathbf{a}_i$ with $m_i \in \mathbb{Q}$ and $n \in \mathbb{Z}$, then the number $|np|$ is the smallest integer s.t.

$$\pm h = \frac{|np|}{nm_1} \qquad \pm k = \frac{|np|}{nm_2} \qquad \pm l = \frac{|np|}{nm_3} \tag{31.2}$$

are three (non-partial) integers. We therefore see, that the tripel $\pm(hkl)$ is not in one-to-one correspondence to a single lattice-plane, but in „infinity-to-one“ correspondence to infinitely many layers of lattice-planes.

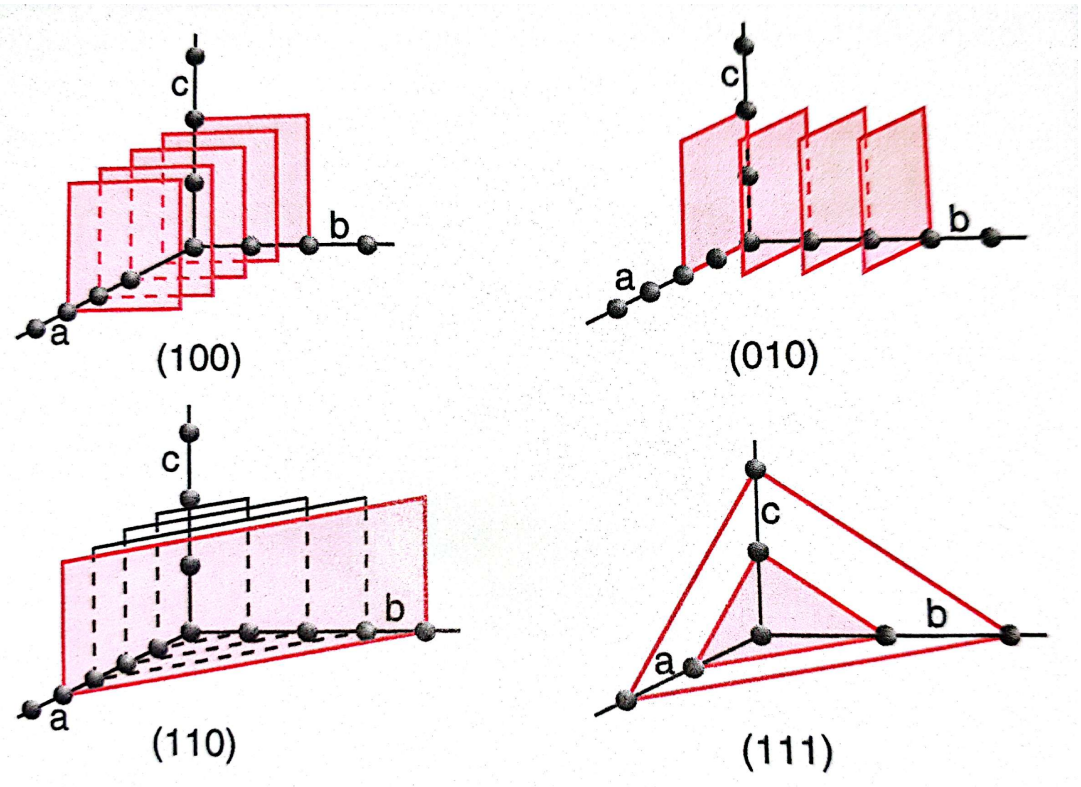


Figure 31.3.: Excerpt from Wolfang Demtröders Experimentalphysik 3.

Lemma 31.5 The reciprocal lattice-vector $\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$ is orthogonal to the planes (hkl).

Proof 31.5 See Appendix, p. 640.

Lemma 31.6 The absolute-value of $\mathbf{G}$ is inversely proportional to the distance d_{hkl} of two neighboring lattice-planes of the layers (hkl) as

$$|\mathbf{G}| = \frac{2\pi}{d_{hkl}}. \tag{31.3}$$

Proof 31.6 The vector $\mathbf{G}/|\mathbf{G}|$ has length one and is orthogonal to the plane. We consider now any lattice-point on the plane as „origin“. A vector, that points to a point in a neighboring plane is, for example, $\mathbf{v} \equiv \frac{\mathbf{a}_1}{h}$ whereas we assume without loss of generality that $h \neq 0$. The distance $d \equiv d_{hkl}$ between those two planes is then given as

$$d_{hkl} = \frac{\mathbf{G}}{G} \cdot \mathbf{v} = \frac{2\pi}{G}. \tag{31.4}$$

Corollary 31.7 For a three dimensional simple cubic lattice we obtain for the distance d_{hkl} between lattice-layers described by the tripel (hkl)

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}. \tag{31.5}$$

Proof 31.7 Follows from the orthogonality of the reciprocal lattice-vectors and the formula in the Lemma.

31.2. The Scattering-Amplitude

31.2.1. A Single Scattering-Center

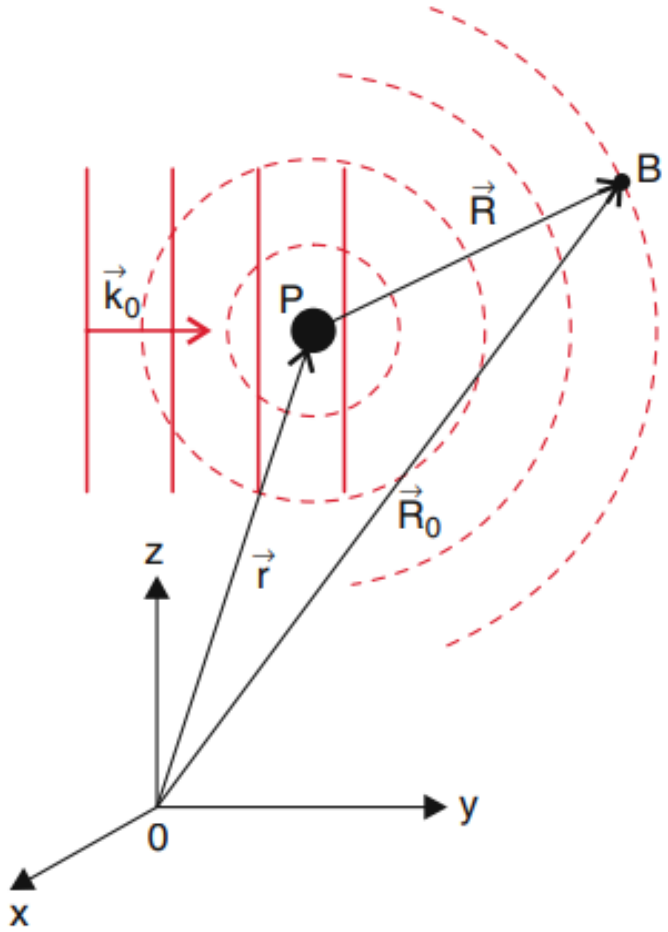


Figure 31.4.: Excerpt from Wolfang Demtröders Experimentalphysik 3.

We consider as in the figure a scattering-center (i.e. a single atom inside a crystal) at the position described by the vector $\mathbf{r}$. If a plane wave

$$\mathbf{E}(\mathbf{x}) = \mathbf{A}_e e^{i\mathbf{k}_0 \cdot \mathbf{x} - \omega t} \tag{31.6}$$

falls into this scattering-center, a fraction f of this plane-wave is being scattered as a spherical wave[1] into all directions. In an observation-point $B(\mathbf{R}_0)$ with $\mathbf{R}_0 \gg \mathbf{r}$ we have for the amplitude A_B of the scattered wave

[1] This is far from obvious. ToBeElaborated.

$$\begin{aligned} A_B &= f\frac{\mathbf{E}(\mathbf{x})}{R}\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}} \\ &= f\frac{\mathbf{A}_e}{R}\mathrm{e}^{\mathrm{i}\mathbf{k}_0\cdot\mathbf{x}-\omega t}\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}} \\ &= f\frac{\mathbf{A}_e}{R}\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}_0}\mathrm{e}^{\mathrm{i}\left(\mathbf{k}_0-\mathbf{k}\right)\cdot\mathbf{x}}\mathrm{e}^{-\mathrm{i}\omega t} \\ &= Cf\mathrm{e}^{\mathrm{i}\Delta\mathbf{k}\cdot\mathbf{x}} \end{aligned}$$

whereas we introduced the abbreviations $\Delta\mathbf{k} = \mathbf{k}_0 - \mathbf{k}$ and $C = \left(A_e/R\right)\mathrm{e}^{\mathrm{i}\left(\mathbf{k}\cdot\mathbf{R}_0-\omega t\right)}$.

31.2.2. A Crystal with a mono-atomic basis as Scattering-Centers at Lattice-Positions

In a crystal with a mono-atomic basis, we have many scattering-centers with positions $\mathrm{R}_\mathbf{n} \equiv \sum_j n_j\mathbf{a}_j$. This yields in a calculation analogous to the one above the amplitude A_B of the scattered waves

$$\begin{aligned} A_B &= Cf\sum_{\mathbf{R}_\mathbf{n}\in\mathrm{L_f}}\mathrm{e}^{\mathrm{i}\Delta\mathbf{k}\cdot\mathbf{R}_\mathbf{n}} \\ &= Cf\mathscr{F}_{\mathrm{Lattice}}(\Delta\mathbf{k}), \end{aligned}$$

whereas we introduced the so-called „lattice-factor“ $\mathscr{F}_{\mathrm{L_f}}(\Delta\mathbf{k})$. The usual way to proceed at this point is to argue that that the lattice-factor is non-zero, whenever the Laue-condition

$$\Delta\mathbf{k}\cdot\mathbf{R}_\mathbf{n} \in 2\pi\mathbb{Z} \quad\Longleftrightarrow\quad \Delta\mathbf{k} \equiv \mathbf{G}_{hkl} \in \mathrm{RL}_\infty \tag{31.7}$$

is fulfilled, and averages to zero (due to a so-called „random phase cancellation“) whenever this is not the case, which reads as a formula

$$\mathscr{F}_{\mathrm{Lattice}}(\Delta\mathbf{k}) \approx \begin{cases} N_p & \text{if } \Delta\mathbf{k} \equiv \mathbf{G}_{hkl} \in \mathrm{RL}_\infty \\ 0 & \text{otherwise (due to rpc).} \end{cases} \tag{31.8}$$

It is important to note, that this equation alone gives us nothing else but the Bragg-condition, i.e. implying that the lattice-structure does imply the existence of constructive interference. However, in the next step we will determine proper tools in order to make further conclusions about the type of the crystal-structure.

31.2.3. A Crystal with a many-atomic basis as Scattering-Centers at Crystal-Positions

In a crystal with a potentially many-atomic basis, we have many scattering-centers with positions

$$\mathrm{R}_{\mathbf{n}\kappa} \equiv \sum_j n_j\mathbf{a}_j \quad + \quad \sum_j c_{j\kappa}\mathbf{a}_j \equiv \mathbf{R}_\mathbf{n} \quad + \quad \sum_j c_{j\kappa}\mathbf{a}_j \tag{31.9}$$

with $c_{j\kappa} < 1$. This yields in a calculation analogous to the one above the amplitude A_B of the scattered waves

$$A_B = C \sum_{\mathbf{R_n} \in \mathrm{L_f}} e^{i\Delta\mathbf{k}\cdot\mathbf{R_n}} \sum_{\kappa \in \{1,\dots,r\}} f_\kappa e^{i\Delta\mathbf{k}\cdot(\sum_j c_{j\kappa}\mathbf{a}_j)}$$
$$= C\mathscr{F}_{\mathrm{Lattice}}(\Delta\mathbf{k})\mathscr{F}_{\mathrm{Atomic}}(\Delta\mathbf{k}),$$

whereas we introduced the so-called „atomic scattering-factor“ $\mathscr{F}_{\mathrm{Atomic}}(\Delta\mathbf{k})$.

31.3. The Debye-Scherrer Setup

Copy-Pasted from [Demtröder, Experimentalphysik 3] into DeepL and subsequently Copy-Pasted (and slightly adapted) into this document:

In the case of polycrystalline solids (e.g. pulverized crystalline material such as common salt, diamond powder, etc.), the microcrystals and their lattice planes are are randomly oriented (...), and the Bragg Bragg method can therefore not be used. Here is a method developed by Peter J. W. Debye (1884-1966) and Paul Scherrer (1890-1969) is useful here. The general idea is shown in Fig. 11.29. A thin tube containing the powdered sample is placed placed in the axis of a cylindrical vessel and irradiated with a monochromatic parallel X-ray beam. Only those microcrystals whose orientation is suitable to fulfill the Bragg condition contribute noticeably to the scattered radiation. This means that only at certain angles $2\theta_i$ against the direction of incidence, i.e. on cones with full aperture angles $4\theta_i$, reflected intensity is to be expected. It is measured on a film strip which is attached to the inner wall of the cylindrical container with radius RZ. On the unrolled developed film you can therefore see blackened approximated circular arcs (Fig. 11.29b), from whose radii $R_i \equiv R_C \sin(2\theta_i)$ the angles theta$_i$ and thus, for a known wavelength λ the grid plane spacing d_{hkl} can be determined.

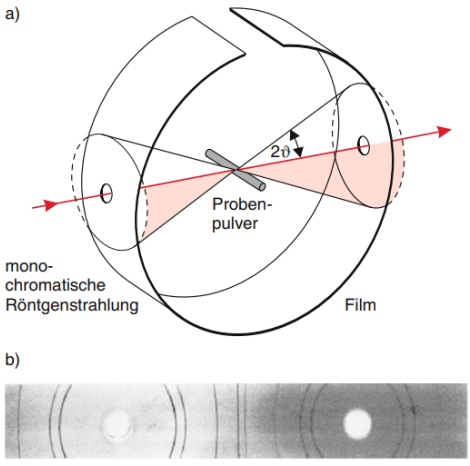


Abb. 11.29a,b. Debye-Scherrer-Verfahren: (**a**) Experimentelle Anordnung; (**b**) Aufnahme der ringförmigen Interferenzmaxima von Kupferpulver

Figure 31.5.: Excerpt from Wolfang Demtröders Experimentalphysik 3.

31.4. Cooking-Recipe to determine the Crystal-Structure from a Debye-Scherrer-Experiment

Given a diffraction pattern N_{counts} vs 2θ, we give a a cooking-recipe on how to determine the crystal-structure, whereas we restrict our attention to cubic lattices with only a single type of atom inside the crystal.

See the Lab-Sheet for the rest.

32. Appendix - Proofs for Part I

Proof 32.1 of Lemma 1.3

Inserting the one equation into the other gives

$$\begin{aligned}\xi_j &= \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \hat{\xi}_n \, \mathrm{e}^{-\mathrm{i}2\pi \frac{n}{N} j} \\ &= \frac{1}{N} \sum_{n=0}^{N-1} \sum_{m=0}^{N-1} \xi_m \, \mathrm{e}^{-\mathrm{i}2\pi \frac{n}{N} j} \, \mathrm{e}^{+\mathrm{i}2\pi \frac{m}{N} n} \\ &= \frac{1}{N} \sum_{n=0}^{N-1} \sum_{m=0}^{N-1} \xi_m \, \exp\left[2\pi \mathrm{i} \frac{1}{N} (mn - jn)\right] \\ &= \frac{1}{N} \sum_{m=0}^{N-1} \xi_m \sum_{n=0}^{N-1} \left(\exp\left[2\pi \mathrm{i} \frac{1}{N} (m-j)\right]\right)^n = \xi_j\end{aligned} \tag{32.1}$$

whereas we used in the last step the finite geometric series

$$\sum_{n=0}^{N-1} \left(\exp\left[2\pi \mathrm{i} \frac{1}{N} (m-j)\right]\right)^n = \begin{cases} N, & m = j \\ \frac{1-\mathrm{e}^{2\pi \mathrm{i}(m-j)}}{1-\mathrm{e}^{2\pi \mathrm{i} \frac{1}{N}(m-j)}} = 0, & m \neq j \end{cases}. \tag{32.2}$$

Proof 32.2 of Lemma 1.11[1]

Using the Fourier-expansion in Equation (1.5) we obtain[2]

$$\mathscr{G}_\zeta(\tau) = \frac{1}{\hbar\beta} \sum_{n=-\infty}^{+\infty} \mathscr{G}_\zeta(\mathrm{i}\omega_n) \, \mathrm{e}^{-\mathrm{i}n\pi\tau/\hbar\beta} \tag{32.3}$$

with coefficients

$$\mathscr{G}_\zeta(\mathrm{i}\omega_n) = \frac{1}{2} \int_{-\hbar\beta}^{+\hbar\beta} \mathrm{d}\tau \, \mathscr{G}_\zeta(\tau) \mathrm{e}^{\mathrm{i}n\pi\tau/\hbar\beta} \tag{32.4}$$

Bosons: $\zeta = +1$

We use that

[1] Reference: [32] p. 110 onwards.

[2] Notice that we have a different-prefactor-convention w.r.t. the equation before. This is *the* prefactor-convention for Matsubara-Green-functions.

$$-\hbar\beta < \tau < 0 \quad \Rightarrow \quad \mathscr{G}_\zeta(\tau) = \mathscr{G}_\zeta(\tau + \hbar\beta) \tag{32.5}$$

and therefore we obtain

$$\mathscr{G}_\zeta(\mathrm{i}\omega_n) = \frac{1}{2}\left[\int_0^{\hbar\beta} \mathrm{d}\tau\, \mathscr{G}_\zeta(\tau)\mathrm{e}^{\mathrm{i}n\pi\tau/\hbar\beta} + \int_{-\hbar\beta}^{0} \mathrm{d}\tau\, \mathscr{G}_\zeta(\tau)\mathrm{e}^{\mathrm{i}n\pi\tau/\hbar\beta}\right] \tag{32.6}$$

For the second term we change variables from $\tau \mapsto \tau + \hbar\beta$ which gives

$$\mathscr{G}_\zeta(\mathrm{i}\omega_n) = \frac{1}{2}\left(1 + \mathrm{e}^{\mathrm{i}n\pi}\right)\int_0^{\hbar\beta} \mathrm{d}\tau\, \mathscr{G}_\zeta(\tau)\mathrm{e}^{\mathrm{i}n\pi\tau/\hbar\beta} \tag{32.7}$$

This expression has the feature that $\mathscr{G}_\zeta(\mathrm{i}\omega_n) = 0$ whenever n is an odd integer. For bosons we hence obtain

$$\begin{aligned}
\mathscr{G}_\zeta(\tau) &= \sum_{\omega_n \in \Omega_{+1}} \mathrm{e}^{-\mathrm{i}\omega_n\tau}\mathscr{G}_\zeta(\mathrm{i}\omega_n), \\
\mathscr{G}_\zeta(\mathrm{i}\omega_n) &= \int_0^{\hbar\beta} \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\omega_n\tau}\mathscr{G}_\zeta(\tau), \\
\Omega_{+1} &= \left\{\omega_n = 2n\pi/\hbar\beta \quad | \quad n \in \mathbb{Z}\right\}.
\end{aligned}$$

Fermions: $\zeta = -1$

We use that

$$-\hbar\beta < \tau < 0 \quad \Rightarrow \quad \mathscr{G}_\zeta(\tau) = -\mathscr{G}_\zeta(\tau + \hbar\beta) \tag{32.8}$$

and therefore we obtain

$$\mathscr{G}_\zeta(\mathrm{i}\omega_n) = \frac{1}{2}\left[\int_0^{\hbar\beta} \mathrm{d}\tau\, \mathscr{G}_\zeta(\tau)\mathrm{e}^{\mathrm{i}n\pi\tau/\hbar\beta} + \int_{-\hbar\beta}^{0} \mathrm{d}\tau\, \mathscr{G}_\zeta(\tau)\mathrm{e}^{\mathrm{i}n\pi\tau/\hbar\beta}\right] \tag{32.9}$$

For the second term we obtain in the same manner

$$\mathscr{G}_\zeta(\mathrm{i}\omega_n) = \frac{1}{2}\left(1 - \mathrm{e}^{\mathrm{i}n\pi}\right)\int_0^{\hbar\beta} \mathrm{d}\tau\, \mathscr{G}_\zeta(\tau)\mathrm{e}^{\mathrm{i}n\pi\tau/\hbar\beta} \tag{32.10}$$

This expression has the feature that $\mathscr{G}_\zeta(\mathrm{i}\omega_n) = 0$ whenever n is an even integer. For fermions we hence obtain

$$\begin{aligned}
\mathscr{G}_\zeta(\tau) &= \sum_{\omega_n \in \Omega_{-1}} \mathrm{e}^{-\mathrm{i}\omega_n\tau}\mathscr{G}_\zeta(\mathrm{i}\omega_n), \\
\mathscr{G}_\zeta(\mathrm{i}\omega_n) &= \int_0^{\hbar\beta} \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\omega_n\tau}\mathscr{G}_\zeta(\tau), \\
\Omega_{+1} &= \left\{\omega_n = (2n+1)\pi/\hbar\beta \quad | \quad n \in \mathbb{Z}\right\}.
\end{aligned}$$

Proof 32.3 of Corollary 1.12

By straight-forward integration we obtain

$$\int_0^{\hbar\beta} \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\tau\omega_m} = \begin{cases} \dfrac{1}{\mathrm{i}\omega_m}\left(\mathrm{e}^{\mathrm{i}\tau\omega_m} - 1\right) & \text{for } \omega_m \neq 0 \\ \hbar\beta & \text{for } \omega_m = 0 \end{cases} \tag{32.11}$$

hence we have proven the identity.

Proof 32.4 of Lemma 1.16

We obtain in usual Dirac-notation

$$\begin{aligned} \left\langle\, \tau \,|\, \mathscr{G}_\zeta \,\right\rangle &= \mathscr{G}_\zeta(\tau) \\ &= \sum_{\omega_n \in \Omega_\zeta} \left\langle\, \tau \,|\, \mathrm{i}\omega_n \,\right\rangle \left\langle\, \mathrm{i}\omega_n \,|\, \mathscr{G}_\zeta \,\right\rangle \\ &= \frac{1}{\hbar\beta} \sum_{\omega_n \in \Omega_\zeta} \mathscr{G}_\zeta(\mathrm{i}\omega_n) \mathrm{e}^{-\mathrm{i}\omega_n\tau} \end{aligned}$$

and also

$$\begin{aligned} \left\langle\, \tau \,|\, \tau' \,\right\rangle &= \delta(\tau - \tau') \\ &= \frac{1}{\hbar\beta} \sum_{\omega_n \in \Omega_\zeta} \mathrm{e}^{-\mathrm{i}\omega_n\tau + \mathrm{i}\omega_n\tau'} \\ &= \frac{1}{\hbar\beta} \sum_{\omega_n \in \Omega_\zeta} \mathrm{e}^{\mathrm{i}\omega_n(\tau - \tau')} \end{aligned}$$

Proof 32.5 of Lemma 2.11 To prove the canonical commutation relations:

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij},$$

we start with the definitions of the position and momentum operators:

$$\hat{x}_i = x_i, \quad \hat{p}_j = -i\hbar\frac{\partial}{\partial x_j}.$$

The commutator is defined as:

$$[\hat{x}_i, \hat{p}_j] = \hat{x}_i\hat{p}_j - \hat{p}_j\hat{x}_i.$$

Applying this to a test function $f(x)$, we have:

$$[\hat{x}_i, \hat{p}_j]f(x) = x_i \left(-i\hbar \frac{\partial f}{\partial x_j}\right) - \left(-i\hbar \frac{\partial}{\partial x_j}(x_i f(x))\right).$$

Expanding the derivative $\frac{\partial}{\partial x_j}(x_i f(x))$ using the product rule:

$$\frac{\partial}{\partial x_j}(x_i f(x)) = \delta_{ij} f(x) + x_i \frac{\partial f}{\partial x_j}.$$

Substituting back, we get:

$$[\hat{x}_i, \hat{p}_j]f(x) = -i\hbar x_i \frac{\partial f}{\partial x_j} + i\hbar \left(\delta_{ij} f(x) + x_i \frac{\partial f}{\partial x_j}\right).$$

Simplifying:

$$[\hat{x}_i, \hat{p}_j]f(x) = i\hbar \delta_{ij} f(x).$$

Thus, we conclude:

$$[\hat{x}_i, \hat{p}_j] = i\hbar \delta_{ij}.$$

Proof 32.6 of Theorem 2.15 For concreteness we consider a single particle with Hamilton-function given as $H = \frac{p^2}{2m} + V(x)$. The proof can be straightfowardly generalized to many-particle systems with more complicated Hamilton-functions. Substituting the product ansatz $\psi(\mathbf{x}, t) = \psi(\mathbf{x})\phi(t)$ into the time-dependent Schrödinger equation:

$$\mathrm{i}\hbar \frac{\partial \psi(\mathbf{x}, t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla_{\mathbf{x}}^2 + V(\mathbf{x})\right)\psi(\mathbf{x}, t), \tag{32.12}$$

we obtain

$$\mathrm{i}\hbar \frac{\partial}{\partial t}\left(\psi(\mathbf{x})\phi(t)\right) = \psi(\mathbf{x})\left(-\frac{\hbar^2}{2m}\nabla_{\mathbf{x}}^2\psi(\mathbf{x}) + V(\mathbf{x})\psi(\mathbf{x})\right). \tag{32.13}$$

Using the product rule for differentiation on the left-hand side gives:

$$\mathrm{i}\hbar\psi(\mathbf{x})\frac{\mathrm{d}\phi(t)}{\mathrm{d}t} = \phi(t)\left(-\frac{\hbar^2}{2m}\nabla_{\mathbf{x}}^2\psi(\mathbf{x}) + V(\mathbf{x})\psi(\mathbf{x})\right). \tag{32.14}$$

Dividing through by $\psi(\mathbf{x})\phi(t)$, we get:

$$\mathrm{i}\hbar \frac{1}{\phi(t)}\frac{\mathrm{d}\phi(t)}{\mathrm{d}t} = \frac{-\frac{\hbar^2}{2m}\nabla_{\mathbf{x}}^2\psi(\mathbf{x}) + V(\mathbf{x})\psi(\mathbf{x})}{\psi(\mathbf{x})}. \tag{32.15}$$

The left-hand side is a function of t only, while the right-hand side is a function of $\mathbf{x}$ only. Hence, both must equal a constant, say E. This gives two separate equations:

$$\mathrm{i}\hbar \frac{1}{\phi(t)} \frac{\mathrm{d}\phi(t)}{\mathrm{d}t} = E, \tag{32.16}$$

$$-\frac{\hbar^2}{2m} \nabla_{\mathbf{x}}^2 \psi(\mathbf{x}) + V(\mathbf{x})\psi(\mathbf{x}) = E\psi(\mathbf{x}). \tag{32.17}$$

The first equation simplifies to

$$\frac{\mathrm{d}\phi(t)}{\mathrm{d}t} = -\frac{\mathrm{i}E}{\hbar}\phi(t), \tag{32.18}$$

which has the solution

$$\phi(t) = e^{-\mathrm{i}Et/\hbar}. \tag{32.19}$$

The second equation is the time-independent Schrödinger equation:

$$E\psi(\mathbf{x}) = H\psi(\mathbf{x}). \tag{32.20}$$

Thus, the theorem is proven.

Proof 32.7 of Corollary 2.16 A stationary state is defined as a quantum state for which the expectation value of any observable $\hat{O}$ is constant in time. The expectation value is given by

$$\langle \hat{O} \rangle(t) = \int \psi^*(\mathbf{x}, t) \hat{O} \psi(\mathbf{x}, t)\, d^{d_{\mathbf{x}}}. \tag{32.21}$$

Substituting $\psi(\mathbf{x}, t) = \psi(\mathbf{x})\phi(t)$ and $\phi(t) = e^{-\mathrm{i}Et/\hbar}$ gives

$$\psi^*(\mathbf{x}, t) = \psi^*(\mathbf{x}) e^{\mathrm{i}Et/\hbar}, \quad \psi(\mathbf{x}, t) = \psi(\mathbf{x}) e^{-\mathrm{i}Et/\hbar}. \tag{32.22}$$

The time-dependent factors cancel out:

$$\langle \hat{O} \rangle(t) = \int \psi^*(\mathbf{x}) \hat{O} \psi(\mathbf{x})\, d^{d_{\mathbf{x}}}. \tag{32.23}$$

Since $\psi(\mathbf{x})$ is time-independent, the expectation value $\langle \hat{O} \rangle(t)$ is constant in time. Therefore, the state is stationary, and the corollary is proven.

Proof 32.8 of Theorem 2.25 We first note the auxiliary identities

$$\frac{\mathrm{d}}{\mathrm{d}t}U(t,0) = -\frac{i}{\hbar}HU(t,0)$$
$$\frac{\mathrm{d}}{\mathrm{d}t}U(t,0)^\dagger = \frac{\mathrm{d}}{\mathrm{d}t}U(0,t) = \frac{i}{\hbar}U(0,t)H = \frac{i}{\hbar}U(t,0)^\dagger H$$

Then it follows

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}X_{\mathrm{H}}(t) &= \frac{\mathrm{d}}{\mathrm{d}t}U(t,0)^\dagger X(t)U(t,0) \\
&= \left(\frac{\mathrm{d}}{\mathrm{d}t}U(t,0)^\dagger\right)X(t)U(t,0) + U(t,0)^\dagger\left(\frac{\mathrm{d}}{\mathrm{d}t}X(t)\right)U(t,0) + U(t,0)^\dagger X(t)\left(\frac{\mathrm{d}}{\mathrm{d}t}U(t,0)\right) \\
&= \frac{i}{\hbar}U(t,0)^\dagger HX(t)U(t,0) + U(t,0)^\dagger\left(\frac{\mathrm{d}}{\mathrm{d}t}X(t)\right)U(t,0) + U(t,0)^\dagger X(t)\left(-\frac{i}{\hbar}HU(t,0)\right) \\
&= \frac{i}{\hbar}U(t,0)^\dagger\left(HX(t) - X(t)H\right)U(t,0) + U(t,0)^\dagger\left(\frac{\mathrm{d}}{\mathrm{d}t}X(t)\right)U(t,0) \\
&= \frac{i}{\hbar}U(t,0)^\dagger\left[H, X(t)\right]U(t,0) + U(t,0)^\dagger\left(\frac{\mathrm{d}}{\mathrm{d}t}X(t)\right)U(t,0) \\
&= -\frac{i}{\hbar}\left[X, H\right]_{\mathrm{H}}(t) + U(t,0)^\dagger\left(\frac{\mathrm{d}}{\mathrm{d}t}X(t)\right)U(t,0)
\end{aligned}$$

Proof 32.9 of Corollary 3.13

To be done: Needs to be updated such that the details are fine.

- Cf. the weblink for the details of the proof:

  `https://en.wikipedia.org/wiki/Fourier_series#Fourier_series_of_a_Bravais-lattice-periodi function`

- TBD: Fixing the details of the proof with the notes. Cf. Waste-Folder-1

We provide the proof for the three-dimensional case[3]. The one- and two-dimensional cases can be proven analogously.[4]

We define a new function g as,

$$g(x_1, x_2, x_3) := f\left(x_1 \frac{\mathbf{a}_1}{a_1} + x_2 \frac{\mathbf{a}_2}{a_2} + x_3 \frac{\mathbf{a}_3}{a_3}\right).$$

This new function, $g(x_1, x_2, x_3)$, is now a function of three variables, each of which has periodicity a_1, a_2, and a_3 respectively:

$$g(x_1, x_2, x_3) = g(x_1 + a_1, x_2, x_3) = g(x_1, x_2 + a_2, x_3) = g(x_1, x_2, x_3 + a_3).$$

This enables us to build up a set of Fourier coefficients, each being indexed by three independent integers m_1, m_2, m_3. If we write a series for g on the interval $[0, a_1]$ for x_1, we can define the following:

$$h^{\text{one}}(m_1, x_2, x_3) \equiv \frac{1}{a_1} \int_0^{a_1} g(x_1, x_2, x_3) \cdot e^{-i2\pi \frac{m_1}{a_1} x_1} \, dx_1.$$

And then we can write:

$$g(x_1, x_2, x_3) = \sum_{m_1=-\infty}^{\infty} h^{\text{one}}(m_1, x_2, x_3) \cdot e^{\text{i}2\pi \frac{m_1}{a_1} x_1}.$$

Further defining:

$$\begin{aligned} h^{\text{two}}(m_1, m_2, x_3) &\equiv \frac{1}{a_2} \int_0^{a_2} h^{\text{one}}(m_1, x_2, x_3) \cdot e^{-\text{i}2\pi \frac{m_2}{a_2} x_2} \, dx_2 \\ &= \frac{1}{a_2} \int_0^{a_2} dx_2 \frac{1}{a_1} \int_0^{a_1} dx_1 g(x_1, x_2, x_3) \cdot e^{-\text{i}2\pi \frac{m_1}{a_1} x_1} \cdot e^{-\text{i}2\pi \frac{m_2}{a_2} x_2} \end{aligned}$$

We can write g once again as:

$$g(x_1, x_2, x_3) = \sum_{m_1=-\infty}^{\infty} \sum_{m_2=-\infty}^{\infty} h^{\text{two}}(m_1, m_2, x_3) \cdot e^{\text{i}2\pi \frac{m_1}{a_1} x_1} \cdot e^{\text{i}2\pi \frac{m_2}{a_2} x_2}$$

[3] Cf. [85] in Waste-Folder 3.

[4] TBD: Add the proof for the one- and two-dimensional cases.

Finally, applying the same for the third coordinate, we define:

$$\begin{aligned} h^{\text{three}}(m_1,m_2,m_3) &\equiv \frac{1}{a_3}\int_0^{a_3} h^{\text{two}}(m_1,m_2,x_3)\cdot e^{-\mathrm{i}2\pi\frac{m_3}{a_3}x_3}\,dx_3 \\ &= \frac{1}{a_3}\int_0^{a_3} dx_3 \frac{1}{a_2}\int_0^{a_2} dx_2 \frac{1}{a_1}\int_0^{a_1} dx_1 g(x_1,x_2,x_3)\cdot e^{-\mathrm{i}2\pi\frac{m_1}{a_1}x_1}\cdot e^{-\mathrm{i}2\pi\frac{m_2}{a_2}x_2}\cdot e^{-\mathrm{i}2\pi\frac{m_3}{a_3}x_3} \end{aligned}$$

We write g as:

$$\begin{aligned} g(x_1,x_2,x_3) &= \sum_{m_1=-\infty}^{\infty}\sum_{m_2=-\infty}^{\infty}\sum_{m_3=-\infty}^{\infty} h^{\text{three}}(m_1,m_2,m_3)\cdot e^{\mathrm{i}2\pi\frac{m_1}{a_1}x_1}\cdot e^{\mathrm{i}2\pi\frac{m_2}{a_2}x_2}\cdot e^{\mathrm{i}2\pi\frac{m_3}{a_3}x_3}. \\ &= \sum_{m_1,m_2,m_3\in\mathbb{Z}} h^{\text{three}}(m_1,m_2,m_3)\cdot e^{i2\pi\left(\frac{m_1}{a_1}x_1+\frac{m_2}{a_2}x_2+\frac{m_3}{a_3}x_3\right)}. \end{aligned}$$

Now, every reciprocal lattice vector can be written as

$\mathbf{G} = m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3$, where m_i are integers and $\mathbf{b}_i$ are reciprocal lattice vectors to satisfy $\mathbf{b}_i\cdot\mathbf{a}_j = 2\pi\delta_{ij}$ ($\delta_{ij}=1$ for $i=j$, and $\delta_{ij}=0$ for $i\neq j$). Then for any arbitrary reciprocal lattice vector $\mathbf{G}$ and arbitrary position vector $\mathbf{r} = \left(x_1\frac{\mathbf{a}_1}{a_1} + x_2\frac{\mathbf{a}_2}{a_2} + x_3\frac{\mathbf{a}_3}{a_3}\right)$ in the original Bravais lattice space, their scalar product is:

$$\mathbf{G}\cdot\mathbf{r} = (m_1\mathbf{g}_1 + m_2\mathbf{g}_2 + m_3\mathbf{g}_3)\cdot\left(x_1\frac{\mathbf{a}_1}{a_1} + x_2\frac{\mathbf{a}_2}{a_2} + x_3\frac{\mathbf{a}_3}{a_3}\right) = 2\pi\left(x_1\frac{m_1}{a_1} + x_2\frac{m_2}{a_2} + x_3\frac{m_3}{a_3}\right).$$

So it is clear that in our expansion of $g(x_1,x_2,x_3) = f(\mathbf{r})$, the sum is actually over reciprocal lattice vectors:

$$f(\mathbf{r}) = \sum_{\mathbf{G}} h(\mathbf{G})\cdot e^{i\mathbf{G}\cdot\mathbf{r}},$$

where

$$h(\mathbf{G}) = \frac{1}{a_3}\int_0^{a_3} dx_3\,\frac{1}{a_2}\int_0^{a_2} dx_2\,\frac{1}{a_1}\int_0^{a_1} dx_1\, f\left(x_1\frac{\mathbf{a}_1}{a_1} + x_2\frac{\mathbf{a}_2}{a_2} + x_3\frac{\mathbf{a}_3}{a_3}\right)\cdot e^{-i\mathbf{G}\cdot\mathbf{r}}.$$

Assuming

$$\mathbf{r} = (x,y,z) = a_1x_1 + a_2x_2 + a_3x_3,$$

we can solve this system of three linear equations for x,y,z in terms of x_1,x_2,x_3 in order to calculate the volume element in the original Cartesian coordinate system. Once we have x,y,z in terms of x_1,x_2,x_3, we can calculate the Jacobian determinant:

$$\begin{vmatrix} \frac{\partial x_1}{\partial x} & \frac{\partial x_1}{\partial y} & \frac{\partial x_1}{\partial z} \\ \frac{\partial x_2}{\partial x} & \frac{\partial x_2}{\partial y} & \frac{\partial x_2}{\partial z} \\ \frac{\partial x_3}{\partial x} & \frac{\partial x_3}{\partial y} & \frac{\partial x_3}{\partial z} \end{vmatrix}$$

which after some calculation and applying some non-trivial cross-product identities (TBDone) can be shown to be equal to:

$$\frac{a_1 a_2 a_3}{a_1 \cdot (a_2 \times a_3)}.$$

(It may be advantageous for the sake of simplifying calculations to work in such a Cartesian coordinate system in which it just so happens that a_1 is parallel to the x-axis, a_2 lies in the xy-plane, and a_3 has components of all three axes). The denominator is exactly the volume of the primitive unit cell which is enclosed by the three primitive vectors a_1, a_2, a_3. In particular, we now know that:

$$dx_1 dx_2 dx_3 = \frac{a_1 a_2 a_3}{a_1 \cdot (a_2 \times a_3)}\, dx\, dy\, dz.$$

We can write now $\hat{h}(\mathbf{G})$ as an integral with the traditional coordinate system over the volume of the primitive cell, instead of with the x_1, x_2, x_3 variables:

$$\hat{h}(\mathbf{G}) = \frac{1}{a_1 \cdot (a_2 \times a_3)} \int_C e^{-i\mathbf{G}\cdot\mathbf{r}} f(\mathbf{r})\, d^3 r,$$

writing $d^3 r$ for the volume element $dx\, dy\, dz$; and where C is the primitive unit cell, thus, $a_1 \cdot (a_2 \times a_3)$ is the volume of the primitive unit cell.

Proof 32.10 of Theorem 4.8 We compute

$$\begin{aligned} 0 &= (H - E)\,\psi(\mathbf{r}, \boldsymbol{\tau}) \\ &= \sum_{\alpha \in \mathscr{A}} \left(H_0 + T_{\mathrm{a}} - E\right) \chi_\alpha(\boldsymbol{\tau}) \phi_{\alpha,\boldsymbol{\tau}}(\mathbf{r}) \\ &= \sum_{\alpha \in \mathscr{A}} \left(\epsilon_{\alpha,\boldsymbol{\tau}} + T_{\mathrm{a}} - E\right) \chi_\alpha(\boldsymbol{\tau}) \phi_{\alpha,\boldsymbol{\tau}}(\mathbf{r}) \\ &= \dots \end{aligned}$$

We now use the general Leibniz-rule and compute

$$\Delta_{\boldsymbol{\tau}_i}\Big[\chi_\alpha(\boldsymbol{\tau})\phi_{\alpha,\boldsymbol{\tau}}(\mathbf{r})\Big] \quad = \quad \big[\Delta_{\boldsymbol{\tau}_i}\chi_\alpha(\boldsymbol{\tau})\big]\phi_{\alpha,\boldsymbol{\tau}}(\mathbf{r}) + \big[\nabla_{\boldsymbol{\tau}_i}\chi_\alpha(\boldsymbol{\tau})\big] \cdot \big[\nabla_{\boldsymbol{\tau}_i}\phi_{\alpha,\boldsymbol{\tau}}(\mathbf{r})\big] + \chi_\alpha(\boldsymbol{\tau})\big[\Delta_{\boldsymbol{\tau}_i}\phi_{\alpha,\boldsymbol{\tau}}(\mathbf{r})\big] \tag{32.24}$$

and therefore obtain

$$\begin{aligned} \mathrm{T}_a\,\chi_\alpha(\boldsymbol{\tau})\phi_{\alpha,\boldsymbol{\tau}}(\mathbf{r}) &= \sum_{i=1}^{N_a} -\frac{\hbar^2}{2M_i}\big[\Delta_{\boldsymbol{\tau}_i}\chi_\alpha(\boldsymbol{\tau})\big]\phi_{\alpha,\boldsymbol{\tau}}(\mathbf{r}) \quad + \quad \text{remaining terms which will be neglected} \\ &\approx \sum_{i=1}^{N_a} -\frac{\hbar^2}{2M_i}\big[\Delta_{\boldsymbol{\tau}_i}\chi_\alpha(\boldsymbol{\tau})\big]\phi_{\alpha,\boldsymbol{\tau}}(\mathbf{r}) \end{aligned} \tag{32.25}$$

Inserting this in the expression above yields

$$\dots = \sum_{\alpha \in \mathscr{A}} \Big[\left(\epsilon_{\alpha,\boldsymbol{\tau}} + T_{\mathrm{a}} - E\right) \chi_\alpha(\boldsymbol{\tau})\Big]\phi_{\alpha,\boldsymbol{\tau}}(\mathbf{r}) \tag{32.26}$$

multiplying with $\phi^*_{\beta,\boldsymbol{\tau}}(\mathbf{r})$ and integrating over the electronic coordinates yields

$$\sum_{\alpha \in \mathscr{A}} \Big[\left(\epsilon_{\alpha,\boldsymbol{\tau}} + T_{\mathrm{a}} - E\right) \chi_\alpha(\boldsymbol{\tau})\Big] \int \mathrm{d}\mathbf{r}\phi^*_{\beta,\boldsymbol{\tau}}(\mathbf{r})\phi_{\alpha,\boldsymbol{\tau}}(\mathbf{r}) = \left(\epsilon_{\beta,\boldsymbol{\tau}} + T_{\mathrm{a}} - E\right) \chi_\beta(\boldsymbol{\tau}) = 0 \iff \left(T_{\mathrm{a}} + \epsilon_{\beta,\boldsymbol{\tau}}\right) \chi_\beta(\boldsymbol{\tau}) = E\chi_\beta(\boldsymbol{\tau}) \tag{32.27}$$

Proof 32.11 of Corollary 5.18 The kinetic energy term is straightforward from Lemma 5.17. The potential energy term is a bit more involved, since we have to use the different expansion formulae Equations (5.25) and (5.27) for the coordinates. However, by direct calculation one has

$$
\begin{aligned}
V_{\text{eff}}(\tau) &\approx \frac{1}{2} \sum_{\substack{\mathbf{R_n},\mathbf{R_{n'}}\in \mathrm{L} \\ \kappa,\kappa'\in\{1,\dots,r\} \\ \alpha,\alpha'\in\{1,2,3\}}} \Delta\tau_{\mathbf{n}\kappa\alpha} \left(\frac{\partial^2 V_{\text{eff}}}{\partial\tau_{\mathbf{n}\kappa\alpha}\partial\tau_{\mathbf{n'}\kappa'\alpha'}} \right)(\mathbf{R})\, \Delta\tau_{\mathbf{n'}\kappa'\alpha'} \\
&= \frac{1}{2} \sum_{\substack{\kappa,\kappa'\in\{1,\dots,r\} \\ \alpha,\alpha'\in\{1,2,3\}}} \sqrt{M_\kappa M_{\kappa'}} \sum_{\mathbf{R_n},\mathbf{R_{n'}}\in \mathrm{L}} \Delta\tau_{\mathbf{n}\kappa\alpha}\, D_{\kappa\alpha,\,\kappa'\alpha'}(\mathbf{R_n}-\mathbf{R_{n'}})\, \Delta\tau_{\mathbf{n'}\kappa'\alpha'} \\
&= \frac{1}{2}\frac{1}{N_p^2} \sum_{\substack{\kappa,\kappa'\in\{1,\dots,r\} \\ \alpha,\alpha'\in\{1,2,3\}}} \sqrt{M_\kappa M_{\kappa'}} \sum_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3\in \mathrm{Q}} \Delta\tau_{-\mathbf{q}_1\kappa\alpha}\, D_{\kappa\alpha,\,\kappa'\alpha'}(\mathbf{q}_2)\, \Delta\tau_{\mathbf{q}_3\kappa'\alpha'} \sum_{\mathbf{R_n},\mathbf{R_{n'}}\in \mathrm{L}} \mathrm{e}^{\mathrm{i}\mathbf{R_n}(\mathbf{q}_1-\mathbf{q}_2)}\mathrm{e}^{-\mathrm{i}\mathbf{R_{n'}}(+\mathbf{q}_3-\mathbf{q}_2)} \\
&= \frac{1}{2} \sum_{\substack{\kappa,\kappa'\in\{1,\dots,r\} \\ \alpha,\alpha'\in\{1,2,3\}}} \sqrt{M_\kappa M_{\kappa'}} \sum_{\mathbf{q}\in \mathrm{Q}} \Delta\tau_{-\mathbf{q}\kappa\alpha}\, D_{\kappa\alpha,\,\kappa'\alpha'}(\mathbf{q})\, \Delta\tau_{\mathbf{q}\kappa'\alpha'} \\
&= \frac{1}{2} \sum_{\mathbf{q}\in \mathrm{Q}} \sum_{\substack{\kappa,\kappa'\in\{1,\dots,r\} \\ \alpha,\alpha'\in\{1,2,3\}}} \Delta\tau_{-\mathbf{q}\kappa\alpha} \frac{D_{\kappa\alpha,\,\kappa'\alpha'}(\mathbf{q})}{\sqrt{M_\kappa M_{\kappa'}}^{-1}}\, \Delta\tau_{\mathbf{q}\kappa'\alpha'}
\end{aligned}
$$

proving the claim.

Proof 32.12 of Lemma 5.19 By direct calculation one obtains with the symmetry of the real-space-dynamical-matrix from Remark 5.6.1, together with the translation invariance from Theorem 5.15, through a long chain of equations

$$
\begin{aligned}
\left(D^{\mathrm{T}}(\mathbf{q})\right)_{\kappa\alpha,\kappa'\alpha'} = D_{\kappa'\alpha',\kappa\alpha}(\mathbf{q}) &= \sum_{\mathbf{R_n}\in \mathrm{L_f}} D_{\kappa'\alpha',\kappa\alpha}(\mathbf{R_n})\mathrm{e}^{+\mathrm{i}\mathbf{q}\cdot\mathbf{R_n}} = \sum_{\mathbf{R_n}\in \mathrm{L_f}} D_{\mathbf{n}\kappa'\alpha',\mathbf{0}\kappa\alpha}\mathrm{e}^{+\mathrm{i}\mathbf{q}\cdot\mathbf{R_n}} = \sum_{\mathbf{R_n}\in \mathrm{L_f}} D_{\mathbf{0}\kappa'\alpha',-\mathbf{n}\kappa\alpha}\mathrm{e}^{+\mathrm{i}\mathbf{q}\cdot\mathbf{R_n}} = \dots \\
\dots &\overset{\mathbf{R_n}\mapsto-\mathbf{R_n}}{=} \sum_{\mathbf{R_n}\in \mathrm{L_f}} D_{\mathbf{0}\kappa'\alpha',\mathbf{n}\kappa\alpha}\mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{R_n}} \overset{D\text{ symmetric}}{=} \sum_{\mathbf{R_n}\in \mathrm{L_f}} D_{\mathbf{n}\kappa\alpha,\mathbf{0}\kappa'\alpha'}\mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{R_n}} \\
&= \sum_{\mathbf{R_n}\in \mathrm{L_f}} D_{\kappa\alpha,\kappa'\alpha'}(\mathbf{R_n})\mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{R_n}} = \left(D_{\kappa\alpha,\kappa'\alpha'}(\mathbf{q})\right)^*
\end{aligned}
$$

Proof 32.13 of Lemma 5.23

$D_{\kappa\alpha,\,\kappa'\alpha'}(\mathbf{q})$ is hermitian, according to Lemma 5.19. We obtain further with Equation (5.25) and the fact that the dynamical matrix is real-valued in real-space as follows from Equation (5.2)

$$
D_{\kappa\alpha,\,\kappa'\alpha'}(\mathbf{q}) \equiv \sum_{\mathbf{R_n}\in \mathrm{L_f}} D_{\kappa\alpha,\,\kappa'\alpha'}(\mathbf{R_n})\mathrm{e}^{\mathrm{i}\mathbf{q}\mathbf{R}_n} \quad \Rightarrow \quad D_{\kappa\alpha,\,\kappa'\alpha'}(-\mathbf{q}) = D^*_{\kappa\alpha,\,\kappa'\alpha'}(\mathbf{q}) \tag{32.28}
$$

Thus we obtain for $\nu \in \{1,\dots,rd_x\}$ the equations

$$
D(\mathbf{q})e_{:\nu}(\mathbf{q}) = \omega_\nu^2(\mathbf{q})e_{:\nu}(\mathbf{q}) \quad \Longleftrightarrow \quad D(-\mathbf{q})e^*_{:\nu}(\mathbf{q}) = \omega_\nu^2(\mathbf{q})e^*_{:\nu}(\mathbf{q}) \tag{32.29}
$$

which lets us conclude that the eigenvectors $\{\mathbf{e}_{:,1}(-\mathbf{q}), \mathbf{e}_{:,2}(-\mathbf{q}), \dots, \mathbf{e}_{:,rd_x}(-\mathbf{q})\}$ of $D(-\mathbf{q})$ are given by the complex conjugates of the eigenvectors of $D(\mathbf{q})$, and that $\omega_\nu^2(-\mathbf{q}) = \omega_\nu^2(\mathbf{q})$, proving the theorem.

Proof 32.14 of Lemma 5.25

- For the inverse-relation, we find with Lemma 5.22 that

$$\Delta\boldsymbol{\tau}_{\mathbf{q}\kappa\alpha} = \sum_{\nu'} e_{\kappa\alpha,\nu'}(\mathbf{q}) u_{\mathbf{q}\nu'} \frac{1}{\sqrt{M_\kappa}} \tag{32.30}$$

$$= \sum_{\kappa'\alpha'} \underbrace{\sum_{\nu'} e^*_{\kappa'\alpha',\nu'}(\mathbf{q}) e_{\kappa\alpha,\nu'}(\mathbf{q})}_{=\delta_{\kappa'\kappa}\delta_{\alpha'\alpha}} \sqrt{\frac{M_{\kappa'}}{M_\kappa}} \Delta\boldsymbol{\tau}_{\mathbf{q}\kappa'\alpha'} \tag{32.31}$$

$$= \sum_{\kappa'\alpha'} \delta_{\kappa'\kappa}\delta_{\alpha'\alpha} \sqrt{\frac{M_{\kappa'}}{M_\kappa}} \Delta\boldsymbol{\tau}_{\mathbf{q}\kappa'\alpha'} \tag{32.32}$$

$$= \Delta\boldsymbol{\tau}_{\mathbf{q}\kappa\alpha} \tag{32.33}$$

- The second auxiliary identity is evident from Remark 5.16.2.
- For the derivative-relations, we find that

$$u_{\mathbf{q}\nu} = \sum_{\kappa'\alpha'} e^*_{\kappa'\alpha',\nu}(\mathbf{q}) \sqrt{M_{\kappa'}} \Delta\boldsymbol{\tau}_{\mathbf{q}\kappa'\alpha'} \tag{32.34}$$

which implies

$$\frac{\partial}{\partial \Delta\boldsymbol{\tau}_{\mathbf{q}\kappa\alpha}} = \sum_{\nu'} \frac{\partial u_{\mathbf{q}\nu'}}{\partial \Delta\boldsymbol{\tau}_{\mathbf{q}\kappa\alpha}} \frac{\partial}{\partial u_{\mathbf{q}\nu'}} = \sum_{\nu'} e^*_{\kappa\alpha,\nu'}(\mathbf{q}) \sqrt{M_\kappa} \frac{\partial}{\partial u_{\mathbf{q}\nu'}} \tag{32.35}$$

which proves the left side of the identity. Now we come to the right side, and compute straight forwardly as well

$$\Delta\boldsymbol{\tau}_{\mathbf{q}\kappa\alpha} = \sum_{\nu'} e_{\kappa\alpha,\nu'}(\mathbf{q}) u_{\mathbf{q}\nu'} \frac{1}{\sqrt{M_\kappa}} \tag{32.36}$$

which implies

$$\frac{\partial}{\partial u_{\mathbf{q}\nu}} = \sum_{\kappa'\alpha'} \frac{\partial \Delta\boldsymbol{\tau}_{\mathbf{q}\kappa'\alpha'}}{\partial u_{\mathbf{q}\nu}} \frac{\partial}{\partial \Delta\boldsymbol{\tau}_{\mathbf{q}\kappa'\alpha'}} = \sum_{\kappa'\alpha'} e_{\kappa'\alpha',\nu}(\mathbf{q}) \frac{1}{\sqrt{M_{\kappa'}}} \frac{\partial}{\partial \Delta\boldsymbol{\tau}_{\mathbf{q}\kappa'\alpha'}} \tag{32.37}$$

- For the preservation of the CCR, we fist note that

$$\left[\tau_{\mathbf{n}\kappa\alpha}, -\mathrm{i}\hbar \frac{\partial}{\partial \tau_{\mathbf{n}'\kappa'\alpha'}}\right] = +\mathrm{i}\hbar\delta_{\mathbf{n}\mathbf{n}'}\delta_{\kappa\kappa'}\delta_{\alpha\alpha'}, \tag{32.38}$$

it follows

$$\left[u_{\mathbf{q}\nu}, -\mathrm{i}\hbar\frac{\partial}{\partial u_{\mathbf{q}'\nu'}}\right] = \frac{1}{N_p}\sum_{\substack{nn'\\ \kappa\kappa'\\ \alpha\alpha'}} e^*_{\kappa\alpha,\nu}(\mathbf{q})\sqrt{M_\kappa}\mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{R}_n}\left[\left(\tau_{n\kappa\alpha} - R_{n\kappa\alpha}\right), \quad e_{\kappa'\alpha',\nu'}(\mathbf{q}')\,\mathrm{e}^{\mathrm{i}\mathbf{q}'\mathbf{R}_{\mathbf{n}'}}\frac{1}{\sqrt{M_{\kappa'}}}\frac{\partial}{\partial\tau_{\mathbf{n}'\kappa'\alpha'}}(-\mathrm{i}\hbar)\right] \tag{32.39}$$

$$= \frac{1}{N_p}\sum_{\substack{\mathbf{n},\mathbf{n}'\\ \kappa,\kappa'\\ \alpha,\alpha'}} e^*_{\kappa\alpha,\nu}(\mathbf{q})\sqrt{\frac{M_\kappa}{M_{\kappa'}}}\mathrm{e}^{\mathrm{i}(\mathbf{q}'\mathbf{R}_{\mathbf{n}'}-\mathbf{q}\mathbf{R}_{\mathbf{n}})}\underbrace{\left[\tau_{\mathbf{n}\kappa\alpha}, \quad -\mathrm{i}\hbar\frac{\partial}{\partial\tau_{\mathbf{n}'\kappa'\alpha'}}\right]}_{=\delta_{\mathbf{n},\mathbf{n}'}\delta_{\kappa,\kappa'}\delta_{\alpha,\alpha'}\mathrm{i}\hbar} e_{\kappa'\alpha',\nu'}(\mathbf{q}') \tag{32.40}$$

$$= \frac{1}{N_p}\sum_{\substack{\mathbf{n}\\ \kappa,\alpha}} e^*_{\kappa\alpha,\nu}(\mathbf{q})\sqrt{\frac{M_\kappa}{M_{\kappa'}}}\mathrm{e}^{\mathrm{i}\mathbf{R}_n(\mathbf{q}'-\mathbf{q})}e_{\kappa\alpha,\nu'}(\mathbf{q}')\mathrm{i}\hbar \tag{32.41}$$

$$= \frac{1}{N_p}\underbrace{\sum_{\kappa\alpha} e^*_{\kappa\alpha,\nu}(\mathbf{q})e_{\kappa\alpha,\nu'}(\mathbf{q}')}_{=\delta_{\nu\nu'}}\delta_{\mathbf{q}\mathbf{q}'}\mathrm{i}\hbar \tag{32.42}$$

$$= \delta_{\nu\nu'}\delta_{\mathbf{q}\mathbf{q}'}\mathrm{i}\hbar \tag{32.43}$$

Implying

$$-\mathrm{i}\hbar\left[u_{\mathbf{q}\nu}, \frac{\partial}{\partial u_{\mathbf{q}'\nu'}}\right] = \mathrm{i}\hbar\delta_{\nu\nu'}\delta_{\mathbf{q}\mathbf{q}'} \quad \Longleftrightarrow \quad \left[u_{\mathbf{q}\nu}, \frac{\partial}{\partial u_{\mathbf{q}'\nu'}}\right] = -\delta_{\nu\nu'}\delta_{\mathbf{q}\mathbf{q}'} \tag{32.44}$$

Proof 32.15 of Lemma 5.26

- For the identity $\tau_{\mathbf{n}\kappa\alpha} = \ldots$:

  We simply have to summarize all the coordinate-changes. Those were …

$$\begin{aligned}
\tau_{\mathbf{n}\kappa\alpha} &\xrightarrow{\text{Translation}} && \Delta\tau_{\mathbf{n}\kappa\alpha} := \tau_{\mathbf{n}\kappa\alpha} - R_{\mathbf{n}\kappa\alpha} \\
&\xrightarrow{\text{Fourier}} && \Delta\tau_{\mathbf{q}\kappa\alpha} := \frac{1}{\sqrt{N_p}}\sum_{\mathbf{n}}\Delta\tau_{\mathbf{n}\kappa\alpha}\mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{R}_n} \\
&\xrightarrow{\text{Eigenmodes and rescaling}} && u_{\mathbf{q}\nu} := \sum_{\kappa\alpha} e^*_{\kappa\alpha,\nu}(\mathbf{q})\sqrt{M_\kappa}\Delta\tau_{\mathbf{q}\kappa\alpha}
\end{aligned}$$

  Now combining the equations gives

$$\tau_{\mathbf{n}\kappa\alpha} \equiv R_{\mathbf{n}\kappa\alpha} + \Delta\tau_{\mathbf{n}\kappa\alpha} \tag{32.45}$$

$$= R_{\mathbf{n}\kappa\alpha} + \frac{1}{\sqrt{N_p}} \sum_{\mathbf{q}} \underbrace{\Delta\tau_{\mathbf{q}\kappa\alpha}}_{= \sum_{\nu'} e_{\kappa\alpha,\nu'}(\mathbf{q}) u_{\mathbf{q}\nu'} \frac{1}{\sqrt{M_\kappa}}} \mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{R}_\mathbf{n}} \tag{32.46}$$

$$= R_{\mathbf{n}\kappa\alpha} + \frac{1}{\sqrt{N_p}} \sum_{\substack{\mathbf{q} \\ \nu'}} e_{\kappa\alpha,\nu'}(\mathbf{q}) \mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{R}_n} \frac{1}{\sqrt{M_\kappa}} u_{\mathbf{q}\nu'} \tag{32.47}$$

which is the left hand side of Equation (5.38). Combining equations from the other side, gives the right hand side of the equation.

- For the identity $u_{\mathbf{q}\nu} = \ldots$: Taking the individual inverses one gets the relation

$$u_{\mathbf{q}\nu} = \sum_{\kappa'\alpha'} e^*_{\kappa'\alpha',\nu}(\mathbf{q}) \sqrt{M_{\kappa'}} \Delta\boldsymbol{\tau}_{\mathbf{q}\kappa'\alpha'} \tag{32.48}$$

$$= \sum_{\substack{\kappa'\alpha' \\ \mathbf{n}}} e^*_{\kappa'\alpha',\nu}(\mathbf{q}) \sqrt{M_{\kappa'}} \mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{R}_n} \frac{1}{\sqrt{N_p}} \underbrace{\Delta\boldsymbol{\tau}_{n\kappa'\alpha'}}_{=\left(\boldsymbol{\tau}_{n\kappa'\alpha'} - \mathbf{R}_{\mathbf{n}\kappa'\alpha'}\right)} \tag{32.49}$$

$$= \frac{1}{\sqrt{N_p}} \sum_{\substack{\mathbf{R}_\mathbf{n} \in L \\ \kappa'\alpha'}} e^*_{\kappa'\alpha',\nu}(\mathbf{q}) \sqrt{M_{\kappa'}} \mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{R}_n} \left(\boldsymbol{\tau}_{n\kappa'\alpha'} - \mathbf{R}_{\mathbf{n}\kappa'\alpha'}\right) \tag{32.50}$$

We can also simply insert the equation and see that it describely corrects the inverse relation:

$$u_{\mathbf{q}\nu} = \sum_{\kappa'\alpha'} e^*_{\kappa'\alpha',\nu}(\mathbf{q}) \sqrt{M_{\kappa'}} \Delta\tau_{\mathbf{q}\kappa'\alpha'} \tag{32.51}$$

$$= \sum_{\kappa'\alpha'} e^*_{\kappa'\alpha',\nu}(\mathbf{q}) \sqrt{M_{\kappa'}} \sum_{\nu''} e_{\kappa'\alpha',\nu''}(\mathbf{q}) u_{\mathbf{q}\nu''} \frac{1}{\sqrt{M_{\kappa'}}} \tag{32.52}$$

$$= \sum_{\nu''} u_{\mathbf{q}\nu''} \sqrt{\frac{M_{\kappa'}}{M_{\kappa'}}} \underbrace{\sum_{\kappa'\alpha'} \mathrm{e}^*_{\kappa'\alpha',\nu}(\mathbf{q}) \mathrm{e}_{\kappa'\alpha',\nu''}(\mathbf{q})}_{\delta_{\nu\nu''}} \tag{32.53}$$

$$= u_{\mathbf{q}\nu} \tag{32.54}$$

- For the identity $\frac{1}{\partial\tau_{\mathbf{n}\kappa\alpha}} = \ldots$:

  Formula: If $x_i = x_i\left(x'_1, \ldots, x'_n\right)$ then

$$\frac{\partial}{\partial x'_i} = \sum_j \frac{\partial x_j}{\partial x'_i} \frac{\partial}{\partial x_j}$$

  Therefore

$$\frac{\partial}{\partial \tau_{n\kappa\alpha}} = \frac{\partial}{\partial \left(\Delta\tau_{\mathbf{n}\kappa\alpha}\right)} \underbrace{\frac{\partial \left(\Delta\tau_{\mathbf{n}\kappa\alpha}\right)}{\partial \boldsymbol{\tau}_{\mathbf{n}\kappa\alpha}}}_{=1} = \frac{\partial}{\partial \left(\Delta\tau_{\mathbf{n}\kappa\alpha}\right)} \tag{32.55}$$

$$\frac{\partial}{\partial \left(\Delta\tau_{\mathbf{n}\kappa\alpha}\right)} = \sum_{\mathbf{q}} \frac{\partial}{\partial \left(\Delta\tau_{\mathbf{q}\kappa\alpha}\right)} \underbrace{\frac{\partial \left(\Delta\tau_{\mathbf{q}\kappa\alpha}\right)}{\partial \left(\Delta\tau_{\mathbf{n}\kappa\alpha}\right)}}_{=\mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{R}_\mathbf{n}}\frac{1}{\sqrt{N_p}}} = \frac{1}{\sqrt{N_p}} \sum_{\mathbf{q}} \mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{R}_\mathbf{n}} \frac{\partial}{\partial \left(\Delta\tau_{\mathbf{q}\kappa\alpha}\right)} \tag{32.56}$$

$$\frac{\partial}{\partial \left(\Delta\tau_{\mathbf{q}\kappa\alpha}\right)} = \sum_{\nu'} \frac{\partial}{\partial u_{\mathbf{q}\nu'}} \underbrace{\frac{\partial u_{\mathbf{q}\nu'}}{\partial \left(\Delta\tau_{\mathbf{q}\kappa\alpha}\right)}}_{=\sqrt{M_\kappa} e^*_{\kappa\alpha,\nu'}(\mathbf{q})} = \sum_{\nu'} \sqrt{M_\kappa} e^*_{\kappa\alpha,\nu'}(\mathbf{q}) \frac{\partial}{\partial u_{\mathbf{q}\nu'}} \tag{32.57}$$

Combining these equations yields the desired result as

$$\frac{\partial}{\partial \tau_{n\kappa\alpha}} = \frac{\partial}{\partial \left(\Delta\tau_{n\kappa\alpha}\right)} \tag{32.58}$$

$$= \frac{1}{\sqrt{N_p}} \sum_{\mathbf{q}} \mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{R}_n} \underbrace{\frac{\partial}{\partial \left(\Delta\tau_{\mathbf{q}\kappa\alpha}\right)}}_{= \sum_{\mu} \sqrt{M_\kappa} e^*_{\kappa\alpha,\mu}(\mathbf{q}) \frac{\partial}{\partial u_{\mathbf{q}\mu}}} \tag{32.59}$$

$$= \frac{\sqrt{M_\kappa}}{\sqrt{N_p}} \sum_{\substack{\mathbf{q} \\ \mu}} \mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{R}_n} e^*_{\kappa\alpha,\mu}(\mathbf{q}) \frac{\partial}{\partial u_{\mathbf{q}\mu}} \tag{32.60}$$

- For the identity $\frac{\partial}{\partial u_{\mathbf{q}\nu}} = \ldots$:

$$\frac{\partial}{\partial u_{\mathbf{q}\nu}} = \sum_{\substack{\mathbf{R}_\mathbf{n} \in \mathrm{L_f} \\ \kappa',\alpha'}} \frac{\partial}{\partial \tau_{\mathbf{n}\kappa'\alpha'}} \underbrace{\frac{\partial \tau_{\mathbf{n}\kappa'\alpha'}}{\partial u_{\mathbf{q}\nu}}}_{= \frac{1}{\sqrt{N_p}} e^*_{\kappa'\alpha',\nu}(\mathbf{q}) \frac{1}{\sqrt{M_{\kappa'}}} \mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{R}_\mathbf{n}}} \tag{32.61}$$

$$= \frac{1}{\sqrt{N_p}} \sum_{\substack{\mathbf{R}_\mathbf{n} \in L \\ \kappa'\alpha'}} e_{\kappa'\alpha',\nu}(\mathbf{q}) \mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{R}_\mathbf{n}} \frac{1}{\sqrt{M_{\kappa'}}} \frac{\partial}{\partial \tau_{\mathbf{n}\kappa'\alpha'}} \tag{32.62}$$

Proof 32.16 of Corollary 5.27 We can the terms appearing in the kinetic and potential energy expression through their new coordinates as

$$\Delta\tau^*_{\mathbf{q}\kappa\alpha} = \sum_{\nu} e^*_{\kappa\alpha,\nu}(\mathbf{q}) u^*_{\mathbf{q}\nu} \frac{1}{\sqrt{M_\kappa}}, \qquad \Delta\tau_{\mathbf{q}\kappa'\alpha'} = \sum_{\nu} e_{\kappa'\alpha',\nu}(\mathbf{q}) u_{\mathbf{q}\nu} \frac{1}{\sqrt{M_{\kappa'}}} \tag{32.63}$$

with $u_{\mathbf{q}\nu}$ as new coordinates.

Potential Energy Term:

Inserting this into the expression for the potential energy gives

$$\frac{1}{2}\sum_{\mathbf{q}}\sum_{\substack{\kappa\kappa'\\ \alpha\alpha'}}\Delta\tau^*_{\mathbf{q}\kappa\alpha}\frac{D_{\kappa\alpha,\,\kappa'\alpha'}(\mathbf{q})}{\sqrt{M_\kappa M_{\kappa'}}^{-1}}\Delta\tau_{\mathbf{q}\kappa'\alpha'} = \frac{1}{2}\sum_{\mathbf{q}}\sum_{\substack{\kappa\kappa'\\ \alpha\alpha'\\ \nu\nu'}} e^*_{\kappa\alpha,\nu}(\mathbf{q})u^*_{\mathbf{q}\nu}D_{\kappa\alpha,\,\kappa'\alpha'}(\mathbf{q})e_{\kappa'\alpha',\nu'}(\mathbf{q})u_{\mathbf{q}\nu'} \tag{32.64}$$

$$= \dots \tag{32.65}$$

Performing the sum over $\kappa'\alpha'$ (i.e. using Equation (5.31)) gives

$$\dots = \frac{1}{2}\sum_{\mathbf{q}}\sum_{\substack{\kappa\alpha\\ \nu\nu'}} e^*_{\kappa\alpha,\nu}(\mathbf{q})u^*_{\mathbf{q}\nu}\omega^2_\nu(\mathbf{q})e_{\kappa\alpha,\nu'}(\mathbf{q})u_{\mathbf{q}\nu'} = \dots \tag{32.66}$$

Now we use Equation (5.32)

$$\sum_{\kappa\alpha} e^*_{\kappa\alpha,\nu}(\mathbf{q})e_{\kappa\alpha,\nu'}(\mathbf{q}) = \delta_{\nu,\nu'} \qquad (**) \tag{32.67}$$

such that we obtain

$$\dots = \frac{1}{2}\sum_{\mathbf{q}\nu} u^*_{\mathbf{q}\nu}\omega^2_\nu(\mathbf{q})u_{\mathbf{q}\nu} = \frac{1}{2}\sum_{\mathbf{q}\nu}\omega^2_\nu(\mathbf{q})u_{-\mathbf{q}\nu}u_{\mathbf{q}\nu} \tag{32.68}$$

Kinetic Energy Term:

Before we proceed let's pay attention to the Momentum again:

$$T_e \equiv \sum_{\substack{\mathbf{R}_\mathbf{n}\in L\\ \kappa\alpha}} -\frac{\hbar^2}{2M_\kappa}\frac{\partial^2}{\partial\tau^2_{\mathbf{n}\kappa\alpha}} \tag{32.69}$$

$$\equiv \sum_{\mathbf{n}\kappa\alpha}\frac{\partial}{\partial\tau_{\mathbf{n}\kappa\alpha}}\left(-\frac{\hbar^2}{2M_\kappa}\right)\frac{\partial}{\partial\tau_{\mathbf{n}\kappa\alpha}} \tag{32.70}$$

Then it follows

$$T_e = \sum_{n\kappa\alpha}\frac{\partial}{\partial\tau_{n\kappa\alpha}}\left(-\frac{\hbar^2}{2M_\kappa}\right)\frac{\partial}{\partial\tau_{n\kappa\alpha}} \tag{32.71}$$

With $\sum_{\kappa\alpha} \equiv \sum_{\nu}$

$$T_e = \sum_{\substack{\mathbf{q}\mathbf{q}'\\ \mu\mu'\\ n\nu}} \left(-\frac{\hbar^2}{2M_\kappa}\right)\left(\frac{M_\kappa}{N_p}\right) \mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{R}_n} e^*_{\nu\mu}(\mathbf{q}) \frac{\partial}{\partial u_{\mathbf{q}\mu}} \mathrm{e}^{-\mathrm{i}\mathbf{q}'\mathbf{R}_n} e^*_{\nu\mu'}(\mathbf{q}') \frac{\partial}{\partial u_{\mathbf{q}'\mu}} \tag{32.72}$$

$$= \sum_{\substack{\mathbf{q}\mathbf{q}'\\ \mu\mu'\\ \nu}} \underbrace{\sum_n \mathrm{e}^{-\mathrm{i}\mathbf{R}_n(\mathbf{q}+\mathbf{q}')}}_{=N_p\delta_{\mathrm{q}+\mathrm{q}',0}} \left(-\frac{\hbar^2}{2N_p}\right) e^*_{\nu\mu}(\mathbf{q}) \frac{\partial}{\partial u_{\mathbf{q}\mu}} e^*_{\nu\mu'}(\mathbf{q}') \frac{\partial}{\partial u_{\mathbf{q}'\mu}} \tag{32.73}$$

$$= \sum_{\substack{\mathbf{q}\\ \mu\mu'\\ \nu}} -\frac{\hbar^2}{2} e^*_{\nu\mu}(\mathbf{q}) \underbrace{e^*_{\nu\mu'}(-\mathbf{q})}_{=e_{\nu\mu'}(\mathbf{q})} \frac{\partial}{\partial u_{\mathbf{q}\mu}} \frac{\partial}{\partial u_{-\mathbf{q}\mu}} \tag{32.74}$$

$$= \sum_{\substack{\mathbf{q}\\ \mu\mu'}} -\frac{\hbar^2}{2} \underbrace{\sum_\nu e^*_{\nu\mu}(\mathbf{q}) e_{\nu\mu'}(\mathbf{q})}_{=\delta_{\mu\mu'}} \frac{\partial}{\partial u_{\mathbf{q}\mu}} \frac{\partial}{\partial u_{-\mathbf{q}\mu}} \tag{32.75}$$

$$= \sum_{\mathbf{q}\mu} -\frac{\hbar^2}{2} \frac{\partial}{\partial u_{\mathbf{q}\mu}} \frac{\partial}{\partial u_{-\mathbf{q}\mu}} \tag{32.76}$$

Proof 32.17 of Lemma 5.29

Proof of CCR:

$$\left[a_{\mathbf{q}\mu}, a^\dagger_{\mathbf{q}\mu}\right] = \sqrt{\frac{\omega_\mu(\mathbf{q})\,\omega_{\mu'}(\mathbf{q}')}{(2\hbar)^2}} \left(\frac{\hbar}{\omega_\mu(\mathbf{q})} \underbrace{\left[\frac{\partial}{\partial u_{-\mathbf{q}\mu}}, u_{-\mathbf{q}'\mu'}\right]}_{=\delta_{\mu\mu'}\delta_{\mathbf{q}\mathbf{q}'}} - \frac{\hbar}{\omega_{\mu'}(\mathbf{q}')} \left[u_{\mathbf{q}\mu}, \frac{\partial}{\partial u_{\mathbf{q}\mu}}\right] \right) \tag{32.77}$$

$$= \sqrt{\frac{\omega_\mu(\mathbf{q})\,\omega_{\mu'}(\mathbf{q}')}{(2\hbar)^2}} \hbar \left(\frac{\delta_{\mathbf{q}\mathbf{q}'}\delta_{\mu\mu'}}{\omega_\mu(\mathbf{q})} + \frac{\delta_{\mathbf{q}\mathbf{q}'}\delta_{\mu\mu'}}{\omega_{\mu'}(\mathbf{q}')} \right) \tag{32.78}$$

$$= \delta_{\mathbf{q}\mathbf{q}'}\delta_{\mu\mu'} \tag{32.79}$$

Proof of the inversion Formulae:

$$u_{\mathbf{q}\mu} = \left(a_{\mathbf{q}\mu} + a^\dagger_{-\mathbf{q}\mu}\right) \sqrt{\frac{\hbar}{2\omega_\mu(\mathbf{q})}} \tag{32.80}$$

Proof:

$$\left(a_{\mathbf{q}\mu} + a^{\dagger}_{-\mathbf{q}\mu}\right)\sqrt{\frac{\hbar}{2\omega_\mu(\mathbf{q})}} \tag{32.81}$$

$$= \left(\sqrt{\frac{\omega_\mu(\mathbf{q})}{2\hbar}}\left(u_{\mathbf{q}\mu} + \frac{\hbar}{\omega_\mu(\mathbf{q})}\frac{\partial}{\partial u_{-\mathbf{q}\mu}}\right) + \sqrt{\frac{\omega_\mu(-\mathbf{q})}{2\hbar}}\left(u_{\mathbf{q}\mu} - \frac{\hbar}{\omega_\mu(-\mathbf{q})}\frac{\partial}{\partial u_{-\mathbf{q}\mu}}\right)\right)\sqrt{\frac{\hbar}{2\omega_\mu(\mathbf{q})}} \tag{32.82}$$

$$\overset{\text{symmetry of }\omega_\mu}{=} \sqrt{\frac{\omega_\mu(\mathbf{q})}{2\hbar}}\left(\left(u_{\mathbf{q}\mu} + \frac{\hbar}{\omega_\mu(\mathbf{q})}\frac{\partial}{\partial u_{-\mathbf{q}\mu}}\right) + \left(u_{\mathbf{q}\mu} - \frac{\hbar}{\omega_\mu(\mathbf{q})}\frac{\partial}{\partial u_{-\mathbf{q}\mu}}\right)\right)\sqrt{\frac{\hbar}{2\omega_\mu(\mathbf{q})}} \tag{32.83}$$

$$= \sqrt{\frac{\omega_\mu(\mathbf{q})}{2\hbar}}\left(u_{\mathbf{q}\mu} + u_{\mathbf{q}\mu}\right)\sqrt{\frac{\hbar}{2\omega_\mu(\mathbf{q})}} \tag{32.84}$$

$$= u_{\mathbf{q}\mu} \tag{32.85}$$

Now the other identity:

$$\frac{\partial}{\partial u_{\mathbf{q}\mu}} = \left(a_{-\mathbf{q}\mu} - a^{\dagger}_{\mathbf{q}\mu}\right)\sqrt{\frac{\omega_\mu(\mathbf{q})}{2\hbar}} \tag{32.86}$$

By straight forward computation we find

$$\left(a_{-\mathbf{q}\mu} - a^{\dagger}_{\mathbf{q}\mu}\right)\sqrt{\frac{\omega_\mu(\mathbf{q})}{2\hbar}} \tag{32.87}$$

$$= \left(\sqrt{\frac{\omega_\mu(-\mathbf{q})}{2\hbar}}\left(u_{-\mathbf{q}\mu} + \frac{\hbar}{\omega_\mu(-\mathbf{q})}\frac{\partial}{\partial u_{\mathbf{q}\mu}}\right) - \sqrt{\frac{\omega_\mu(\mathbf{q})}{2\hbar}}\left(u_{-\mathbf{q}\mu} - \frac{\hbar}{\omega_\mu(\mathbf{q})}\frac{\partial}{\partial u_{\mathbf{q}\mu}}\right)\right)\sqrt{\frac{\omega_\mu(\mathbf{q})}{2\hbar}} \tag{32.88}$$

$$\overset{\text{symmetry of }\omega_\mu}{=} \sqrt{\frac{\omega_\mu(\mathbf{q})}{2\hbar}}\left(\left(u_{-\mathbf{q}\mu} + \frac{\hbar}{\omega_\mu(\mathbf{q})}\frac{\partial}{\partial u_{\mathbf{q}\mu}}\right) - \left(u_{-\mathbf{q}\mu} - \frac{\hbar}{\omega_\mu(\mathbf{q})}\frac{\partial}{\partial u_{\mathbf{q}\mu}}\right)\right)\sqrt{\frac{\omega_\mu(\mathbf{q})}{2\hbar}} \tag{32.89}$$

$$= \sqrt{\frac{\omega_\mu(\mathbf{q})}{2\hbar}}\left(\frac{2\hbar}{\omega_\mu(\mathbf{q})}\frac{\partial}{\partial u_{\mathbf{q}\mu}}\right)\sqrt{\frac{\omega_\mu(\mathbf{q})}{2\hbar}} \tag{32.90}$$

$$= \frac{\partial}{\partial u_{\mathbf{q}\mu}} \tag{32.91}$$

Proof 32.18 of Corollary 5.30

$$H \approx \sum_{\mathrm{q}\mu} \left(-\frac{\hbar^2}{2} \frac{\partial}{\partial u_{\mathbf{q}\mu}} \frac{\partial}{\partial u_{-\mathbf{q}\mu}} + \frac{1}{2}\omega_\mu^2(\mathrm{q})\, u_{\mathbf{q}\mu} u_{-\mathbf{q}\mu} \right) \tag{32.92}$$

$$= \sum_{\mathrm{q}\mu} -\frac{\hbar^2}{2} \left(a_{-\mathbf{q}\mu} - a_{\mathbf{q}\mu}^\dagger \right) \sqrt{\frac{\omega_\mu(\mathbf{q})}{2\hbar}} \left(a_{\mathbf{q}\mu} - a_{-\mathbf{q}\mu}^\dagger \right) \sqrt{\frac{\omega_\mu(-\mathbf{q})}{2\hbar}} \tag{32.93}$$

$$+ \frac{1}{2}\omega_\mu^2(\mathrm{q}) \left(a_{\mathbf{q}\mu} + a_{-\mathbf{q}\mu}^\dagger \right) \sqrt{\frac{\hbar}{2\omega_\mu(\mathbf{q})}} \left(a_{-\mathbf{q}\mu} + a_{\mathbf{q}\mu}^\dagger \right) \sqrt{\frac{\hbar}{2\omega_\mu(-\mathbf{q})}} \tag{32.94}$$

$$= \sum_{\mathrm{q}\mu} -\frac{\hbar\omega_\mu(\mathrm{q})}{4} \left(a_{-\mathbf{q}\mu} - a_{\mathbf{q}\mu}^\dagger \right) \left(a_{\mathbf{q}\mu} - a_{-\mathbf{q}\mu}^\dagger \right) \tag{32.95}$$

$$+ \frac{\hbar\omega_\mu(\mathrm{q})}{4} \left(a_{\mathbf{q}\mu} + a_{-\mathbf{q}\mu}^\dagger \right) \left(a_{-\mathbf{q}\mu} + a_{\mathbf{q}\mu}^\dagger \right) \tag{32.96}$$

$$= \sum_{\mathrm{q}\mu} \frac{\hbar\omega_\mu(\mathrm{q})}{4} \left(-a_{-\mathbf{q}\mu} a_{\mathbf{q}\mu} + a_{-\mathbf{q}\mu} a_{-\mathbf{q}\mu}^\dagger + a_{\mathbf{q}\mu}^\dagger a_{\mathbf{q}\mu} - a_{\mathbf{q}\mu}^\dagger a_{-\mathbf{q}\mu}^\dagger + a_{\mathbf{q}\mu} a_{-\mathbf{q}\mu} + a_{\mathbf{q}\mu} a_{\mathbf{q}\mu}^\dagger + a_{-\mathbf{q}\mu}^\dagger a_{-\mathbf{q}\mu} + a_{-\mathbf{q}\mu}^\dagger a_{\mathbf{q}\mu}^\dagger \right) \tag{32.97}$$

$$= \sum_{\mathrm{q}\mu} \frac{\hbar\omega_\mu(\mathrm{q})}{4} \left(\underbrace{a_{-\mathbf{q}\mu} a_{-\mathbf{q}\mu}^\dagger}_{=1+a_{-\mathbf{q}\mu}^\dagger a_{-\mathbf{q}\mu}} + a_{\mathbf{q}\mu}^\dagger a_{\mathbf{q}\mu} \underbrace{+ a_{\mathbf{q}\mu} a_{\mathbf{q}\mu}^\dagger}_{=1+a_{\mathbf{q}\mu}^\dagger a_{\mathbf{q}\mu}} + a_{-\mathbf{q}\mu}^\dagger a_{-\mathbf{q}\mu} \right) \tag{32.98}$$

$$= \sum_{\mathrm{q}\mu} \frac{\hbar\omega_\mu(\mathrm{q})}{4} \left(2 + 4 a_{\mathbf{q}\mu}^\dagger a_{\mathbf{q}\mu} \right) \tag{32.99}$$

$$= \sum_{\mathrm{q}\mu} \hbar\omega_\mu(\mathrm{q}) \left(a_{\mathbf{q}\mu}^\dagger a_{\mathbf{q}\mu} + \frac{1}{2} \right) \tag{32.100}$$

Proof 32.19 of Lemma 5.31

Combining the derived equations we obtain

$$\Delta\boldsymbol{\tau}_{\mathbf{n}\nu} = \frac{1}{\sqrt{N_p}} \sum_{\substack{\mathbf{q} \\ \nu'}} e_{\nu\nu'}(\mathbf{q}) \mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{R}_n} \frac{1}{\sqrt{M_\nu}} \underbrace{u_{\mathbf{q}\nu'}}_{= \left(a_{\mathbf{q}\nu'} + a_{-\mathbf{q}\nu'}^\dagger \right) \sqrt{\frac{\hbar}{2\omega_{\nu'}(\mathbf{q})}}} \tag{32.101}$$

$$= \frac{1}{\sqrt{N_p}} \sum_{\substack{\mathbf{q} \\ \nu'}} \sqrt{\frac{\hbar}{2M_\nu\omega_{\nu'}(\mathbf{q})}} e_{\nu\nu'}(\mathbf{q}) \mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{R}_n} \left(a_{\mathbf{q}\nu'} + a_{-\mathbf{q}\nu'}^\dagger \right) \tag{32.102}$$

33. Appendix - Proofs for Part II

Proof 33.1 of Theorem 7.7[1]

The factorization of the Fock-space into polynomial expressions of different orders is a direct consequence of the contruction.

The fermionic ($\zeta = -1$) case.

One way to find out the number of linearly independent elements in $\Lambda^n(\mathcal{H})$ is by direct counting. Linearity allows any element in $\omega = \Lambda^n(\mathcal{H})$ in the following way

$$\omega = \sum_{1 \leq i_1, \ldots, i_n \leq \mathrm{d}_{\mathcal{H}}} \omega_{i_1,\ldots,i_n} |i_1 \textcircled{\zeta} \cdots \textcircled{\zeta} i_n\rangle \tag{33.1}$$

Due to the defining relation $vv' + v'v = 0$ for all $v, v' \in \mathcal{H}$, any two elements $|i_1 \textcircled{\zeta} \cdots \textcircled{\zeta} i_n\rangle$, $|i'_1 \textcircled{\zeta} \cdots \textcircled{\zeta} i'_n\rangle$ are equal to zero, if one basis element appears more than one time $|i_j \textcircled{\zeta} \cdots \textcircled{\zeta} i_j\rangle = 0$. Thus, the number of possible non-zero combinations for $|i_1 \textcircled{\zeta} \cdots \textcircled{\zeta} i_n\rangle$ is

$$\begin{aligned}\# \left\{ |i_1 \textcircled{\zeta} \cdots \textcircled{\zeta} i_n\rangle \,\middle|\, i_1, \ldots, i_n \in \{1, \ldots, \mathrm{d}_{\mathcal{H}}\} \wedge \nexists j, j' \in \{1, \ldots, n\} \,:\, i_j = i_{j'} \right\} &= \mathrm{d}_{\mathcal{H}} \cdot (\mathrm{d}_{\mathcal{H}} - 1) \cdot \ldots \cdot (\mathrm{d}_{\mathcal{H}} - n + 1) \\ &= \frac{\mathrm{d}_{\mathcal{H}}!}{(\mathrm{d}_{\mathcal{H}} - n)!}.\end{aligned}$$

We now notice the following things:

- Every element $|i_1 \textcircled{\zeta} \cdots \textcircled{\zeta} i_n\rangle$ can be re-ordered as $|\tilde{i}_1 \textcircled{\zeta} \cdots \textcircled{\zeta} \tilde{i}_n\rangle$ such that $\tilde{i}_1 < \ldots < \tilde{i}_n$.
- The number of ways to reorder elements as $|i_1 \textcircled{\zeta} \cdots \textcircled{\zeta} i_n\rangle$ is $n!$ (due to the dimension of the symmetric group).

Hence $\omega = \Lambda^n(\mathcal{H})$ can be rewritten as

$$\omega = \sum_{1 \leq i_1 < \ldots < i_n \leq \mathrm{d}_{\mathcal{H}}} \tilde{\omega}_{i_1,\ldots,i_n} |i_1 \textcircled{\zeta} \cdots \textcircled{\zeta} i_n\rangle \tag{33.2}$$

Hence we obtain

$$\# \left\{ |i_1 \textcircled{\zeta} \cdots \textcircled{\zeta} i_n\rangle \,\middle|\, 1 \leq i_1 < \ldots < i_n \leq \mathrm{d}_{\mathcal{H}} \right\} = \binom{\mathrm{d}_{\mathcal{H}}}{n} = \dim_{\mathbb{C}} \Lambda^n(\mathcal{H}).$$

The bosonic ($\zeta = +1$) case.

[1] References: For the Bosonic part: See Zirnbauer 2018 / 2019 Sheet 09 Exercise 2 a). For the fermionic part: See Zirnbauer SS 2020, Sheet 6 Exercise 3 a).

Notice first, that the identity to prove can be written as

$$\dim_{\mathbb{C}} \mathrm{S}^n(\mathcal{H}) = \binom{\mathrm{d}_{\mathcal{H}} + n - 1}{n} = \# \left\{ (x_1, \dots, x_{\mathrm{d}_{\mathcal{H}}}) \quad \middle| \quad \sum_{i=1}^{\mathrm{d}_{\mathcal{H}}} x_i = n \quad \wedge \quad x_1, \dots, x_{\mathrm{d}_{\mathcal{H}}} \geq 0 \right\} \tag{33.3}$$

by induction. Since we have two integers $\mathrm{d}_{\mathcal{H}}$, n to vary, we need to perform the induction-start on the lines

$$\left\{ (n, \mathrm{d}_{\mathcal{H}}) \in \mathbb{N}_+^2 \quad | \quad n \in \{1, \dots, \infty\} \wedge \mathrm{d}_{\mathcal{H}} = 1 \right\} \tag{33.4}$$

and

$$\left\{ (n, \mathrm{d}_{\mathcal{H}}) \in \mathbb{N}_+^2 \quad | \quad n = 1 \wedge \mathrm{d}_{\mathcal{H}} \in \{1, \dots, \infty\} \right\} \tag{33.5}$$

This is fulfilled

Now we prove that

$$\# \left\{ (x_1, \dots, x_{\mathrm{d}_{\mathcal{H}}}, x_{\mathrm{d}_{\mathcal{H}}+1}) \quad \middle| \quad \sum_{i=1}^{\mathrm{d}_{\mathcal{H}}+1} x_i = n+1 \quad \wedge \quad x_1, \dots, x_{\mathrm{d}_{\mathcal{H}}}, x_{\mathrm{d}_{\mathcal{H}}+1} \geq 0 \right\} = \binom{\mathrm{d}_{\mathcal{H}} + n + 1}{n+1} \tag{33.6}$$

under the assumption that Equation (33.3) is true for $(n+1, \mathrm{d}_{\mathcal{H}})$ and $(n, \mathrm{d}_{\mathcal{H}}+1)$. TBD: Adding sketch. For this, we decompose the set

$$\# \left\{ (x_1, \dots, x_{\mathrm{d}_{\mathcal{H}}}, x_{\mathrm{d}_{\mathcal{H}}+1}) \quad \middle| \quad \sum_{i=1}^{\mathrm{d}_{\mathcal{H}}+1} x_i = n+1 \quad \wedge \quad x_1, \dots, x_{\mathrm{d}_{\mathcal{H}}}, x_{\mathrm{d}_{\mathcal{H}}+1} \geq 0 \right\} \tag{33.7}$$

into the two cases $x_1 = 0$ and $x_1 \geq 1$.

- Case 1: We consider the set

$$\# \left\{ (x_2, \dots, x_{\mathrm{d}_{\mathcal{H}}}, x_{\mathrm{d}_{\mathcal{H}}+1}) \quad \middle| \quad \sum_{i=2}^{\mathrm{d}_{\mathcal{H}}+1} x_i = n+1 \quad \wedge \quad x_2, \dots, x_{\mathrm{d}_{\mathcal{H}}}, x_{\mathrm{d}_{\mathcal{H}}+1} \geq 0 \right\} = \binom{\mathrm{d}_{\mathcal{H}} + n}{n+1} \tag{33.8}$$

- Case 2: We have now that $y_1 \equiv x_1 - 1 \geq 0$ We consider the set

$$\# \left\{ (y_1, x_2, \dots, x_{\mathrm{d}_{\mathcal{H}}}, x_{\mathrm{d}_{\mathcal{H}}+1}) \quad \middle| \quad y_1 + \sum_{i=2}^{\mathrm{d}_{\mathcal{H}}+1} x_i = n \quad \wedge \quad y_1, x_2, \dots, x_{\mathrm{d}_{\mathcal{H}}}, x_{\mathrm{d}_{\mathcal{H}}+1} \geq 0 \right\} = \binom{\mathrm{d}_{\mathcal{H}} + n}{n} \tag{33.9}$$

Thus we obtain in total

$$\begin{aligned} \# \left\{ (x_1, \dots, x_{\mathrm{d}_{\mathcal{H}}}, x_{\mathrm{d}_{\mathcal{H}}+1}) \quad \middle| \quad \sum_{i=1}^{\mathrm{d}_{\mathcal{H}}+1} x_i = n+1 \quad \wedge \quad x_1, \dots, x_{\mathrm{d}_{\mathcal{H}}}, x_{\mathrm{d}_{\mathcal{H}}+1} \geq 0 \right\} &= \binom{\mathrm{d}_{\mathcal{H}} + n}{n+1} + \binom{\mathrm{d}_{\mathcal{H}} + n}{n} \\ &= \binom{\mathrm{d}_{\mathcal{H}} + n + 1}{n+1} \end{aligned}$$

Proving the theorem for the bosonic case.

Proof 33.2 of Corollary 7.12

We have to show, that taking two elements $v \equiv \psi$ and $v' \equiv \phi$ (which are then interpreted as many-particle wavefunctions), the condition in Equation (7.7) is still satisfied. This is done by straightforward computation

$$\begin{aligned}\left(\psi \textcircled{\zeta} \phi\right)(x_1, x_2) - \zeta \left(\phi \textcircled{\zeta} \psi\right)(x_1, x_2) &= \sum_{\pi \in \mathrm{S}_2} \mathrm{sign}(\pi)^{1-\theta(\zeta)} \psi(x_{\pi(1)}) \phi(x_{\pi(2)}) - \zeta \sum_{\pi \in \mathrm{S}_2} \mathrm{sign}(\pi)^{1-\theta(\zeta)} \phi(x_{\pi(1)}) \psi(x_{\pi(2)}) \\ &= 0\end{aligned} \tag{33.10}$$

It remains to prove the associativity. This is proven more or less straight-forwardly[2] To Be Done

Proof 33.3 of Lemma 7.14

Introducing $u \equiv v + \phi$ and $u' \equiv v' + \phi'$ we obtain by direct computation

$$\begin{aligned} & B_\zeta(u, u') + \zeta B_\zeta(u', u) \\ = \; & B_\zeta(v + \phi, v' + \phi') + \zeta B_\zeta(v' + \phi', v + \phi) \\ = \; & \phi(v') - \zeta \phi'(v) \quad + \quad \zeta \left(\phi'(v) - \zeta \phi(v')\right) \\ = \; & 0 \end{aligned}$$

Proof 33.4 of Lemma 7.17

Expanding the r.h.s. of the identity yields

$$\begin{aligned}[A, B]_\zeta C + \zeta B [A, C]_\zeta &= (AB - \zeta BA) C + \zeta B (AC - \zeta CA) \\ &= ABC - \zeta^2 BCA \\ &= ABC - BCA \\ &= [A, BC]\end{aligned}$$

Proof 33.5 of Notation 7.21 One fixes the elements $u \equiv |i\rangle + 0$ and $u' \equiv 0 + \langle j|$ and immediately obtains the relations by considering their commutators.

Proof 33.6 of Theorem 7.23 Recall that a mapping

$$\begin{aligned}\Phi : \; \mathscr{A}_\zeta(\mathcal{H} \oplus \mathcal{H}^*, B_\zeta) \times \mathscr{F}_\zeta &\to \mathscr{F}_\zeta \\ (g, v) &\mapsto \Phi(g, v) \equiv g \cdot v\end{aligned}$$

qualifies as a representation, iff

[2] See, for example, [53].

1. for all $g \in \mathscr{A}_\zeta(\mathcal{H} \oplus \mathcal{H}^*, B_\zeta)$ the map

$$\begin{aligned}\Phi(g): \mathscr{F}_\zeta &\mapsto \mathscr{F}_\zeta \\ v &\mapsto \Phi(g, v)\end{aligned}$$

   is linear over $\mathbb{C}$,

2. for all $g_1, g_2 \in \mathscr{A}_\zeta(\mathcal{H} \oplus \mathcal{H}^*, B_\zeta)$ and $v \in \mathscr{F}_\zeta$ one has

$$\begin{aligned}e \cdot v &= v \\ g_1 \cdot (g_2 \cdot v) &= (g_1 g_2) \cdot v\end{aligned}$$

   whereas $e \equiv 1 \equiv 1_{\mathbb{C}}$ is the identity in the algebra.

The first property is obviously fulfilled, as we defined our representation on the basis-elements and extended the definition by linearity. The identity condition is also fulfilled by applying the definition for multiplication with scalars. For the third condition there are two non-trivial cases:

1. $g_1 \equiv w + 0$, $g_2 \equiv 0 + \phi$
2. $g_1 \equiv 0 + \phi$, $g_2 \equiv w + 0$

and we have to check in each case whether $v \in \mathbb{C}$, $v \in \mathcal{H}$ or $v \in \mathscr{F}_\zeta^n$ for $n \geq 2$.

Case 1:

In this case we obtain

$$\begin{aligned}g_1 g_2 w &= (w + 0)(0 + \phi) \cdot v \\ &\equiv \iota(w)\epsilon(\phi) \cdot v = \dots\end{aligned}$$

which gives for each type of v:

- $v \in \mathbb{C}$: $\dots = 0$.
- $v \in \mathcal{H}$: $\dots = \iota(w) \cdot \phi(v) = w \cdot_\zeta \phi(v)$
- $v \equiv v_1 \cdot_\zeta v_2 \in \mathscr{F}_\zeta^n$ for $n \geq 2$: $\dots =$

TBContinued.

Proof 33.7 of Theorem 7.24 TBD.

Proof 33.8 of Corollary 7.26 TBD. With computation-rules of determinants / permanents.

Proof 33.9 of Corollary 7.29 TBD. Recall that the hermitian adjoint of an operator w.r.t. a scalar-product is defined as TBWritten.

Proof 33.10 of Theorem 7.34 TBD. The states form obviously a basis, since every element in the Fock-space can be expanded w.r.t. the states. Now to the orthonormality: TBDone.

Proof 33.11 of Corollary 7.37 TBD.

Proof 33.12 of Lemma 7.38 TBD.

Proof 33.13 of Lemma 7.39 TBD.

Proof 33.14 of Corollary 7.37 TBD.

Proof 33.15 of Corollary 7.45 TBD.

Proof 33.16 of Corollary 7.46 TBD.

Proof 33.17 of Theorem 7.48 TBD.

Proof 33.18 of Theorem 8.9

TBUpdated w.r.t. the ensemble Hamiltonian.

We first note the auxiliary identities

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}U(t,0) &= -\frac{\mathrm{i}}{\hbar}HU(t,0)\\ \frac{\mathrm{d}}{\mathrm{d}t}U(t,0)^\dagger = \frac{\mathrm{d}}{\mathrm{d}t}U(0,t) &= \frac{\mathrm{i}}{\hbar}U(0,t)H = \frac{\mathrm{i}}{\hbar}U(t,0)^\dagger H\end{aligned}$$

Then it follows

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}X_{\mathrm{H}}(t) &= \frac{\mathrm{d}}{\mathrm{d}t}U(t,0)^\dagger X(t)U(t,0)\\ &= \left(\frac{\mathrm{d}}{\mathrm{d}t}U(t,0)^\dagger\right)X(t)U(t,0) + U(t,0)^\dagger\left(\frac{\mathrm{d}}{\mathrm{d}t}X(t)\right)U(t,0) + U(t,0)^\dagger X(t)\left(\frac{\mathrm{d}}{\mathrm{d}t}U(t,0)\right)\\ &= \frac{\mathrm{i}}{\hbar}U(t,0)^\dagger HX(t)U(t,0) + U(t,0)^\dagger\left(\frac{\mathrm{d}}{\mathrm{d}t}X(t)\right)U(t,0) + U(t,0)^\dagger X(t)\left(-\frac{\mathrm{i}}{\hbar}HU(t,0)\right)\\ &= \frac{\mathrm{i}}{\hbar}U(t,0)^\dagger\left(HX(t) - X(t)H\right)U(t,0) + U(t,0)^\dagger\left(\frac{\mathrm{d}}{\mathrm{d}t}X(t)\right)U(t,0)\\ &= \frac{\mathrm{i}}{\hbar}U(t,0)^\dagger\left[H,X(t)\right]U(t,0) + U(t,0)^\dagger\left(\frac{\mathrm{d}}{\mathrm{d}t}X(t)\right)U(t,0)\\ &= -\frac{\mathrm{i}}{\hbar}\left[X,H\right]_{\mathrm{H}}(t) + U(t,0)^\dagger\left(\frac{\mathrm{d}}{\mathrm{d}t}X(t)\right)U(t,0)\end{aligned}$$

Proof 33.19 of Theorem 8.24

TBUpdated w.r.t. the ensemble Hamiltonian.

Analogously to the real-time theorem we first note the auxiliary identities

$$\frac{\mathrm{d}}{\mathrm{d}\tau}U(\tau,0) = -\frac{1}{\hbar}HU(\tau,0)$$
$$\frac{\mathrm{d}}{\mathrm{d}\tau}U(0,\tau) = \frac{1}{\hbar}U(0,\tau)H$$

Then it follows

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\tau}X_{\mathrm{H}}(\tau) &= \frac{\mathrm{d}}{\mathrm{d}t}U(0,\tau)X(\tau)U(\tau,0) \\
&= \left(\frac{\mathrm{d}}{\mathrm{d}\tau}U(0,\tau)\right)X(\tau)U(\tau,0) + U(0,\tau)\left(\frac{\mathrm{d}}{\mathrm{d}\tau}X(\tau)\right)U(\tau,0) + U(0,\tau)X(\tau)\left(\frac{\mathrm{d}}{\mathrm{d}\tau}U(\tau,0)\right) \\
&= \frac{1}{\hbar}U(0,\tau)HX(\tau)U(\tau,0) + U(0,\tau)\left(\frac{\mathrm{d}}{\mathrm{d}\tau}X(\tau)\right)U(\tau,0) + U(0,\tau)X(\tau)\left(-\frac{1}{\hbar}HU(\tau,0)\right) \\
&= \frac{1}{\hbar}U(0,\tau)\left(HX(\tau) - X(\tau)H\right)U(\tau,0) + U(0,\tau)\left(\frac{\mathrm{d}}{\mathrm{d}t}X(\tau)\right)U(\tau,0) \\
&= \frac{1}{\hbar}U(0,\tau)\left[H, X(\tau)\right]U(\tau,0) + U(0,\tau)\left(\frac{\mathrm{d}}{\mathrm{d}\tau}X(\tau)\right)U(\tau,0) \\
&= -\frac{1}{\hbar}\left[X, H\right]_{\mathrm{H}}(\tau) + U(0,\tau)\left(\frac{\mathrm{d}}{\mathrm{d}\tau}X(\tau)\right)U(\tau,0)
\end{aligned}$$

Proof 33.20 of Lemma 8.28

There is at least two possibilities to prove the lemma.

1. With the Equation of motion-method.
2. With the Baker-Campbell-Hausdorff-series[3].

TBElaborated with Mahan eq. (3.44) and BCH-series TBElaborated with Mahan eq. (3.67) and BCH-series

The Equation of motion-method

We compute with the Heisenberg-equation-of-motion in Equation TBReferenced, and with the identity for statistical commutators

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}c_{\bullet}(t) &= -\frac{\mathrm{i}}{\hbar}\sum_{\alpha\in\mathscr{A}}(\epsilon_\alpha - \mu)[c_{\bullet}, c_\alpha^\dagger c_\alpha]_{\mathrm{H}}(t) \\
&= -\frac{\mathrm{i}}{\hbar}\sum_{\alpha\in\mathscr{A}}(\epsilon_\alpha - \mu)\left([c_{\bullet}, c_\alpha^\dagger]_\zeta c_\alpha + \zeta c_\alpha^\dagger[c_{\bullet}, c_\alpha]_\zeta\right)_{\mathrm{H}}(t) \\
&= \frac{\mathrm{i}}{\hbar}(\epsilon_{\bullet} - \mu)c_{\bullet}(t)
\end{aligned}$$

[3] TBElaborated with Mahan eq. (3.44) and Zirnbauers exercise-sheet

with the initial conditions $c_\alpha(t=0) = c_\alpha$ we see, that

$$c_\bullet(t) = \mathrm{e}^{-\mathrm{i}(\epsilon_\bullet - \mu)t/\hbar} c_\bullet \tag{33.11}$$

is a solution of the differential equation. Taking the hermitian conjugate proves the other identity.

The Baker-Campbell-Hausdorff-method

TBD.

Other references related to this[4]

Proof 33.21 of Lemma 8.37

We compute the hermitian conjugate of the interaction-term as

$$\begin{aligned}
\left(H_{\text{el-ph}}\right)^\dagger &= \sum_{\substack{\mathbf{k},\mathbf{q}\in Q \\ \sigma\in\{\uparrow,\downarrow\} \\ \nu\in\{1,\dots,rd_{\mathbf{x}}\} \\ n,m\in\{1,\dots,\infty\}}} \frac{g^*_{mn\nu}(\mathbf{k},\mathbf{q})}{\sqrt{N_p}} c^\dagger_{n\sigma}(\mathbf{k}) c_{m\sigma}(\mathbf{k}+\mathbf{q}) \left(b_\nu(-\mathbf{q}) + b^\dagger_\nu(+\mathbf{q})\right) \\
&= \sum_{\substack{\mathbf{k},\mathbf{q}\in Q \\ \sigma\in\{\uparrow,\downarrow\} \\ \nu\in\{1,\dots,rd_{\mathbf{x}}\} \\ n,m\in\{1,\dots,\infty\}}} \frac{g^*_{mn\nu}(\mathbf{k},-\mathbf{q})}{\sqrt{N_p}} c^\dagger_{n\sigma}(\mathbf{k}) c_{m\sigma}(\mathbf{k}-\mathbf{q}) \left(b_\nu(+\mathbf{q}) + b^\dagger_\nu(-\mathbf{q})\right) \\
&= \sum_{\substack{\mathbf{k},\mathbf{q}\in Q \\ \sigma\in\{\uparrow,\downarrow\} \\ \nu\in\{1,\dots,rd_{\mathbf{x}}\} \\ n,m\in\{1,\dots,\infty\}}} \frac{g^*_{nm\nu}(\mathbf{k}+\mathbf{q},-\mathbf{q})}{\sqrt{N_p}} c^\dagger_{m\sigma}(\mathbf{k}+\mathbf{q}) c_{n\sigma}(\mathbf{k}) \left(b_\nu(\mathbf{q}) + b^\dagger_\nu(-\mathbf{q})\right)
\end{aligned}$$

whereas we used $\mathbf{q} \mapsto -\mathbf{q}$, in the second equation sign and $\mathbf{k} \mapsto \mathbf{k}+\mathbf{q}$ and $m \leftrightarrow n$ in the third equation sign.

Therefore we obtain

$$g_{mn\nu}(\mathbf{k},\mathbf{q}) = g^*_{nm\nu}(\mathbf{k}+\mathbf{q},-\mathbf{q})$$

Proof 33.22 of Lemma 9.65

For this proof, see also the literature[5]. We first rewrite

$$\mathrm{n}^\zeta(x) = \frac{1}{\mathrm{e}^x - \zeta} = (\mathrm{e}^x - \zeta)^{-1} \tag{33.12}$$

and then compute for the first identity

[4] TBCopied: cf. Zirnbauer AQM, 2018, 2019, Sheet 10 Exercise 1b).

[5] Cf. Mahan Eqs. (3.236), (3.237).

$$\frac{\mathrm{d}}{\mathrm{d}x}\,\mathrm{n}^{\zeta}(x) = -1\cdot\frac{1}{(\mathrm{e}^{x}-\zeta)^{2}}\cdot\mathrm{e}^{x} = \frac{-1}{4}\cdot\frac{2\mathrm{e}^{x/2}}{\mathrm{e}^{x}-\zeta}\cdot\frac{2\mathrm{e}^{x/2}}{\mathrm{e}^{x}-\zeta} = \frac{-1}{4}\zeta\mathrm{ch}^{2}\left(\frac{x}{2}\right) \tag{33.13}$$

For the second identity we simplify the appearing expressions in another way as

$$\frac{\mathrm{d}}{\mathrm{d}x}\,\mathrm{n}^{\zeta}(x) = -1\cdot\frac{1}{(\mathrm{e}^{x}-\zeta)^{2}}\cdot\mathrm{e}^{x} = -\cdot\frac{1}{\mathrm{e}^{x}-\zeta}\cdot\frac{\mathrm{e}^{x}-\zeta+\zeta}{\mathrm{e}^{x}-\zeta} = -\,\mathrm{n}^{\zeta}(x)\cdot\left(1+\zeta\,\mathrm{n}^{\zeta}(x)\right) \tag{33.14}$$

Proof 33.23 of Lemma 9.65

We compute

$$\mathrm{F}_{\hbar\beta}(\bullet+\mathrm{i}\omega_{n}) = \frac{1}{\mathrm{e}^{\hbar\beta(\bullet+\mathrm{i}\omega_{n})}+1} = \frac{1}{-\mathrm{e}^{\hbar\beta\bullet}+1} = -\,\mathrm{B}_{\hbar\beta}(\bullet)$$

and

$$\mathrm{F}_{\hbar\beta}(\mathrm{i}\omega_{n}-\bullet)-\mathrm{B}_{\hbar\beta}(\bullet) = \frac{1}{\mathrm{e}^{\hbar\beta(\mathrm{i}\omega_{n}-\bullet)}+1}-\frac{1}{\mathrm{e}^{\hbar\beta\bullet}-1} = \frac{1}{1-\mathrm{e}^{-\hbar\beta\bullet}}-\frac{1}{\mathrm{e}^{\hbar\beta\bullet}-1} = \frac{\mathrm{e}^{-\hbar\beta\bullet}-1}{\mathrm{e}^{-\hbar\beta\bullet}-1} = 1$$

For the third identity we still have to digitalize / create the proof.

Proof 33.24 of Lemma 9.66

We define $x = \hbar\beta\omega = \frac{\hbar\omega}{k_{\mathrm{B}}T}$ such that we obtain

$$\frac{\mathrm{d}x}{\mathrm{d}T} = \hbar\omega\,\frac{\mathrm{d}\beta}{\mathrm{d}T} = \hbar\omega\,\frac{\mathrm{d}}{\mathrm{d}T}\left(\frac{1}{k_{\mathrm{B}}T}\right) = -\frac{\hbar\omega}{k_{\mathrm{B}}T^{2}}. \tag{33.15}$$

and

$$\mathrm{n}^{\zeta}_{\hbar\beta}(\omega) = \mathrm{n}^{\zeta}(x) \tag{33.16}$$

and therefore

$$\frac{\mathrm{d}}{\mathrm{d}T}\,\mathrm{n}^{\zeta}_{\hbar\beta}(\omega) = \frac{\mathrm{d}}{\mathrm{d}T}\,\mathrm{n}^{\zeta}(x) = \frac{\mathrm{d}}{\mathrm{d}x}\,\mathrm{n}^{\zeta}(x)\cdot\frac{\mathrm{d}x}{\mathrm{d}T} \tag{33.17}$$

Combining this with Lemma 9.63 yields the desired result.

Proof 33.25 of Corollary 9.67 We recall the definition of the Bose-function

$$\mathrm{B}_{\hbar\beta}(z) = \frac{1}{\mathrm{e}^{\hbar\beta z}-1} = \left(\mathrm{e}^{\hbar\beta z}-1\right)^{-1} \tag{33.18}$$

and compute straightforwardly

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}z}\,\mathrm{B}_{\hbar\beta}(z) &= -\left(\mathrm{e}^{\hbar\beta z}-1\right)^{-2}\cdot\underbrace{\frac{\mathrm{d}}{\mathrm{d}z}\mathrm{e}^{\hbar\beta z}}_{\hbar\beta\mathrm{e}^{\hbar\beta z}}\\ &= -\hbar\beta\frac{\mathrm{e}^{\hbar\beta z}-1+1}{\left(\mathrm{e}^{\hbar\beta z}-1\right)^{2}}\\ &= -\hbar\beta\Big[\,\mathrm{B}_{\hbar\beta}(z)+\mathrm{B}^{2}_{\hbar\beta}(z\Big]\\ &= -\hbar\beta\,\mathrm{B}_{\hbar\beta}(z)\Big[1+\mathrm{B}_{\hbar\beta}(z)\Big]\end{aligned} \tag{33.19}$$

For the Fermi-function the computation is analogous.

Proof 33.26 of Lemma 12.3 With the cyclicity of the trace, and the Baker-Campbell-Hausdorff-formula, the proof is straightforward: [TBElaborated...]

Proof 33.27 of Lemma 12.4

See Waste-Folder 1, topic 10.

The proofs are more or less straightforward by simply writing out the underlying equations. We obtain for the individual Green-functions

$$\begin{aligned}G(A,A') &= -\frac{\mathrm{i}}{\hbar}\langle\theta(t-t')c_\alpha(t)c^\dagger_{\alpha'}(t')+\zeta\theta(t'-t)c^\dagger_{\alpha'}(t')c_\alpha(t)\rangle\\ &= \theta(t-t')G^{>}(A,A')+\theta(t'-t)G^{<}(A,A')\end{aligned}$$

$$\begin{aligned}G^{\overline{\mathbb{T}}}(A,A') &= -\frac{\mathrm{i}}{\hbar}\langle\theta(t'-t)c_\alpha(t)c^\dagger_{\alpha'}(t')+\zeta\theta(t-t')c^\dagger_{\alpha'}(t')c_\alpha(t)\rangle\\ &= \theta(t'-t)G^{>}(A,A')+\theta(t-t')G^{<}(A,A')\end{aligned}$$

$$G^{\mathrm{ret}}(A,A') = -\frac{\mathrm{i}}{\hbar}\theta(t-t')\langle c_\alpha(t)c^\dagger_{\alpha'}(t')-\zeta c^\dagger_{\alpha'}(t')c_\alpha(t)\rangle$$

$$G^{\mathrm{adv}}(A,A') = +\frac{\mathrm{i}}{\hbar}\theta(t'-t)\langle c_\alpha(t)c^\dagger_{\alpha'}(t')-\zeta c^\dagger_{\alpha'}(t')c_\alpha(t)\rangle$$

(i) We obtain for the retarded Green-function

$$G^{\mathrm{ret}}_{\alpha,\alpha'}(t,t') = -\frac{\mathrm{i}}{\hbar}\theta(t-t')\langle c_\alpha(t)c^\dagger_{\alpha'}(t')-\zeta c^\dagger_{\alpha'}(t')c_\alpha(t)\rangle \tag{33.20}$$

and for the advanced Green-function

$$G^{\mathrm{adv}}_{\alpha,\alpha'}(t,t') = +\frac{\mathrm{i}}{\hbar}\theta(t'-t)\langle c_\alpha(t)c^\dagger_{\alpha'}(t') - \zeta c^\dagger_{\alpha'}(t')c_\alpha(t)\rangle \tag{33.21}$$

and hence

$$\begin{aligned}\left(G^{\mathrm{adv}}_{\alpha',\alpha}(t',t)\right)^\dagger &= \left(+\frac{\mathrm{i}}{\hbar}\theta(t-t')\langle c_{\alpha'}(t')c^\dagger_\alpha(t) + c^\dagger_\alpha(t)c_{\alpha'}(t')\rangle\right)^\dagger \\ &= -\frac{\mathrm{i}}{\hbar}\theta(t-t')\langle c_\alpha(t)c^\dagger_{\alpha'}(t') + c^\dagger_{\alpha'}(t')c_\alpha(t)\rangle = G^{\mathrm{ret}}_{\alpha,\alpha'}(t,t')\end{aligned}$$

Therefore we obtain

$$G^{\mathrm{ret}}_{\alpha,\alpha'}(t,t') = \left(G^{\mathrm{adv}}_{\alpha',\alpha}(t',t)\right)^\dagger \Longleftrightarrow G^{\mathrm{ret}}(A,A') = \left(G^{\mathrm{adv}}(A',A)\right)^\dagger \tag{33.22}$$

(ii) We obtain further

$$\begin{aligned}\left(G^{++} - G^{-+}\right)(A,A') &= -\frac{\mathrm{i}}{\hbar}\langle\left(\theta(t-t')-1\right)c_\alpha(t)c_{\alpha'}(t') + \zeta\theta(t'-t)c_{\alpha'}(t')c_\alpha(t)\rangle \\ &= -\frac{\mathrm{i}}{\hbar}\langle -\theta(t'-t)c_\alpha(t)c_{\alpha'}(t') + \zeta\theta(t'-t)c_{\alpha'}(t')c_\alpha(t)\rangle \\ &= \frac{\mathrm{i}}{\hbar}\theta(t'-t)\langle c_\alpha(t)c_{\alpha'}(t') - \zeta c_{\alpha'}(t')c_\alpha(t)\rangle\end{aligned}$$

(iii) We obtain further

$$\begin{aligned}\left(G^{++} - G^{--}\right)(A,A') &= -\frac{\mathrm{i}}{\hbar}\langle -\theta(t'-t)c_\alpha(t)c_{\alpha'}(t') + \left(-\zeta\theta(t-t')+\zeta\right)c_{\alpha'}(t')c_\alpha(t)\rangle \\ &= -\frac{\mathrm{i}}{\hbar}\langle -\theta(t'-t)c_\alpha(t)c_{\alpha'}(t') + \zeta\theta(t'-t)c_{\alpha'}(t')c_\alpha(t)\rangle \\ &= +\frac{\mathrm{i}}{\hbar}\theta(t'-t)\langle c_\alpha(t)c_{\alpha'}(t') - \zeta c_{\alpha'}(t')c_\alpha(t)\rangle\end{aligned}$$

(iv) We obtain further

$$\begin{aligned}\left(G^{++} - G^{-+}\right)(A,A') &= -\frac{\mathrm{i}}{\hbar}\langle \zeta c_{\alpha'}(t')c_\alpha(t) - c_\alpha(t)c_{\alpha'}(t')\rangle \\ &= \frac{\mathrm{i}}{\hbar}\langle c_\alpha(t)c_{\alpha'}(t') - \zeta\theta(t'-t)c_{\alpha'}(t')c_\alpha(t)\rangle\end{aligned}$$

(v) We obtain further

$$\begin{aligned}\left(G^{++}-G^{+-}\right)(A,A') &= -\frac{\mathrm{i}}{\hbar}\langle\theta(t-t')c_\alpha(t)c_{\alpha'}(t')+\zeta\left(\theta(t'-t)-1\right)c_{\alpha'}(t')c_\alpha(t)\rangle\\ &= -\frac{\mathrm{i}}{\hbar}\theta(t-t')\langle c_\alpha(t)c_{\alpha'}(t')-\zeta c_{\alpha'}(t')c_\alpha(t)\rangle\end{aligned}$$

(vi) We obtain further

$$\begin{aligned}\left(G^{-+}-G^{--}\right)(A,A') &= -\frac{\mathrm{i}}{\hbar}\langle\left(1-\theta(t'-t)\right)c_\alpha(t)c_{\alpha'}(t')-\zeta\theta(t-t')c_{\alpha'}(t')c_\alpha(t)\rangle\\ &= -\frac{\mathrm{i}}{\hbar}\theta(t-t')\langle c_\alpha(t)c_{\alpha'}(t')-\zeta c_{\alpha'}(t')c_\alpha(t)\rangle\end{aligned}$$

and therefore we obtain

$$\theta(t-t')\left(G^{-+}-G^{+-}\right)(A,A') = -\frac{\mathrm{i}}{\hbar}\theta(t-t')\langle c_\alpha(t)c_{\alpha'}(t')-\zeta c_{\alpha'}(t')c_\alpha(t)\rangle$$

ToBeSorted. The last two identities follow from combining the results we just obtained TBDone.

Proof 33.28 of Lemma 12.6

The time-ordered Green-function

With the equation of motion technique, we consider the definition

$$\mathbb{R}\ni t\mapsto G^{\mathbb{T}}_{\alpha,\alpha'}(t) = -\frac{\mathrm{i}}{\hbar}\frac{\mathrm{Tr}_{\mathscr{F}_\zeta}\,\mathrm{e}^{-\beta(H-\mu N)}\left[\theta(t)\,c_\alpha(t)\,c^\dagger_{\alpha'}(0)+\zeta\,\theta(-t)\,c^\dagger_{\alpha'}(0)\,c_\alpha(t)\right]}{\mathrm{Tr}_{\mathscr{F}_\zeta}\,\mathrm{e}^{-\beta(H-\mu N)}}\in\mathbb{C}$$

and want to calculate its derivative. We therefore calculate first

$$\begin{aligned}\partial_t\,\mathrm{T}_t\,c_\alpha(t)\,c^\dagger_{\alpha'}(0) &\propto \partial_t\left[\theta(t)\,c_\alpha(t)\,c^\dagger_{\alpha'}(0)+\zeta\,\theta(-t)\,c^\dagger_{\alpha'}(0)\,c_\alpha(t)\right]\\ &= \delta(t)c_\alpha(t)\,c^\dagger_{\alpha'}(0)-\zeta\delta(-t)c^\dagger_{\alpha'}(0)\,c_\alpha(t)-\frac{\mathrm{i}}{\hbar}\theta(t)\left[c_\alpha,H-\mu\right]_{\mathrm{H}}(t)c^\dagger_{\alpha'}(0)-\frac{\mathrm{i}}{\hbar}\theta(-t)\zeta c^\dagger_{\alpha'}(0)\left[c_\alpha,H-\mu\right]_{\mathrm{H}}(t)\\ &= \delta(t)\left[c_\alpha(t)\,,c^\dagger_{\alpha'}(0)\right]_\zeta-\frac{\mathrm{i}}{\hbar}\,\mathrm{T}_t\left(\left[c_\alpha,H-\mu\right]_{\mathrm{H}}(t)\,c^\dagger_{\alpha'}(0)\right)\end{aligned}$$

whereas we used the statistical commutator from Definition TBD and the Heisenberg-equation-of-motions from Lemma TBD. This gives the equation of motion

$$\partial_t G^{\mathbb{T}}_{\alpha,\alpha'}(t) = -\frac{\mathrm{i}}{\hbar}\delta(t)\delta_{\alpha,\alpha'} \quad - \quad \frac{1}{\hbar}\left\langle \mathrm{T}_t \left[c_\alpha, \frac{H-\mu N}{\hbar}\right]_{\mathrm{H}}(t) c^\dagger_{\alpha'}(0) \right\rangle \tag{33.23}$$

The anti-time-ordered Green-function

With the equation of motion technique, we consider the definition

$$\mathbb{R} \ni t \mapsto G^{\overline{\mathbb{T}}}_{\alpha,\alpha'}(t) = -\frac{\mathrm{i}}{\hbar}\frac{\mathrm{Tr}_{\mathscr{F}_\zeta}\, \mathrm{e}^{-\beta(H-\mu N)}\Big[\theta(-t)\, c_\alpha(t)\, c^\dagger_{\alpha'}(0) + \zeta\, \theta(+t)\, c^\dagger_{\alpha'}(0)\, c_\alpha(t)\Big]}{\mathrm{Tr}_{\mathscr{F}_\zeta}\, \mathrm{e}^{-\beta(H-\mu N)}} \in \mathbb{C}$$

and want to calculate its derivative. We therefore calculate first

$$\begin{aligned}
\partial_t \overline{\mathrm{T}}_t c_\alpha(t)\, c^\dagger_{\alpha'}(0) &\propto \partial_t \Big[\theta(-t)\, c_\alpha(t)\, c^\dagger_{\alpha'}(0) + \zeta\, \theta(+t)\, c^\dagger_{\alpha'}(0)\, c_\alpha(t)\Big] \\
&= -\delta(-t) c_\alpha(t)\, c^\dagger_{\alpha'}(0) + \zeta\delta(t) c^\dagger_{\alpha'}(0)\, c_\alpha(t) - \frac{\mathrm{i}}{\hbar}\theta(-t)\big[c_\alpha, H-\mu\big]_{\mathrm{H}}(t) c^\dagger_{\alpha'}(0) - \frac{\mathrm{i}}{\hbar}\theta(t)\zeta c^\dagger_{\alpha'}(0)\big[c_\alpha, H-\mu\big]_{\mathrm{H}}(t) \\
&= -\delta(-t)\big[c_\alpha(t)\,, c^\dagger_{\alpha'}(0)\big]_\zeta - \frac{\mathrm{i}}{\hbar}\overline{\mathrm{T}}_t\left(\big[c_\alpha, H-\mu\big]_{\mathrm{H}}(t)\, c^\dagger_{\alpha'}(0)\right)
\end{aligned}$$

whereas we used the statistical commutator from Definition TBD and the Heisenberg-equation-of-motions from Lemma TBD. This gives the equation of motion

$$\partial_t G^{\overline{\mathbb{T}}}_{\alpha,\alpha'}(t) = \frac{\mathrm{i}}{\hbar}\delta(t)\delta_{\alpha,\alpha'} \quad - \quad \frac{1}{\hbar}\left\langle \overline{\mathrm{T}}_t \big[c_\alpha, \frac{H-\mu N}{\hbar}\big]_{\mathrm{H}}(t) c^\dagger_{\alpha'}(0) \right\rangle \tag{33.24}$$

The retarded Green-function

With the equation of motion technique, we consider the definition

$$\mathbb{R} \ni t \mapsto G^{\mathrm{ret}}_{\alpha,\alpha'}(t) = -\frac{\mathrm{i}}{\hbar}\theta(t)\frac{\mathrm{Tr}_{\mathscr{F}_\zeta}\, \mathrm{e}^{-\beta(H-\mu N)}\Big[c_\alpha(t)\, c^\dagger_{\alpha'}(0) - \zeta\, c^\dagger_{\alpha'}(0)\, c_\alpha(t)\Big]}{\mathrm{Tr}_{\mathscr{F}_\zeta}\, \mathrm{e}^{-\beta(H-\mu N)}} \in \mathbb{C}$$

and want to calculate its derivative. We therefore calculate first

$$\begin{aligned}
\partial_t \theta(t)\big[c_\alpha(t),\, c^\dagger_{\alpha'}(0)\big]_\zeta &= \delta(t)\big[c_\alpha(t),\, c^\dagger_{\alpha'}(0)\big]_\zeta + \theta(t)\big[\partial_t c_\alpha(t),\, c^\dagger_{\alpha'}(0)\big]_\zeta \\
&= \delta(t)\delta_{\alpha,\alpha'} - \frac{\mathrm{i}}{\hbar}\theta(t)\Big[\big[c_\alpha, H-\mu\big]_{\mathrm{H}}(t), c^\dagger_{\alpha'}(0)\Big]_\zeta
\end{aligned}$$

whereas we used the statistical commutator from Definition TBD and the Heisenberg-equation-of-motions from Lemma TBD. This gives the equation of motion

$$\partial_t G^{\text{ret}}_{\alpha,\alpha'}(t) = -\frac{\mathrm{i}}{\hbar}\delta(t)\delta_{\alpha,\alpha'} \quad - \quad \frac{1}{\hbar}\theta(t)\left\langle \left[\left[c_\alpha, H-\mu\right]_{\mathrm{H}}(t), c^\dagger_{\alpha'}(0)\right]_\zeta \right\rangle \tag{33.25}$$

The advanced Green-function

With the equation of motion technique, we consider the definition

$$\mathbb{R} \ni t \mapsto G^{\text{adv}}_{\alpha,\alpha'}(t) = \frac{\mathrm{i}}{\hbar}\theta(-t)\frac{\mathrm{Tr}_{\mathscr{F}_\zeta}\, \mathrm{e}^{-\beta(H-\mu N)}\left[c_\alpha(t)\, c^\dagger_{\alpha'}(0) - \zeta\, c^\dagger_{\alpha'}(0)\, c_\alpha(t)\right]}{\mathrm{Tr}_{\mathscr{F}_\zeta}\, \mathrm{e}^{-\beta(H-\mu N)}} \in \mathbb{C}$$

and want to calculate its derivative. We therefore calculate first

$$\begin{aligned}\partial_t\theta(-t)\left[c_\alpha(t),\, c^\dagger_{\alpha'}(0)\right]_\zeta &= -\delta(-t)\left[c_\alpha(t),\, c^\dagger_{\alpha'}(0)\right]_\zeta + \theta(-t)\left[\partial_t c_\alpha(t),\, c^\dagger_{\alpha'}(0)\right]_\zeta \\ &= -\delta(-t)\delta_{\alpha,\alpha'} - \frac{\mathrm{i}}{\hbar}\theta(-t)\left[\left[c_\alpha, H-\mu\right]_{\mathrm{H}}(t), c^\dagger_{\alpha'}(0)\right]_\zeta\end{aligned}$$

whereas we used the statistical commutator from Definition TBD and the Heisenberg-equation-of-motions from Lemma TBD. This gives the equation of motion

$$\partial_t G^{\text{adv}}_{\alpha,\alpha'}(t) = -\frac{\mathrm{i}}{\hbar}\delta(-t)\delta_{\alpha,\alpha'} \quad + \quad \frac{1}{\hbar}\theta(-t)\left\langle \left[\left[c_\alpha, H-\mu\right]_{\mathrm{H}}(t), c^\dagger_{\alpha'}(0)\right]_\zeta \right\rangle \tag{33.26}$$

Proof 33.29 of Corollary 12.8 Recall that we have, *for example* (we could use any other one as well) for the time-ordered-Green-function

$$G_{i,j}(t,t') = -\frac{-\mathrm{i}}{\hbar}\left\langle \mathrm{T}_t\, c_i(t) c^\dagger_j(t')\right\rangle \tag{33.27}$$

and therefore we obtain

$$\begin{aligned}\widetilde{G}_{\alpha,\beta}(t,t') &= -\frac{-\mathrm{i}}{\hbar}\left\langle \mathrm{T}_t\, c_\alpha(t) c^\dagger_\beta(t')\right\rangle \\ &= -\frac{-\mathrm{i}}{\hbar}\sum_{i,j} U^*_{i,\alpha}U_{j,\beta}\left\langle \mathrm{T}_t\, c_i(t) c^\dagger_j(t')\right\rangle \\ &= \sum_{i,j} U^*_{i,\alpha} G_{i,j}(t,t') U_{j,\beta}\end{aligned} \tag{33.28}$$

Proof 33.30 of Theorem 12.9

See Waste-Folder 1, topic 5.

We start with the lesser Green-function and we focus on the case $\alpha = \alpha'$ since it is easy to see that the expectation-value is diagonal in these indices. This gives (lightening the notation) which gives

$$G^{<} = -\frac{\mathrm{i}}{\hbar}\zeta \mathrm{e}^{-\mathrm{i}-\xi t/\hbar}\frac{1}{Z}\sum_{j\in\mathbb{N}}\left\langle j \mid \mathrm{e}^{-\beta(\epsilon-\mu)c^{\dagger}c}c^{\dagger}c \mid j\right\rangle = \dots \tag{33.29}$$

Now we simplify

$$\begin{aligned}
\frac{1}{Z}\sum_{j\in\mathbb{N}}\left\langle j \mid \mathrm{e}^{-\beta(\epsilon-\mu)c^{\dagger}c}c^{\dagger}c \mid j\right\rangle &= \frac{\sum_{j\in\mathbb{N}} j\mathrm{e}^{-\beta(\epsilon-\mu)j}}{\sum_{j\in\mathbb{N}}\mathrm{e}^{-\beta(\epsilon-\mu)j}} \\
&= -\partial_x \log \sum_{j\in\mathbb{N}} \mathrm{e}^{-\beta(\epsilon-\mu)x}\Big|_{x=\beta(\epsilon-\mu)} \\
&= -\partial_x \log \frac{1}{(1-\zeta\mathrm{e}^{-x})^{\zeta}}\Big|_{x=\beta(\epsilon-\mu)} \\
&= -\partial_x \log (1-\zeta\mathrm{e}^{-x})^{-\zeta}\Big|_{x=\beta(\epsilon-\mu)} \\
&= \zeta\partial_x \log (1-\zeta\mathrm{e}^{-x})\Big|_{x=\beta(\epsilon-\mu)} \\
&= \zeta^2 \frac{\mathrm{e}^{-x}}{1-\zeta}\Big|_{x=\beta(\epsilon-\mu)} \\
&= \mathrm{n}^{\zeta}_{\hbar\beta}(\xi)
\end{aligned} \tag{33.30}$$

whereas in the last step we used Notation 9.62. This yields therefore

$$\dots = -\frac{\mathrm{i}}{\hbar}\zeta \mathrm{e}^{-\mathrm{i}\xi t/\hbar}\,\mathrm{n}^{\zeta}_{\hbar\beta}(\xi) \tag{33.31}$$

We compute further

$$\begin{aligned}
\frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}\xi t/\hbar} &= \frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}\xi t/\hbar}\left\langle [c, c^{\dagger}]_{\zeta}\right\rangle \\
&= \frac{\mathrm{i}}{\hbar}\left\langle c(t)c^{\dagger}\right\rangle - \zeta\frac{\mathrm{i}}{\hbar}\left\langle c^{\dagger}c(t)\right\rangle \\
&= -G^{>}(t) + G^{<}(t)
\end{aligned} \tag{33.32}$$

which can be rewritten as

$$\begin{aligned}
G^{>}(t) &= G^{<}(t) - \frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}\xi t/\hbar} \\
&= -\frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}\xi t/\hbar}\left(\zeta\,\mathrm{n}^{\zeta}_{\hbar\beta}(\xi) + 1\right)
\end{aligned} \tag{33.33}$$

This then gives eventually

$$\begin{aligned}
G^{\mathbb{T}}(t) &= \theta(t)G^{>}(t) + \theta(-t)G^{<} \\
&= -\frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}\xi t/\hbar}\left(\left(1+\zeta\,\mathrm{n}^{\zeta}_{\hbar\beta}(\xi)\right)\theta(t) + \theta(-t)\zeta\,\mathrm{n}^{\zeta}_{\hbar\beta}(\xi)\right)
\end{aligned} \tag{33.34}$$

And further we obtain

$$\begin{aligned}
G^{\mathrm{ret}}(t) &= \theta(t)\left(G^{>}(t) - G^{<}(t)\right) \\
&= \theta(t)\left(-\frac{\mathrm{i}}{\hbar}\right)\mathrm{e}^{-\mathrm{i}\xi t/\hbar}
\end{aligned} \tag{33.35}$$

and we also obtain

$$\begin{aligned} G^{\text{adv}}(t) &= \theta(-t)\left(G^{<}(t) - G^{>}(t)\right) \\ &= \theta(-t)\left(\frac{\mathrm{i}}{\hbar}\right)\mathrm{e}^{-\mathrm{i}\xi t/\hbar} \end{aligned} \tag{33.36}$$

Now we transition to the frequency-versions of these equations and obtain

$$\begin{aligned} G^{<}(\omega) &= \int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t} G^{<}(t) \\ &= -\frac{\mathrm{i}}{\hbar}\zeta\, \mathrm{n}^{\zeta}_{\hbar\beta}(\xi) \underbrace{\int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t - \mathrm{i}\xi t/\hbar}}_{=2\pi\delta(\omega-\xi/\hbar)} \end{aligned} \tag{33.37}$$

and likewise we obtain

$$\begin{aligned} G^{>}(\omega) &= \int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t} G^{>}(t) \\ &= -\frac{\mathrm{i}}{\hbar}\left(1 + \zeta\, \mathrm{n}^{\zeta}_{\hbar\beta}(\xi)\right) \underbrace{\int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t - \mathrm{i}\xi t/\hbar}}_{=2\pi\delta(\omega-\xi/\hbar)} \end{aligned} \tag{33.38}$$

The identities for G^{ret} and G^{adv} follow by computing the integral. For the time-ordered Green-function we obtain

$$\begin{aligned} G^{\mathbb{T}}_{\eta}(\omega) &= \int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t} G^{\mathbb{T}}_{\eta}(t) \\ &= \int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t} G^{\mathbb{T}}(t) \mathrm{e}^{-\eta|t|} \\ &= -\frac{\mathrm{i}}{\hbar}\left(1 + \zeta\, \mathrm{n}^{\zeta}_{\hbar\beta}(\omega)\right) \int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t} \mathrm{e}^{-\eta|t|} \mathrm{e}^{-\mathrm{i}\xi t/\hbar}\theta(t) \\ &+ \zeta\left(-\frac{\mathrm{i}}{\hbar}\right) \mathrm{n}^{\zeta}_{\hbar\beta}(\omega) \int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t} \mathrm{e}^{-\eta|t|} \mathrm{e}^{-\mathrm{i}t\xi/\hbar}\theta(-t) \\ &= \frac{1 - \zeta\, \mathrm{n}^{\zeta}_{\hbar\beta}(\omega)}{\hbar} \frac{1}{\omega + \mathrm{i}\eta - \xi/\hbar} - \zeta \frac{\mathrm{n}^{\zeta}_{\hbar\beta}(\omega)}{\hbar} \frac{1}{\omega - \mathrm{i}\eta - \xi/\hbar} \end{aligned} \tag{33.39}$$

Lastly we obtain

$$\begin{aligned} G^{\overline{\mathbb{T}}}(t) &= \theta(-t)G^{>}(t) + \theta(t)G^{<} \\ &= -\frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\mathrm{i}\xi t/\hbar}\left(\theta(-t)\left(1 + \zeta\, \mathrm{n}^{\zeta}_{\hbar\beta}(\omega)\right) + \theta(t)\zeta\, \mathrm{n}^{\zeta}_{\hbar\beta}(\omega)\right) \end{aligned} \tag{33.40}$$

and

$$
\begin{aligned}
G_{\eta}^{\overline{\mathbb{T}}}(\omega) &= \int \mathrm{d}t\, G_{\eta}^{\overline{\mathbb{T}}}(t) \\
&= \int \mathrm{d}t\, G^{\overline{\mathbb{T}}}(t) \mathrm{e}^{-\eta|t|} \\
&= -\frac{\mathrm{i}}{\hbar}\left(1+\zeta\, \mathrm{n}_{\hbar\beta}^{\zeta}(\omega)\right) \int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t} \mathrm{e}^{-\mathrm{i}\xi t/\hbar} \mathrm{e}^{-\eta|t|} \theta(-t) \\
&= -\frac{\mathrm{i}}{\hbar} \zeta\, \mathrm{n}_{\hbar\beta}^{\zeta}(\omega) \int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t} \mathrm{e}^{-\mathrm{i}\xi t/\hbar} \mathrm{e}^{-\eta|t|} \theta(t) \\
&= -\frac{1+\zeta\, \mathrm{n}_{\hbar\beta}^{\zeta}(\omega)}{\hbar} \frac{1}{\omega - \mathrm{i}\eta - \xi/\hbar} + \frac{\zeta\, \mathrm{n}_{\hbar\beta}^{\zeta}(\omega)}{\hbar} \frac{1}{\omega + \mathrm{i}\eta - \xi/\hbar}
\end{aligned}
\tag{33.41}
$$

Proof 33.0 of Lemma 12.13 We consider the unit-vector

$$
\frac{\boldsymbol{\epsilon}}{\epsilon} \equiv \mathbf{n} \equiv n_x \mathbf{e}_x + n_y \mathbf{e}_y + n_z \mathbf{e}_z \in \mathrm{S}^2 \subset \mathbb{R}^3
$$

and find that

$$
H \equiv H(\mathbf{n}) := \epsilon_0 \sigma_0 + \epsilon \mathbf{n} \cdot \boldsymbol{\sigma} = \epsilon_0 \sigma_0 + \epsilon \left(n_x \sigma_x + n_y \sigma_y + n_z \sigma_z\right).
$$

Therefore, if $|\lambda\rangle$ is an eigenstate of $\mathbf{n} \cdot \boldsymbol{\sigma}$ with eigenvalue λ then it follows

$$
\epsilon_0 \sigma_0 + \epsilon \left(n_x \sigma_x + n_y \sigma_y + n_z \sigma_z\right) |\lambda\rangle = \left(\epsilon_0 \sigma_0 + \epsilon \lambda\right) |\lambda\rangle
$$

therefore $|\lambda\rangle$ is also ein eigenvalue of H with eigenvalue $\left(\epsilon_0 \sigma_0 + \epsilon \lambda\right)$.

Proof 33.0 of Lemma 12.15 We compute the eigenvalues of the 2×2-matrix:

$$
\mathbf{n} \cdot \boldsymbol{\sigma} = \begin{pmatrix} n_z & -\mathrm{i}n_y + n_x \\ +\mathrm{i}n_y + n_x & -n_z \end{pmatrix}
$$

by solving the characteristic equation

$$
\begin{aligned}
&\mathrm{Det}\left(\mathbf{n} \cdot \boldsymbol{\sigma} - \lambda \cdot \mathbf{1}_{2\times 2}\right) = \mathrm{Det} \begin{pmatrix} n_z - \lambda & -\mathrm{i}n_y + n_x \\ +\mathrm{i}n_y + n_x & -n_z - \lambda \end{pmatrix} \overset{\text{Binomial Formulae}}{=} \lambda^2 - n_z^2 - (n_x^2 + n_y^2) = \lambda^2 - \mathbf{n}^2 = 0 \\
&\iff \lambda^2 = \mathbf{n}^2 = 1 \iff \lambda_{\pm} = \pm 1
\end{aligned}
$$

Now we compute the eigenstates of $\mathbf{n} \cdot \boldsymbol{\sigma}$:

$$\begin{aligned}\mathrm{Kern}\left(\mathbf{n}\cdot\boldsymbol{\sigma}-(\pm 1)\cdot\mathbf{1}_{2\times 2}\right) &= \mathrm{Kern}\begin{pmatrix} n_z\mp 1 & -\mathrm{i}n_y+n_x \\ 0 & 0\end{pmatrix} \\ &= \left\{\begin{pmatrix} v_1 \\ v_2\end{pmatrix}\in\mathbb{C}^2 \,|\, (n_z\mp 1)v_1+(-\mathrm{i}n_y+n_x)v_2=0\right\} \\ &= \mathrm{Span}_{\alpha\in\mathbb{C}}\left\{\begin{pmatrix} \alpha \\ \frac{-(n_z\mp 1)\alpha}{n_x-\mathrm{i}n_y}\end{pmatrix}\right\} \qquad (\star)\end{aligned}$$

The eigenstate to the eigenvalue $+1$:

We multiply a "clever one"

$$\frac{1}{n_x-\mathrm{i}n_y}=\frac{n_x+\mathrm{i}n_y}{n_x^2+n_y^2}=\frac{(\cos(\phi)+\mathrm{i}\sin(\phi))\sin(\theta)}{\left(\cos^2(\phi)+\sin^2(\phi)\right)\sin^2(\theta)}=\frac{\mathrm{e}^{\mathrm{i}\phi}}{\sin(\theta)}$$

In order to reproduce the control result, we consider[6] the eigenvector in $(\star)$ with $\alpha=\cos\frac{\theta}{2}$. Then it follows for the eigenvector

$$\begin{aligned}|\uparrow_{\mathbf{n}}\rangle &= \cos\frac{\theta}{2}|\uparrow\rangle+\frac{(1-n_z)\cos\frac{\theta}{2}}{n_x-\mathrm{i}n_y}|\downarrow\rangle \\ &= \cos\frac{\theta}{2}|\uparrow\rangle+\frac{(1-\cos(\theta))\cos(\frac{\theta}{2})}{\sin(\theta)}\mathrm{e}^{\mathrm{i}\phi}|\downarrow\rangle \\ &= \cos\frac{\theta}{2}|\uparrow\rangle+\sin\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\phi}|\downarrow\rangle\end{aligned}$$

whereas in the last equation-sign we used a standard-result[7] in the last step. This eigenstate is also normalized as one finds

$$\langle\uparrow_{\mathbf{n}}|\uparrow_{\mathbf{n}}\rangle=\left(\cos\frac{\theta}{2}\langle\uparrow|+\sin\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\phi}\langle\downarrow|\right)\left(\cos\frac{\theta}{2}|\uparrow\rangle+\sin\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\phi}|\downarrow\rangle\right)=\cos^2\frac{\theta}{2}+\sin^2\frac{\theta}{2}=1.$$

The eigenstate to the eigenvalue -1:

This eigenstate can be concluded by demanding orthogonality to $|\uparrow_{\mathbf{n}}\rangle$. One finds that

$$|\downarrow_{\mathbf{n}}\rangle=\sin\frac{\theta}{2}|\uparrow\rangle-\cos\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\phi}|\downarrow\rangle$$

is orthogonal since

$$\langle\downarrow_{\mathbf{n}}|\uparrow_{\mathbf{n}}\rangle=\left(\sin\frac{\theta}{2}\langle\uparrow|-\cos\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\phi}\langle\downarrow|\right)\left(\cos\frac{\theta}{2}|\uparrow\rangle+\sin\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\phi}|\downarrow\rangle\right)=\sin\frac{\theta}{2}\cos\frac{\theta}{2}-\cos\frac{\theta}{2}\sin\frac{\theta}{2}\mathrm{e}^{0}=0$$

[6] Recall that a complex eigenvector is only unique up to a complex phase.
[7] See [59].

Analogously one finds that $|\downarrow_{\mathbf{n}}\rangle$ is normalized.

Remark: In the limit $\mathbf{n} \to \mathbf{e}_z$ one obtains states, that are in the same equivalence-class of states as the usual ones of the third Pauli-matrix.

Proof 33.0 of Corollary 12.16 The equations

$$\begin{aligned} |\uparrow_n\rangle &= \cos\frac{\theta}{2}|\uparrow\rangle + \sin\frac{\theta}{2}e^{i\phi}|\downarrow\rangle \\ |\downarrow_n\rangle &= \sin\frac{\theta}{2}|\uparrow\rangle - \cos\frac{\theta}{2}e^{i\phi}|\downarrow\rangle \end{aligned}$$

can be rewritten in matrix-form as

$$\begin{aligned} \begin{pmatrix} |\uparrow_n\rangle \\ |\downarrow_n\rangle \end{pmatrix} &= \begin{pmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2}e^{i\phi} \\ \sin\frac{\theta}{2} & -\cos\frac{\theta}{2}e^{i\phi} \end{pmatrix} \begin{pmatrix} |\uparrow\rangle \\ |\downarrow\rangle \end{pmatrix} \\ \iff \begin{pmatrix} |\uparrow\rangle \\ |\downarrow\rangle \end{pmatrix} &= \begin{pmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2} \\ \sin\frac{\theta}{2}e^{-i\phi} & -\cos\frac{\theta}{2}e^{-i\phi} \end{pmatrix} \begin{pmatrix} |\uparrow_n\rangle \\ |\downarrow_n\rangle \end{pmatrix} \end{aligned}$$

since the determinant of the first matrix is equal to $-e^{i\phi}$, and therefore we have

$$\begin{aligned} |\uparrow\rangle &= \cos\frac{\theta}{2}|\uparrow_n\rangle + \sin\frac{\theta}{2}|\downarrow_n\rangle \\ |\downarrow\rangle &= \sin\frac{\theta}{2}e^{-i\phi}|\uparrow_n\rangle - \cos\frac{\theta}{2}e^{-i\phi}|\downarrow_n\rangle \end{aligned}$$

Proof 33.0 of Corollary 29.115 One finds

$$\begin{aligned} (\omega - \xi_\downarrow)\cos^2\frac{\theta}{2} + (\omega - \xi_\uparrow)\sin^2\frac{\theta}{2} &= \omega - (\epsilon_0 - \epsilon_z)\cos^2\frac{\theta}{2} - (\epsilon_0 + \epsilon_z)\sin^2\frac{\theta}{2} \\ &= \omega - \epsilon_0 + \epsilon_z(\cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2}) \\ &= \omega - \epsilon_0 + \epsilon_z \end{aligned}$$

whereas we used $\cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2} = \cos\theta$, etc. for the other entries.

Proof 33.31 of Theorem 12.21

The Lesser Temporal Green-function

Starting from Definition 12.19

$$D^{<}_{\substack{\nu,\nu' \\ \mathbf{q},\mathbf{q}'}}(t) = -\frac{\mathrm{i}}{\hbar}\left\langle A^{\dagger}_{\nu'}(0,\mathbf{q}')A_{\nu}(t,\mathbf{q})\right\rangle . \tag{33.42}$$

we simply insert Definition 12.18 for the displacement-operators

$$A_{\nu}(\mathbf{q}) = c_{\mathbf{q}\nu} + c^{\dagger}_{-\mathbf{q}\nu}, \qquad A^{\dagger}_{\nu'}(\mathbf{q}') = c^{\dagger}_{\mathbf{q}'\nu'} + c_{-\mathbf{q}'\nu'}. \tag{33.43}$$

and we use that for the non-interacting phonon Hamiltonian from Remark 8.28.4

$$H_0 = \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} \Omega_{\mathbf{q}\nu}\, c^{\dagger}_{\mathbf{q}\nu}c_{\mathbf{q}\nu}, \qquad \text{with } \Omega_{\mathbf{q}\nu} = \hbar\omega_{\mathbf{q}\nu}, \tag{33.44}$$

the Heisenberg operators evolve according to Lemma 8.27 as

$$c_{\mathbf{q}\nu}(t) = e^{-\mathrm{i}\omega_{\mathbf{q}\nu}t}c_{\mathbf{q}\nu}, \qquad c^{\dagger}_{\mathbf{q}\nu}(t) = e^{+\mathrm{i}\omega_{\mathbf{q}\nu}t}c^{\dagger}_{\mathbf{q}\nu}. \tag{33.45}$$

Consequently we find for the time-evolution of the displacement-operators the equation,

$$A_{\nu}(t,\mathbf{q}) = e^{-\mathrm{i}\omega_{\mathbf{q}\nu}t}c_{\mathbf{q}\nu} + e^{+\mathrm{i}\omega_{-\mathbf{q}\nu}t}c^{\dagger}_{-\mathbf{q}\nu}. \tag{33.46}$$

Assuming that time-reversal symmetry is not broken, we obtain with Remark 8.28.6 that $\omega_{-\mathbf{q}\nu} = \omega_{\mathbf{q}\nu}$, such that we obtain

$$D^{<}_{\substack{\nu\nu' \\ \mathbf{q},\mathbf{q}'}}(t) = -\frac{\mathrm{i}}{\hbar}\left\langle \left(c^{\dagger}_{\mathbf{q}'\nu'} + c_{-\mathbf{q}'\nu'}\right)\left(e^{-\mathrm{i}\omega_{\mathbf{q}\nu}t}c_{\mathbf{q}\nu} + e^{+\mathrm{i}\omega_{\mathbf{q}\nu}t}c^{\dagger}_{-\mathbf{q}\nu}\right)\right\rangle \tag{33.47}$$

$$= -\frac{\mathrm{i}}{\hbar}\left[e^{-\mathrm{i}\omega_{\mathbf{q}\nu}t}\left\langle c^{\dagger}_{\mathbf{q}'\nu'}c_{\mathbf{q}\nu}\right\rangle + e^{+\mathrm{i}\omega_{\mathbf{q}\nu}t}\left\langle c_{-\mathbf{q}'\nu'}c^{\dagger}_{-\mathbf{q}\nu}\right\rangle\right]. \tag{33.48}$$

whereas we used in the last equation that we don't have any interaction-terms, the anomalous expectation values vanish, i.e.

$$\left\langle c^{\dagger}_{\mathbf{q}'\nu'}c^{\dagger}_{-\mathbf{q}\nu}\right\rangle = \left\langle c_{-\mathbf{q}'\nu'}c_{\mathbf{q}\nu}\right\rangle = 0. \tag{33.49}$$

For the other expectation-value we obtain the regular case of non-interacting bosons with Remark 12.9.1,

$$\left\langle c^\dagger_{\mathbf{q}'\nu'} c_{\mathbf{q}\nu} \right\rangle = \delta_{\mathbf{q},\mathbf{q}'}\delta_{\nu,\nu'}\, \mathrm{B}_\beta(\Omega_{\mathbf{q}\nu}), \qquad \text{and } \left\langle c_{-\mathbf{q}'\nu'} c^\dagger_{-\mathbf{q}\nu} \right\rangle = \delta_{\mathbf{q},\mathbf{q}'}\delta_{\nu,\nu'} \left[\mathrm{B}_\beta(\Omega_{\mathbf{q}\nu}) + 1\right], \tag{33.50}$$

whereas we used the CCR in Equation (10.4) and with the Bose-function from Notation 9.64. Therefore we obtain

$$D^<_{\substack{\nu\nu' \\ \mathbf{q},\mathbf{q}'}}(t) = -\frac{\mathrm{i}}{\hbar}\delta_{\nu,\nu'}\delta_{\mathbf{q},\mathbf{q}'}\left[\mathrm{B}_\beta(\Omega_{\mathbf{q}\nu})e^{-\mathrm{i}\omega_{\mathbf{q}\nu}t} + \left(\mathrm{B}_\beta(\Omega_{\mathbf{q}\nu}) + 1\right)e^{+\mathrm{i}\omega_{\mathbf{q}\nu}t}\right]. \tag{33.51}$$

Thus the Green function is diagonal in momentum and branch indices,

$$D^<_{\substack{\nu\nu' \\ \mathbf{q},\mathbf{q}'}}(t) = \delta_{\nu,\nu'}\delta_{\mathbf{q},\mathbf{q}'}D^<_{\mathbf{q}\nu}(t), \qquad \text{with} \qquad D^<_{\mathbf{q}\nu}(t) = -\frac{\mathrm{i}}{\hbar}\left[\left(\mathrm{B}_\beta(\Omega_{\mathbf{q}\nu}) + 1\right)e^{+\mathrm{i}\omega_{\mathbf{q}\nu}t} + \mathrm{B}_\beta(\Omega_{\mathbf{q}\nu})e^{-\mathrm{i}\omega_{\mathbf{q}\nu}t}\right]. \tag{33.52}$$

The Greater Temporal Green-function

Starting from Definition 12.19

$$D^>_{\substack{\nu,\nu' \\ \mathbf{q},\mathbf{q}'}}(t) = -\frac{\mathrm{i}}{\hbar}\left\langle A_\nu(t,\mathbf{q})A^\dagger_{\nu'}(0,\mathbf{q}')\right\rangle. \tag{33.53}$$

Using now Definition 12.18 for the displacement-operators and the Heisenberg-evolution according to Lemma 8.27 as

$$A_\nu(t,\mathbf{q}) = e^{-\mathrm{i}\omega_{\mathbf{q}\nu}t}c_{\mathbf{q}\nu} + e^{+\mathrm{i}\omega_{\mathbf{q}\nu}t}c^\dagger_{-\mathbf{q}\nu},, \qquad A^\dagger_{\nu'}(\mathbf{q}',0) = c^\dagger_{\mathbf{q}'\nu'} + c_{-\mathbf{q}'\nu'}, \tag{33.54}$$

we find

$$D^>_{\substack{\nu,\nu' \\ \mathbf{q},\mathbf{q}'}}(t) = -\frac{\mathrm{i}}{\hbar}\left\langle\left(e^{-\mathrm{i}\omega_{\mathbf{q}\nu}t}c_{\mathbf{q}\nu} + e^{+\mathrm{i}\omega_{\mathbf{q}\nu}t}c^\dagger_{-\mathbf{q}\nu}\right)\left(c^\dagger_{\mathbf{q}'\nu'} + c_{-\mathbf{q}'\nu'}\right)\right\rangle. \tag{33.55}$$

The anomalous expectation values vanish again, i.e.

$$\left\langle c_{\mathbf{q}\nu}c_{-\mathbf{q}'\nu'}\right\rangle = \left\langle c^\dagger_{-\mathbf{q}\nu}c^\dagger_{\mathbf{q}'\nu'}\right\rangle = 0. \tag{33.56}$$

Therefore we obtain

$$D^>_{\substack{\nu,\nu' \\ \mathbf{q},\mathbf{q}'}}(t) = -\frac{\mathrm{i}}{\hbar}\left[e^{-\mathrm{i}\omega_{\mathbf{q}\nu}t}\left\langle c_{\mathbf{q}\nu}c^\dagger_{\mathbf{q}'\nu'}\right\rangle + e^{+\mathrm{i}\omega_{\mathbf{q}\nu}t}\left\langle c^\dagger_{-\mathbf{q}\nu}c_{-\mathbf{q}'\nu'}\right\rangle\right]. \tag{33.57}$$

For thermal bosons we obtain again with Remark 12.9.1

$$\left\langle c_{\mathbf{q}\nu} c^{\dagger}_{\mathbf{q}'\nu'} \right\rangle = \delta_{\mathbf{q},\mathbf{q}'}\delta_{\nu,\nu'} \left[\mathrm{B}_{\beta}(\Omega_{\mathbf{q}\nu}) + 1 \right], \qquad \left\langle c^{\dagger}_{-\mathbf{q}\nu} c_{-\mathbf{q}'\nu'} \right\rangle = \delta_{\nu,\nu'}\delta_{\mathbf{q},\mathbf{q}'}\, \mathrm{B}_{\beta}(\Omega_{\mathbf{q}\nu}), \tag{33.58}$$

with the Bose-function from Notation 9.64. Hence,

$$D^{>}_{\substack{\nu,\nu' \\ \mathbf{q},\mathbf{q}'}}(t) = -\frac{\mathrm{i}}{\hbar}\delta_{\nu,\nu'}\delta_{\mathbf{q},\mathbf{q}'} \left[\left(\mathrm{B}_{\beta}(\omega_{\mathbf{q}\nu}) + 1 \right) e^{-\mathrm{i}\omega_{\mathbf{q}\nu}t} + \mathrm{B}_{\beta}(\omega_{\mathbf{q}\nu}) e^{+\mathrm{i}\omega_{\mathbf{q}\nu}t} \right]. \tag{33.59}$$

Thus,

$$D^{>}_{\substack{\nu,\nu' \\ \mathbf{q},\mathbf{q}'}}(t) = \delta_{\nu,\nu'}\delta_{\mathbf{q},\mathbf{q}'} D^{>}_{\mathbf{q}\nu}(t), \qquad \text{with } D^{>}_{\mathbf{q}\nu}(t) = -\frac{\mathrm{i}}{\hbar} \left[\left(\mathrm{B}_{\beta}(\Omega_{\mathbf{q}\nu}) + 1 \right) e^{-\mathrm{i}\omega_{\mathbf{q}\nu}t} + \mathrm{B}_{\beta}(\Omega_{\mathbf{q}\nu}) e^{+\mathrm{i}\omega_{\mathbf{q}\nu}t} \right]. \tag{33.60}$$

Time- and Anti-Time-Ordered Temporal Green-Functions

For these, we simply use Lemma 12.4 and obtain the desired identities.

Retarded Temporal Green-function

Starting from Definition 12.19

$$D^{\mathrm{ret}}_{\substack{\nu\nu' \\ \mathbf{q},\mathbf{q}'}}(t,t') = -\frac{\mathrm{i}}{\hbar}\,\theta(t-t') \left\langle \left[A_{\nu}(t,\mathbf{q}), A^{\dagger}_{\nu'}(t',\mathbf{q}') \right] \right\rangle. \tag{33.61}$$

Using now Definition 12.18 for the displacement-operators and the Heisenberg-evolution according to Lemma 8.27 as

$$A_{\nu}(t,\mathbf{q}) = e^{-\mathrm{i}\omega_{\mathbf{q}\nu}t} c_{\mathbf{q}\nu} + e^{+\mathrm{i}\omega_{\mathbf{q}\nu}t} c^{\dagger}_{-\mathbf{q}\nu},, \qquad A^{\dagger}_{\nu'}(t',\mathbf{q}') = e^{+\mathrm{i}\omega_{\mathbf{q}'\nu't'}} c^{\dagger}_{\mathbf{q}'\nu'} + e^{-\mathrm{i}\omega_{\mathbf{q}'\nu't'}} c_{-\mathbf{q}'\nu'}, \tag{33.62}$$

the commutator becomes

$$\left[A_{\nu}(t,\mathbf{q}), A^{\dagger}_{\nu'}(t',\mathbf{q}') \right] = e^{-\mathrm{i}\omega_{\mathbf{q}\nu}t} e^{+\mathrm{i}\omega_{\mathbf{q}'\nu't'}} \left[c_{\mathbf{q}\nu}, c^{\dagger}_{\mathbf{q}'\nu'} \right] + e^{+\mathrm{i}\omega_{\mathbf{q}\nu}t} e^{-\mathrm{i}\omega_{\mathbf{q}'\nu't'}} \left[c^{\dagger}_{-\mathbf{q}\nu}, c_{-\mathbf{q}'\nu'} \right]. \tag{33.63}$$

The mixed commutators vanish due to the CCR in Equation (10.4):

$$\left[c_{\mathbf{q}\nu}, c_{-\mathbf{q}'\nu'} \right] = \left[c^{\dagger}_{-\mathbf{q}\nu}, c^{\dagger}_{\mathbf{q}'\nu'} \right] = 0. \tag{33.64}$$

and for the other commutators we obtain

$$\left[c_{\mathbf{q}\nu}, c^{\dagger}_{\mathbf{q}'\nu'} \right] = \delta_{\mathbf{q},\mathbf{q}'}\delta_{\nu,\nu'},, \qquad \left[c^{\dagger}_{-\mathbf{q}\nu}, c_{-\mathbf{q}'\nu'} \right] = -\delta_{\mathbf{q},\mathbf{q}'}\delta_{\nu,\nu'}. \tag{33.65}$$

Therefore,

$$\left[A_\nu(t,\mathbf{q}),A^\dagger_{\nu'}(t',\mathbf{q}')\right]=\delta_{\nu,\nu'}\delta_{\mathbf{q},\mathbf{q}'}\left[e^{-\mathrm{i}\omega_{\mathbf{q}\nu}(t-t')}-e^{+\mathrm{i}\omega_{\mathbf{q}\nu}(t-t')}\right]. \tag{33.66}$$

Using the identity

$$e^{-\mathrm{i}x}-e^{+\mathrm{i}x}=-2\mathrm{i}\sin(x), \tag{33.67}$$

we obtain

$$\left[A_\nu(t,\mathbf{q}),A^\dagger_{\nu'}(t',\mathbf{q}')\right]=-2\mathrm{i}\,\delta_{\nu,\nu'}\delta_{\mathbf{q},\mathbf{q}'}\sin\left(\omega_{\mathbf{q}\nu}(t-t')\right). \tag{33.68}$$

Substitution into the retarded Green-function in Equation (33.61) gives

$$D^{\mathrm{ret}}_{\substack{\nu,\nu'\\ \mathbf{q},\mathbf{q}'}}(t,t')=-\frac{\mathrm{i}}{\hbar}\theta(t-t')\left[-2\mathrm{i}\,\delta_{\mathbf{q},\mathbf{q}'}\delta_{\nu,\nu'}\sin\left(\omega_{\mathbf{q}\nu}(t-t')\right)\right]=-\frac{2}{\hbar}\delta_{\mathbf{q},\mathbf{q}'}\delta_{\nu,\nu'}\theta(t-t')\sin\left[\omega_{\mathbf{q}\nu}(t-t')\right]. \tag{33.69}$$

Hence the retarded Green function is diagonal in momentum and branch indices:

$$D^{\mathrm{ret}}_{\substack{\nu,\nu'\\ \mathbf{q},\mathbf{q}'}}(t,t')=\delta_{\nu,\nu'}\delta_{\mathbf{q},\mathbf{q}'}D^{\mathrm{ret}}_{\mathbf{q}\nu}(t-t'),\qquad\text{with } D^{\mathrm{ret}}_{\mathbf{q}\nu}(t-t')=-\frac{2}{\hbar}\theta(t-t')\sin\left[\omega_{\mathbf{q}\nu}(t-t')\right]. \tag{33.70}$$

Temporal advanced Green-function Derivation

Starting from Definition 12.19

$$D^{\mathrm{adv}}_{\substack{\nu,\nu'\\ \mathbf{q},\mathbf{q}'}}(t,t')=\frac{\mathrm{i}}{\hbar}\,\theta(t'-t)\,\left\langle\left[A_\nu(t,\mathbf{q}),A^\dagger_{\nu'}(t',\mathbf{q}')\right]\right\rangle. \tag{33.71}$$

Notice that the only difference relative to the retarded Green-function is the prefactor. This gives thus for the advanced Green-function

$$D^{\mathrm{adv}}_{\substack{\nu,\nu'\\ \mathbf{q},\mathbf{q}'}}(t,t')=\delta_{\nu,\nu'}\,\delta_{\mathbf{q},\mathbf{q}'}\,D^{\mathrm{adv}}_{\mathbf{q}\nu}(t-t'),\qquad\text{with}\qquad D^{\mathrm{adv}}_{\mathbf{q}\nu}(t-t')=\frac{2}{\hbar}\,\theta(t'-t)\,\sin\left[\omega_{\mathbf{q}\nu}(t-t')\right]. \tag{33.72}$$

The Frequency-Version of the Lesser Green-Function

We start from the already derived temporal expression in Equation (33.52)

$$D^{<}_{\mathbf{q}\nu}(t)=-\frac{\mathrm{i}}{\hbar}\left[\left(\mathrm{B}_\beta(\Omega_{\mathbf{q}\nu})+1\right)e^{+\mathrm{i}\omega_{\mathbf{q}\nu}t}+\mathrm{B}_\beta(\Omega_{\mathbf{q}\nu})e^{-\mathrm{i}\omega_{\mathbf{q}\nu}t}\right]. \tag{33.73}$$

Applying the Fourier transform from Notation 1.17,

$$
\begin{aligned}
D^{<}_{\mathbf{q}\nu}(\omega) &= \int_{-\infty}^{+\infty} \mathrm{d}t\, e^{+\mathrm{i}\omega t} D^{<}_{\mathbf{q}\nu}(t) \\
&= -\frac{\mathrm{i}}{\hbar} \int_{-\infty}^{+\infty} \mathrm{d}t\, e^{+\mathrm{i}\omega t} \left[\left(\mathrm{B}_{\beta}(\Omega_{\mathbf{q}\nu}) + 1 \right) e^{+\mathrm{i}\omega_{\mathbf{q}\nu} t} + \mathrm{B}_{\beta}(\Omega_{\mathbf{q}\nu}) e^{-\mathrm{i}\omega_{\mathbf{q}\nu} t} \right] \\
&= -\frac{\mathrm{i}}{\hbar} \left[\left(\mathrm{B}_{\beta}(\Omega_{\mathbf{q}\nu}) + 1 \right) \int_{-\infty}^{+\infty} \mathrm{d}t\, e^{+\mathrm{i}(\omega+\omega_{\mathbf{q}\nu})t} + \mathrm{B}_{\beta}(\Omega_{\mathbf{q}\nu}) \int_{-\infty}^{+\infty} \mathrm{d}t\, e^{+\mathrm{i}(\omega-\omega_{\mathbf{q}\nu})t} \right].
\end{aligned} \tag{33.74}
$$

Using now Theorem 1.22, i.e.

$$
\int_{-\infty}^{+\infty} \mathrm{d}t\, e^{\mathrm{i}xt} = 2\pi\delta(x), \tag{33.75}
$$

we obtain

$$
D^{<}_{\mathbf{q}\nu}(\omega) = \ldots = -\frac{2\pi i}{\hbar} \left[\left(\mathrm{B}_{\beta}(\Omega_{\mathbf{q}\nu}) + 1 \right) \delta(\omega + \omega_{\mathbf{q}\nu}) + \mathrm{B}_{\beta}(\Omega_{\mathbf{q}\nu}) \delta(\omega - \omega_{\mathbf{q}\nu}) \right]. \tag{33.76}
$$

Therefore we obtain

$$
D^{<}_{\mathbf{q}\nu}(\omega) = -\frac{2\pi i}{\hbar} \left[\left(\mathrm{B}_{\beta}(\Omega_{\mathbf{q}\nu}) + 1 \right) \delta(\omega + \omega_{\mathbf{q}\nu}) + \mathrm{B}_{\beta}(\Omega_{\mathbf{q}\nu}) \delta(\omega - \omega_{\mathbf{q}\nu}) \right]. \tag{33.77}
$$

The Frequency-Version of the Greater Green-Function

We start from the already derived temporal expression in Equation (33.60)

$$
D^{>}_{\mathbf{q}\nu}(t) = -\frac{\mathrm{i}}{\hbar} \left[\left(\mathrm{B}_{\beta}(\Omega_{\mathbf{q}\nu}) + 1 \right) e^{-\mathrm{i}\omega_{\mathbf{q}\nu} t} + \mathrm{B}_{\beta}(\Omega_{\mathbf{q}\nu}) e^{+\mathrm{i}\omega_{\mathbf{q}\nu} t} \right]. \tag{33.78}
$$

Applying the Fourier transform from Notation 1.17,

$$
\begin{aligned}
D^{>}_{\mathbf{q}\nu}(\omega) &= \int_{-\infty}^{+\infty} \mathrm{d}t\, e^{+\mathrm{i}\omega t} D^{>}_{\mathbf{q}\nu}(t) && (33.79) \\
&= -\frac{\mathrm{i}}{\hbar} \int_{-\infty}^{+\infty} \mathrm{d}t\, e^{+\mathrm{i}\omega t} \left[\left(\mathrm{B}_{\beta}(\Omega_{\mathbf{q}\nu}) + 1 \right) e^{-\mathrm{i}\omega_{\mathbf{q}\nu} t} + \mathrm{B}_{\beta}(\Omega_{\mathbf{q}\nu}) e^{+\mathrm{i}\omega_{\mathbf{q}\nu} t} \right] && (33.80) \\
&= -\frac{\mathrm{i}}{\hbar} \left[\left(\mathrm{B}_{\beta}(\Omega_{\mathbf{q}\nu}) + 1 \right) \int_{-\infty}^{+\infty} \mathrm{d}t\, e^{+\mathrm{i}(\omega-\omega_{\mathbf{q}\nu})t} + \mathrm{B}_{\beta}(\Omega_{\mathbf{q}\nu}) \int_{-\infty}^{+\infty} \mathrm{d}t\, e^{+\mathrm{i}(\omega+\omega_{\mathbf{q}\nu})t} \right] && (33.81) \\
&= \ldots && (33.82)
\end{aligned}
$$

Using now Theorem 1.22

$$
\int_{-\infty}^{+\infty} \mathrm{d}t\, e^{\mathrm{i}xt} = 2\pi\delta(x), \tag{33.83}
$$

we obtain

$$D^{>}_{\mathbf{q}\nu}(\omega) = \ldots = -\frac{2\pi i}{\hbar}\left[\left(\mathrm{B}_{\beta}(\Omega_{\mathbf{q}\nu})+1\right)\delta(\omega-\omega_{\mathbf{q}\nu}) + \mathrm{B}_{\beta}(\Omega_{\mathbf{q}\nu})\delta(\omega+\omega_{\mathbf{q}\nu})\right]. \tag{33.84}$$

Therefore we obtain

$$D^{>}_{\mathbf{q}\nu}(\omega) = -\frac{2\pi i}{\hbar}\left[\left(\mathrm{B}_{\beta}(\Omega_{\mathbf{q}\nu})+1\right)\delta(\omega-\omega_{\mathbf{q}\nu}) + \mathrm{B}_{\beta}(\Omega_{\mathbf{q}\nu})\delta(\omega+\omega_{\mathbf{q}\nu})\right]. \tag{33.85}$$

Frequency representation of the time-ordered Green-function

We take the Fourier-transform convention

$$D^{\mathbb{T}}_{\mathbf{q}\nu}(\omega) = \lim_{\eta\to 0^+}\int_{-\infty}^{+\infty} \mathrm{d}t\, e^{+\mathrm{i}\omega t-\eta|t|} D^{\mathbb{T}}_{\mathbf{q}\nu}(t). \tag{33.86}$$

The temporal Green-function is according to Equation (12.27)

$$D^{\mathbb{T}}_{\mathbf{q}\nu}(t) = -\frac{\mathrm{i}}{\hbar}\Big[\theta(t)\big((\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})+1)e^{-\mathrm{i}\omega_{\mathbf{q}\nu}t} + \mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})e^{+\mathrm{i}\omega_{\mathbf{q}\nu}t}\big) + \theta(-t)\big((\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})+1)e^{+\mathrm{i}\omega_{\mathbf{q}\nu}t} + \mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})e^{-\mathrm{i}\omega_{\mathbf{q}\nu}t}\big)\Big]. \tag{33.87}$$

Consequently,

$$\begin{aligned} D^{\mathbb{T}}_{\mathbf{q}\nu}(\omega) = -\frac{\mathrm{i}}{\hbar}\lim_{\eta\to 0^+}\Bigg\{ & (\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})+1)\int_0^{+\infty}\mathrm{d}t\, e^{\mathrm{i}(\omega-\omega_{\mathbf{q}\nu})t-\eta t} \\ & + \mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})\int_0^{+\infty}\mathrm{d}t\, e^{\mathrm{i}(\omega+\omega_{\mathbf{q}\nu})t-\eta t} \\ & + (\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})+1)\int_{-\infty}^{0}\mathrm{d}t\, e^{\mathrm{i}(\omega+\omega_{\mathbf{q}\nu})t+\eta t} \\ & + \mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})\int_{-\infty}^{0}\mathrm{d}t\, e^{\mathrm{i}(\omega-\omega_{\mathbf{q}\nu})t+\eta t}\Bigg\}. \end{aligned} \tag{33.88}$$

The regulated integrals are evaluated analogous to Lemma 1.19 and 1.20

$$\int_0^{+\infty}\mathrm{d}t\, e^{\mathrm{i}xt-\eta t} = \frac{1}{\mathrm{i}x-\eta}\left[\mathrm{e}^{\mathrm{i}xt-\eta t}\right]_0^{\infty} = \frac{-1}{\mathrm{i}x-\eta}\frac{-\mathrm{i}}{\mathrm{i}} = \frac{\mathrm{i}}{x+\mathrm{i}\eta}, \tag{33.89}$$

(33.90)

$$\int_{-\infty}^{0}\mathrm{d}t\, e^{\mathrm{i}xt+\eta t} = \frac{1}{\mathrm{i}x+\eta}\left[\mathrm{e}^{\mathrm{i}xt+\eta t}\right]_0^{\infty} = \frac{-1}{\mathrm{i}x+\eta}\frac{-\mathrm{i}}{\mathrm{i}} = -\frac{\mathrm{i}}{x-\mathrm{i}\eta}. \tag{33.91}$$

Therefore,

$$D^{\mathbb{T}}_{\mathbf{q}\nu}(\omega) = \lim_{\eta\to 0^+} \frac{1}{\hbar}\left[\frac{\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})+1}{\omega-\omega_{\mathbf{q}\nu}+\mathrm{i}\eta} + \frac{\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})}{\omega+\omega_{\mathbf{q}\nu}+\mathrm{i}\eta} - \frac{\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})+1}{\omega+\omega_{\mathbf{q}\nu}-\mathrm{i}\eta} - \frac{\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})}{\omega-\omega_{\mathbf{q}\nu}-\mathrm{i}\eta}\right]. \tag{33.92}$$

Hence,

$$\begin{aligned} D^{\mathbb{T}}_{\mathbf{q}\nu}(\omega) &= \frac{1}{\hbar}\lim_{\eta\to 0^+}\left[\frac{\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})+1}{\omega-\omega_{\mathbf{q}\nu}+\mathrm{i}\eta} + \frac{\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})}{\omega+\omega_{\mathbf{q}\nu}+\mathrm{i}\eta} - \frac{\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})+1}{\omega+\omega_{\mathbf{q}\nu}-\mathrm{i}\eta} - \frac{\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})}{\omega-\omega_{\mathbf{q}\nu}-\mathrm{i}\eta}\right]. \\ &= \frac{1}{\hbar}\lim_{\eta\to 0^+}\sum_{\sigma\in\{+,-\}}\left[\sigma\frac{\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})+1}{\omega-\sigma\omega_{\mathbf{q}\nu}+\sigma\mathrm{i}\eta} + \sigma\frac{\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})}{\omega+\sigma\omega_{\mathbf{q}\nu}+\sigma\mathrm{i}\eta}\right]. \end{aligned} \tag{33.93}$$

Frequency representation of the anti-time-ordered Green-function

We use the same Fourier-transform convention,

$$D^{\overline{\mathbb{T}}}_{\mathbf{q}\nu}(\omega) = \lim_{\eta\to 0^+}\int_{-\infty}^{+\infty}\mathrm{d}t\, e^{+\mathrm{i}\omega t-\eta|t|}D^{\overline{\mathbb{T}}}_{\mathbf{q}\nu}(t). \tag{33.94}$$

The temporal anti-time-ordered Green-function is according to Equation (12.19)

$$\begin{aligned} D^{\overline{\mathbb{T}}}_{\mathbf{q}\nu}(t) = -\frac{\mathrm{i}}{\hbar}\Big[&\theta(-t)\big((\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})+1)e^{-\mathrm{i}\omega_{\mathbf{q}\nu}t} + \mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})e^{+\mathrm{i}\omega_{\mathbf{q}\nu}t}\big) \\ &+ \theta(t)\big((\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})+1)e^{+\mathrm{i}\omega_{\mathbf{q}\nu}t} + \mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})e^{-\mathrm{i}\omega_{\mathbf{q}\nu}t}\big)\Big]. \end{aligned} \tag{33.95}$$

Thus,

$$\begin{aligned} D^{\overline{\mathbb{T}}}_{\mathbf{q}\nu}(\omega) = -\frac{\mathrm{i}}{\hbar}\lim_{\eta\to 0^+}\Bigg\{&(\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})+1)\int_{-\infty}^{0}\mathrm{d}t\, e^{\mathrm{i}(\omega-\omega_{\mathbf{q}\nu})t+\eta t} \\ &+ \mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})\int_{-\infty}^{0}\mathrm{d}t\, e^{\mathrm{i}(\omega+\omega_{\mathbf{q}\nu})t+\eta t} \\ &+ (\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})+1)\int_{0}^{+\infty}\mathrm{d}t\, e^{\mathrm{i}(\omega+\omega_{\mathbf{q}\nu})t-\eta t} \\ &+ \mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})\int_{0}^{+\infty}\mathrm{d}t\, e^{\mathrm{i}(\omega-\omega_{\mathbf{q}\nu})t-\eta t}\Bigg\}. \end{aligned} \tag{33.96}$$

Using the regulated integrals above in Equations (33.89) and (33.91), we find

$$\begin{aligned} D^{\overline{\mathbb{T}}}_{\mathbf{q}\nu}(\omega) = \lim_{\eta\to 0^+}\frac{1}{\hbar}\Bigg[&\frac{\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})}{\omega-\omega_{\mathbf{q}\nu}+\mathrm{i}\eta} + \frac{\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})+1}{\omega+\omega_{\mathbf{q}\nu}+\mathrm{i}\eta} \\ &- \frac{\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})+1}{\omega-\omega_{\mathbf{q}\nu}-\mathrm{i}\eta} - \frac{\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})}{\omega+\omega_{\mathbf{q}\nu}-\mathrm{i}\eta}\Bigg]. \end{aligned} \tag{33.97}$$

Therefore,

$$\begin{aligned} D^{\overline{\mathbb{T}}}_{\mathbf{q}\nu}(\omega) &= \frac{1}{\hbar}\lim_{\eta\to 0^+}\left[\frac{\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})}{\omega-\omega_{\mathbf{q}\nu}+\mathrm{i}\eta}+\frac{\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})+1}{\omega+\omega_{\mathbf{q}\nu}+\mathrm{i}\eta}-\frac{\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})+1}{\omega-\omega_{\mathbf{q}\nu}-\mathrm{i}\eta}-\frac{\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})}{\omega+\omega_{\mathbf{q}\nu}-\mathrm{i}\eta}\right]. \\ &= \frac{1}{\hbar}\lim_{\eta\to 0^+}\sum_{\sigma\in\{+,-\}}\left[\sigma\frac{\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})}{\omega-\sigma\omega_{\mathbf{q}\nu}+\sigma\mathrm{i}\eta}+\sigma\frac{\mathrm{B}_{\hbar\beta}(\Omega_{\mathbf{q}\nu})+1}{\omega+\sigma\omega_{\mathbf{q}\nu}+\sigma\mathrm{i}\eta}\right]. \end{aligned} \tag{33.98}$$

Frequency representation of the retarded Green-function

We use the Fourier-transform convention from Notation 1.17

$$D^{\mathrm{ret}}_{\mathbf{q}\nu}(\omega) = \lim_{\eta\to 0^+}\int_{-\infty}^{+\infty} dt\, e^{+\mathrm{i}\omega t-\eta|t|}D^{\mathrm{ret}}_{\mathbf{q}\nu}(t). \tag{33.99}$$

Starting from the temporal expression in Equation (33.70)

$$D^{\mathrm{ret}}_{\mathbf{q}\nu}(t) = -\frac{2}{\hbar}\theta(t)\sin\left(\omega_{\mathbf{q}\nu}t\right), \tag{33.100}$$

we obtain

$$D^{\mathrm{ret}}_{\mathbf{q}\nu}(\omega) = -\frac{2}{\hbar}\lim_{\eta\to 0^+}\int_0^{+\infty}\mathrm{d}t\, e^{+\mathrm{i}\omega t-\eta t}\sin\left(\omega_{\mathbf{q}\nu}t\right). \tag{33.101}$$

Notice that, omitting the limit, this is formally the same expression as

$$D^{\mathrm{ret}}_{\mathbf{q}\nu}(\omega+\mathrm{i}\eta) = -\frac{2}{\hbar}\int_0^{+\infty}\mathrm{d}t\, e^{+\mathrm{i}\omega t-\eta t}\sin\left(\omega_{\mathbf{q}\nu}t\right). \tag{33.102}$$

for $\eta > 0$. Using now the decomposition again

$$\sin\left(\omega_{\mathbf{q}\nu}t\right) = \frac{1}{2i}\left[e^{+\mathrm{i}\omega_{\mathbf{q}\nu}t}-e^{-\mathrm{i}\omega_{\mathbf{q}\nu}t}\right], \tag{33.103}$$

we find

$$D^{\mathrm{ret}}_{\mathbf{q}\nu}(\omega) = -\frac{1}{i\hbar}\lim_{\eta\to 0^+}\left[\int_0^{+\infty}\mathrm{d}t\, e^{+\mathrm{i}(\omega+\omega_{\mathbf{q}\nu})t-\eta t}-\int_0^{+\infty}\mathrm{d}t\, e^{+\mathrm{i}(\omega-\omega_{\mathbf{q}\nu})t-\eta t}\right]. \tag{33.104}$$

The regulated integral is as in Equation (33.89)

$$\int_0^{+\infty}\mathrm{d}t\, e^{+\mathrm{i}xt-\eta t} = \frac{\mathrm{i}}{x+\mathrm{i}\eta}. \tag{33.105}$$

Therefore,

$$D^{\text{ret}}_{\mathbf{q}\nu}(\omega) = -\frac{1}{i\hbar}\lim_{\eta\to 0^+}\left[\frac{\mathrm{i}}{\omega+\omega_{\mathbf{q}\nu}+\mathrm{i}\eta}-\frac{\mathrm{i}}{\omega-\omega_{\mathbf{q}\nu}+\mathrm{i}\eta}\right] \tag{33.106}$$

$$= \frac{1}{\hbar}\lim_{\eta\to 0^+}\left[\frac{1}{\omega-\omega_{\mathbf{q}\nu}+\mathrm{i}\eta}-\frac{1}{\omega+\omega_{\mathbf{q}\nu}+\mathrm{i}\eta}\right]. \tag{33.107}$$

Hence,

$$D^{\text{ret}}_{\mathbf{q}\nu}(\omega) = \frac{1}{\hbar}\lim_{\eta\to 0^+}\left[\frac{1}{\omega-\omega_{\mathbf{q}\nu}+\mathrm{i}\eta}-\frac{1}{\omega+\omega_{\mathbf{q}\nu}+\mathrm{i}\eta}\right]. \tag{33.108}$$

Notice that this can be further simplified as

$$\begin{aligned} D^{\text{ret}}_{\mathbf{q}\nu}(\omega+\mathrm{i}\epsilon) &= \frac{1}{\hbar}\frac{1}{\omega+\mathrm{i}\epsilon-\omega_\nu(\mathbf{q})}-\frac{1}{\hbar}\frac{1}{\omega+\mathrm{i}\epsilon+\omega_\nu(\mathbf{q})} \\ &= \frac{1}{\hbar}\left[\frac{\omega+\mathrm{i}\epsilon+\omega_\nu(\mathbf{q})-\left(\omega+\mathrm{i}\epsilon-\omega_\nu(\mathbf{q})\right)}{(\omega+\mathrm{i}\epsilon)^2-\omega_\nu^2(\mathbf{q})}\right] \\ &= \frac{1}{\hbar}\frac{2\omega_\nu(\mathbf{q})}{(\omega+\mathrm{i}\epsilon)^2-\omega_\nu^2(\mathbf{q})} \end{aligned} \tag{33.109}$$

Frequency representation of the advanced Green-function

The Fourier transform of the advanced Green-function is according to Notation 1.17

$$D^{\text{adv}}_{\mathbf{q}\nu}(\omega) = \lim_{\eta\to 0^+}\int_{-\infty}^{+\infty} dt\, e^{+\mathrm{i}\omega t-\eta|t|}D^{\text{adv}}_{\mathbf{q}\nu}(t). \tag{33.110}$$

Starting from Equation (33.72)

$$D^{\text{adv}}_{\mathbf{q}\nu}(t) = +\frac{2}{\hbar}\theta(-t)\sin\left(\omega_{\mathbf{q}\nu}t\right), \tag{33.111}$$

we obtain

$$D^{\text{adv}}_{\mathbf{q}\nu}(\omega) = \frac{2}{\hbar}\lim_{\eta\to 0^+}\int_{-\infty}^{0}\mathrm{d}t\, e^{+\mathrm{i}\omega t+\eta t}\sin\left(\omega_{\mathbf{q}\nu}t\right). \tag{33.112}$$

Using the exponential representation of the sine function,

$$D^{\text{adv}}_{\mathbf{q}\nu}(\omega) = \frac{1}{i\hbar}\lim_{\eta\to 0^+}\left[\int_{-\infty}^{0}\mathrm{d}t\, e^{+\mathrm{i}(\omega+\omega_{\mathbf{q}\nu})t+\eta t}-\int_{-\infty}^{0}\mathrm{d}t\, e^{+\mathrm{i}(\omega-\omega_{\mathbf{q}\nu})t+\eta t}\right]. \tag{33.113}$$

The regulated integral over negative times is according to Equation (33.91)

$$\int_{-\infty}^{0} \mathrm{d}t\, e^{+\mathrm{i}xt+\eta t} = -\frac{\mathrm{i}}{x-\mathrm{i}\eta}. \tag{33.114}$$

Consequently,

$$D^{\mathrm{adv}}_{\mathbf{q}\nu}(\omega) = \frac{1}{i\hbar}\lim_{\eta\to 0^+}\left[-\frac{\mathrm{i}}{\omega+\omega_{\mathbf{q}\nu}-\mathrm{i}\eta}+\frac{\mathrm{i}}{\omega-\omega_{\mathbf{q}\nu}-\mathrm{i}\eta}\right] \tag{33.115}$$

$$= \frac{1}{\hbar}\lim_{\eta\to 0^+}\left[\frac{1}{\omega-\omega_{\mathbf{q}\nu}-\mathrm{i}\eta}-\frac{1}{\omega+\omega_{\mathbf{q}\nu}-\mathrm{i}\eta}\right]. \tag{33.116}$$

Hence,

$$\begin{aligned} D^{\mathrm{adv}}_{\mathbf{q}\nu}(\omega) &= \frac{1}{\hbar}\lim_{\eta\to 0^+}\left[\frac{1}{\omega-\omega_{\mathbf{q}\nu}-\mathrm{i}\eta}-\frac{1}{\omega+\omega_{\mathbf{q}\nu}-\mathrm{i}\eta}\right] \\ &= \frac{1}{\hbar}\lim_{\eta\to 0^+}\frac{\omega+\omega_{\mathbf{q}\nu}-\mathrm{i}\eta-\left(\omega-\omega_{\mathbf{q}\nu}-\mathrm{i}\eta\right)}{\left(\omega-\omega_{\mathbf{q}\nu}\right)^2-\mathrm{i}\eta} \\ &= \frac{1}{\hbar}\lim_{\eta\to 0^+}\frac{2\omega_{\mathbf{q}\nu}}{\left(\omega-\omega_{\mathbf{q}\nu}\right)^2-\mathrm{i}\eta} \end{aligned} \tag{33.117}$$

Proof 33.32 of Theorem 13.4 We compute

$$\begin{aligned}\mathscr{G}_{X,X'}(\tau,\tau') &= -\frac{1}{\hbar}\frac{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta(H-\eta\mu N)}\Big[\theta(\tau-\tau')\,X(\tau)\,X'(\tau') + \mathrm{S}_{X,X'}\,\theta(\tau'-\tau)\,X'(\tau')\,X(\tau)\Big]}{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta(H-\eta\mu N)}} \\ &= -\frac{1}{\hbar}\frac{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta(H-\eta\mu N)}\Big[\theta(\tau-\tau')\,X(\tau-\tau')\,X'(0) + \mathrm{S}_{X,X'}\,\theta(\tau'-\tau)\,X'(0)\,X(\tau-\tau')\Big]}{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta(H-\eta\mu N)}}\end{aligned}$$

Therefore the Green-function depends only on time-differences and we can write

$$\mathscr{G}_{X,X'}(\tau,\tau') \equiv \mathscr{G}_{X,X'}(\tau-\tau'). \tag{33.118}$$

With the periodic standard-continuation of the θ-function, we obtain, using the cyclicity property twice, for $-\hbar\beta < \tau < 0$ on the one hand

$$\begin{aligned}\mathscr{G}_{X,X'}(\tau) &= -\frac{\mathrm{S}_{X,X'}}{\hbar}\frac{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta(H-\eta\mu N)}X'(0)\,X(\tau)}{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta(H-\eta\mu N)}} \\ &= -\frac{\mathrm{S}_{X,X'}}{\hbar}\frac{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta(H-\eta\mu N)}X'\,\mathrm{e}^{+\tau(H-\eta\mu N)/\hbar}X\mathrm{e}^{-\tau(H-\eta\mu N)/\hbar}}{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta(H-\mu N)}} \\ &= -\frac{\mathrm{S}_{X,X'}}{\hbar}\frac{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{+\tau(H-\eta\mu N)/\hbar}X\mathrm{e}^{-(\beta+\tau/\hbar)(H-\mu N)}X'}{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta(H-\eta\mu N)}} \\ &= \dots\end{aligned}$$

now we multiply with one: $1 = \mathrm{e}^{\pm\beta(H-\eta\mu N)}$ in order to get

$$\dots = -\frac{\mathrm{S}_{X,X'}}{\hbar}\frac{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta(H-\eta\mu N)}\mathrm{e}^{+(\beta+\tau/\hbar)(H-\eta\mu N)}X\mathrm{e}^{-(\beta+\tau/\hbar)(H-\eta\mu N)}X'}{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta(H-\eta\mu N)}}$$

and we ultimately compute on the other hand (again for $-\hbar\beta < \tau < 0$)

$$\begin{aligned}\mathscr{G}_{X,X'}(\tau+\hbar\beta) &= -\frac{1}{\hbar}\frac{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta(H-\eta\mu N)}X(\tau+\hbar\beta)\,X'(0)}{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta(H-\eta\mu N)}} \\ &= -\frac{1}{\hbar}\frac{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta(H-\eta\mu N)}\mathrm{e}^{+(\tau/\hbar+\beta)(H-\eta\mu N)}X\,\mathrm{e}^{+(\tau/\hbar+\beta)(H-\eta\mu N)}X'}{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta(H-\eta\mu N)}}\end{aligned}$$

and therefore

$$\mathscr{G}_{X,X'}(\tau+\hbar\beta) = \mathrm{S}_{X,X'}\mathscr{G}_{X,X'}(\tau). \tag{33.119}$$

and hence there is a periodic standard-continuation, which is unique, and therefore the originally defined function.

Proof 33.33 of Lemma 13.5

We consider the definition

$$(-\hbar\beta, +\hbar\beta) \ni \tau \mapsto \mathscr{G}_{\alpha,\alpha'}(\tau) = -\frac{1}{\hbar}\frac{\mathrm{Tr}_{\mathscr{F}_\zeta}\, \mathrm{e}^{-\beta(H-\mu N)}\Big[\theta(\tau)\, c_\alpha(\tau)\, c^\dagger_{\alpha'}(0) + \zeta\, \theta(-\tau)\, c^\dagger_{\alpha'}(0)\, c_\alpha(\tau)\Big]}{\mathrm{Tr}_{\mathscr{F}_\zeta}\, \mathrm{e}^{-\beta(H-\mu N)}} \in \mathbb{C}$$

and want to calculate its derivative. We therefore calculate first

$$\begin{aligned}
\partial_\tau\, \mathrm{T}_\tau\, c_\alpha(\tau)\, c^\dagger_{\alpha'}(0) &\propto \partial_\tau\Big[\theta(\tau)\, c_\alpha(\tau)\, c^\dagger_{\alpha'}(0) + \zeta\, \theta(-\tau)\, c^\dagger_{\alpha'}(0)\, c_\alpha(\tau)\Big] \\
&= \delta(\tau) c_\alpha(\tau)\, c^\dagger_{\alpha'}(0) - \zeta\delta(-\tau) c^\dagger_{\alpha'}(0)\, c_\alpha(\tau) - \frac{1}{\hbar}\theta(\tau)\big[c_\alpha, H-\mu\big]_{\mathrm{H}}(\tau) c^\dagger_{\alpha'}(0) - \frac{\zeta}{\hbar}\theta(-\tau) c^\dagger_{\alpha'}(0)\big[c_\alpha, H-\mu\big]_{\mathrm{H}}(\tau) \\
&= \delta(\tau)\big[c_\alpha(\tau)\,, c^\dagger_{\alpha'}(0)\big]_\zeta - \frac{1}{\hbar}\,\mathrm{T}_\tau\,\Big(\big[c_\alpha, H-\mu\big]_{\mathrm{H}}(\tau)\, c^\dagger_{\alpha'}(0)\Big)
\end{aligned}$$

whereas we used the statistical commutator from Definition TBD and the imaginary-time Heisenberg-equation-of-motions from Lemma TBD and the fact. This gives the equation of motion

$$\partial_\tau \mathscr{G}_{\alpha\alpha'}(\tau) = -\frac{1}{\hbar}\delta(\tau)\delta_{\alpha,\alpha'} \quad + \quad \frac{1}{\hbar}\left\langle \mathrm{T}_\tau\, \Big[c_\alpha, \frac{H-\mu N}{\hbar}\Big]_{\mathrm{H}}(\tau) c^\dagger_{\alpha'}(0)\right\rangle \tag{33.120}$$

Proof 33.34 of Theorem 13.6

For Fermions: See Waste-Folder 1, Topic 4, page 8 and Mahan p. 115

For Bosons: See Waste-Folder 1, topic 9.

For both: See Flensberg, page 164f. , Negele and Orland, page 73.

Fermions

For the imaginary-time Green-function one obtains

$$\mathscr{G}(\tau) = -\frac{1}{\hbar}\theta(\tau)\mathrm{e}^{-\xi\tau/\hbar}\left(1 - \mathrm{F}_\beta(\xi)\right) + \frac{1}{\hbar}\theta(-\tau)\mathrm{e}^{-\xi\tau/\hbar}\,\mathrm{F}_\beta(\xi) \tag{33.121}$$

and for the coefficients of the Fourier-series one has

$$\mathscr{G}(\mathrm{i}\omega_n) = \int_0^{\hbar\beta} \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\omega_n\tau}\mathscr{G}(\tau) = -\frac{1}{\hbar}\left(1 - \mathrm{F}_\beta(\xi)\right)\int_0^{\hbar\beta} \mathrm{d}\tau\, \mathrm{e}^{\tau(\mathrm{i}\omega_n - \xi/\hbar)} = \ldots$$

Now we compute

$$\int_0^{\hbar\beta} \mathrm{d}\tau\, \mathrm{e}^{\tau(\mathrm{i}\omega_n - \xi/\hbar)} = \left(-\mathrm{e}^{\beta\xi} - 1\right) \frac{1}{\mathrm{i}\omega_n - \xi/\hbar} = -(1 + \mathrm{e}^{\beta\xi}) \frac{1}{\mathrm{i}\omega_n - \xi/\hbar}$$

which yields

$$\ldots = \frac{1}{\hbar} \frac{(1 - \mathrm{F}_\beta(\xi))(1 + \mathrm{e}^{\beta\xi})}{\mathrm{i}\omega_n - \xi/\hbar} = \frac{1}{\hbar} \frac{1}{\mathrm{i}\omega_n - \xi/\hbar}$$

whereas the last equation-sign is proven in the literature[8].

Bosons

We compute (at the example of a non-interacting phonon-gas)

$$\mathscr{G}_{\substack{\nu,\nu' \\ \mathbf{q},\mathbf{q}'}}(\tau, 0) = -\theta(\tau)\langle c_{\mathbf{q}\nu}(\tau) c^\dagger_{\mathbf{q}'\nu'}(0)\rangle - \theta(-\tau)\langle c^\dagger_{\mathbf{q}'\nu'}(0) c_{\mathbf{q}\nu}(\tau)\rangle = \ldots$$

Now we use

$$c_{\mathbf{q}\nu}(\tau) = \mathrm{e}^{\tau H/\hbar} c_{\mathbf{q}\nu} \mathrm{e}^{-\tau H/\hbar} = \mathrm{e}^{-\tau\omega_{\mathbf{q}\nu}} c_{\mathbf{q}\nu} \tag{33.122}$$

and

$$c^\dagger_{\mathbf{q}\nu}(\tau) = \mathrm{e}^{\tau H/\hbar} c_{\mathbf{q}\nu} \mathrm{e}^{-\tau H/\hbar} = \mathrm{e}^{+\tau\omega_{\mathbf{q}\nu}} c^\dagger_{\mathbf{q}\nu} \tag{33.123}$$

and therefore we obtain

$$-\langle c_{\mathbf{q}\nu}(\tau) c^\dagger_{\mathbf{q}'\nu'}(0)\rangle = -\mathrm{e}^{-\tau\omega_{\mathbf{q}\nu}} \langle c_{\mathbf{q}\nu} c^\dagger_{\mathbf{q}'\nu'}\rangle = -\delta_{\mathbf{q},\mathbf{q}'}\delta_{\nu,\nu'} \mathrm{e}^{-\tau\omega_{\mathbf{q}\nu}} \left(\mathrm{B}_\beta(\hbar\omega_{\mathbf{q}\nu}) + 1\right) \tag{33.124}$$

and

$$-\langle c^\dagger_{\mathbf{q}'\nu'}(0) c_{\mathbf{q}\nu}(\tau)\rangle = -\mathrm{e}^{-\tau\omega_{\mathbf{q}\nu}} \langle c^\dagger_{\mathbf{q}'\nu'} c_{\mathbf{q}\nu}\rangle = -\delta_{\mathbf{q},\mathbf{q}'}\delta_{\nu,\nu'} \mathrm{e}^{-\tau\omega_{\mathbf{q}\nu}} \mathrm{B}_\beta(\hbar\omega_{\mathbf{q}\nu}) \tag{33.125}$$

and therefore we obtain

$$\begin{aligned} \mathscr{G}_{\substack{\nu,\nu' \\ \mathbf{q},\mathbf{q}'}}(\tau, 0) &= \ldots \\ &= -\theta(\tau)\delta_{\mathbf{q},\mathbf{q}'}\delta_{\nu,\nu'} \mathrm{e}^{-\tau\omega_{\mathbf{q}\nu}} \left(\mathrm{B}_\beta(\hbar\omega_{\mathbf{q}\nu}) + 1\right) - \theta(-\tau)\delta_{\mathbf{q},\mathbf{q}'}\delta_{\nu,\nu'} \mathrm{e}^{-\tau\omega_{\mathbf{q}\nu}} \mathrm{B}_\beta(\hbar\omega_{\mathbf{q}\nu}) \end{aligned}$$

Proof 33.35 of Theorem 13.7 We will prove the theorem in two steps. First we will consider the equation of motion of the function to conclude its form. Then we will verify that the function has the correct periodicity.

[8] Cf. [32] page 115. One can also simply write the Equation out and see it immediately.

Fundamental theorems on the uniqueness of differential equations yields then that we have obtained the correct solution. We now evaluate

$$\begin{aligned}\left[c_\alpha, H-\mu\right] &= \sum_{\beta,\beta'} H_{\beta,\beta'}\left[c_\alpha, c_\beta^\dagger c_{\beta'}\right] \quad + \quad \mu \sum_\beta \left[c_\alpha, c_\beta^\dagger c_\beta\right] \\ &= \sum_{\beta,\beta'} H_{\beta,\beta'}\left[c_\alpha, c_\beta^\dagger\right]_\zeta c_{\beta'} \quad + \quad \mu \sum_\beta \left[c_\alpha, c_\beta^\dagger\right]_\zeta c_\beta \\ &= \sum_{\beta'} H_{\alpha,\beta'} c_{\beta'} \quad + \quad \mu c_\alpha\end{aligned}$$

Therefore we obtain

$$\ldots = \delta(\tau)\delta_{\alpha,\alpha'} - \sum_\beta \frac{H_{\alpha,\beta} - \delta_{\alpha,\beta}\mu}{\hbar} \mathrm{T}_\tau \left(c_\beta(\tau) c_{\alpha'}^\dagger(0)\right)$$

which gives combined in total

$$\begin{aligned}\partial_\tau \mathcal{G}_{\alpha,\alpha'}(\tau) = -\delta(\tau)/\hbar\delta_{\alpha,\alpha'} - \sum_\beta \frac{H_{\alpha,\beta} - \delta_{\alpha,\beta}\mu}{\hbar}\mathcal{G}_{\beta,\alpha'}(\tau) \quad &\iff \quad \partial_\tau \mathcal{G}(\tau) = -\delta(\tau)/\hbar - \frac{H-\mu}{\hbar}\mathcal{G}(\tau) \\ &\iff \quad \left(\partial_\tau + \frac{H-\mu}{\hbar}\right)\mathcal{G}(\tau) = -\delta(\tau)/\hbar \\ &\iff \ldots\end{aligned}$$

whereas the r.h.sides are to be understood as matrix-identities. Solving this differential equation w.r.t. the boundary-conditions $\mathcal{G}(\hbar\beta) = \zeta\mathcal{G}(0)$ yields the desired result. We will now use the Dirac-identity for (anti-)periodic functions as[9]

$$\delta(\tau) = \frac{1}{\hbar\beta} \sum_{\omega_n \in \Omega_\zeta} \mathrm{e}^{-\mathrm{i}\omega_n\tau} \tag{33.126}$$

and use the expansion from Lemma TBD to obtain

$$\left(\partial_\tau + \frac{H-\mu}{\hbar}\right)\mathcal{G}(\tau) = -\delta(\tau)/\hbar \iff \frac{1}{\hbar}\sum_{\omega_n\in\Omega_\zeta} \mathrm{e}^{-\mathrm{i}\omega_n\tau}\left(-\mathrm{i}\omega_n + \frac{H-\mu}{\hbar}\right)\mathcal{G}(\mathrm{i}\omega_n) = \frac{1}{\hbar}\sum_{\omega_n\in\Omega_\zeta} \mathrm{e}^{-\mathrm{i}\omega_n\tau}(-1/\hbar)$$

using now that the coefficients of a Fourier-series are unique, one obtains by comparing coefficients

$$\left(-\mathrm{i}\omega_n + \frac{H-\mu}{\hbar}\right)\mathcal{G}(\mathrm{i}\omega_n) = -\frac{1}{\hbar} \quad \iff \quad \mathcal{G}(\mathrm{i}\omega_n) = \frac{1}{\hbar}\left(\frac{1}{\mathrm{i}\omega_n - \frac{H-\mu}{\hbar}}\right)$$

[9] Cf. Waste-Folder 1, topic 34.

Notice that we can't expand the r.h. sides w.r.t. Matsubara-frequencies according to Lemma TBD since we cant use the usual Kronecker-delta-relation since we are only integrating from 0 to $\hbar\beta$.

Equation of Motion Technique for Hybridized Systems

Equations of motion for generalized time-ordered, retarded and advanced Green-functions: Elk-Gasser p. 25

With the equation-of-motion-technique; See Appendix (ToBeReferenced.)

Proof 33.36 of Theorem 13.8 The first (Matsubara-)identity follows from Theorem 13.7 and the rules for inverting 2x2-matrices. For the temporal component, we need to evaluate the Matsubara-sums

$$\mathscr{G}(\tau) = \frac{1}{\hbar\beta} \sum_{\omega_n \in \Omega_{-1}} \mathscr{G}(\mathrm{i}\omega_n) \mathrm{e}^{-\mathrm{i}\omega_n \tau} = \star \tag{33.127}$$

Following Notation 15.17, we consider the function

$$z \mapsto \mathscr{G}(-\mathrm{i}z) = \frac{1}{\hbar} \frac{\left(z - (\epsilon_0 - \mu)\sigma_0/\hbar\right) + \boldsymbol{\epsilon} \cdot \boldsymbol{\sigma}/\hbar}{\left(z - \omega_+\right)\left(z - \omega_-\right)} \mathrm{e}^{-z\tau} \tag{33.128}$$

with

$$\omega_\pm = \left(\pm\epsilon + \epsilon_0 - \mu\right)/\hbar \tag{33.129}$$

Notice that we are now in the situation of Theorem 15.20, with

$$f_{-1}(z) = g_{-1}(z)\mathscr{G}(-\mathrm{i}z) \quad \text{and} \quad g_{-1}(z) = \hbar\beta\, \mathrm{n}^{-1}_{\hbar\beta}(z) = \hbar\beta\, \mathrm{F}_{\hbar\beta}(z) \tag{33.130}$$

which gives us two cases:

Case 1: $\omega_- \neq \omega_+$

$$\begin{aligned}
\star &= \sum_{k=\pm} \mathrm{Res}\left(f_{-1}(z), z = z_k\right) \\
&= \frac{1}{\hbar} \sum_{k=\pm} \frac{\left(z - (\epsilon_0 - \mu)/\hbar\right)\sigma_0 + \boldsymbol{\epsilon} \cdot \boldsymbol{\sigma}/\hbar}{\left(z - \omega_+\right)\left(z - \omega_-\right)} \mathrm{e}^{-z\tau} \left(z - z_k\right) \mathrm{F}_{\hbar\beta}(z)\Big|_{z=z_k} \\
&= \frac{1}{\hbar} \frac{\left(\omega_+ - (\epsilon_0 - \mu)/\hbar\right)\sigma_0 + \boldsymbol{\epsilon} \cdot \boldsymbol{\sigma}/\hbar}{\left(\omega_+ - \omega_-\right)} \mathrm{e}^{-\omega_+\tau}\, \mathrm{F}_{\hbar\beta}(\omega_+) \\
&+ \frac{1}{\hbar} \frac{\left(\omega_- - (\epsilon_0 - \mu)/\hbar\right)\sigma_0 + \boldsymbol{\epsilon} \cdot \boldsymbol{\sigma}/\hbar}{\left(\omega_- - \omega_+\right)} \mathrm{e}^{-\omega_-\tau}\, \mathrm{F}_{\hbar\beta}(\omega_-)
\end{aligned} \tag{33.131}$$

Case 2: $\omega_- = \omega_+ = \omega_\bullet$

Then we have the function

$$z \mapsto \mathscr{G}(-\mathrm{i}z) = \frac{1}{\hbar} \frac{\sigma_0}{z - \omega_\bullet} \mathrm{e}^{-z\tau} \tag{33.132}$$

and therefore we obtain with the Residue-theorem

$$\star = +1 \operatorname{Res}\left(f_{-1}(z), z = \omega_\bullet\right) = \frac{\sigma_0}{\hbar} \mathrm{e}^{-z\tau} \mathrm{F}_{\hbar\beta}(z)\Big|_{z=\omega_\bullet} \tag{33.133}$$

It is not that obvious that both expressions coincide in the limit $\epsilon \to 0$. Their agreement follows however from the differentiability of the (complex) Fermi-function.

Proofs to Section 7.2

Proof 33.37 of Theorem 13.10 By direct computation[10] we obtain

$$\begin{aligned}
\mathscr{D}_{\substack{0 \\ \alpha,\alpha'}}(\tau) &= \frac{-\theta(\tau)}{\hbar} \langle A_\alpha(\tau)\, A^\dagger_{\alpha'}(0)\rangle + \theta(-\tau) \langle A^\dagger_{\alpha'}(0)\, A_\alpha(\tau)\rangle \\
&= \frac{-\theta(\tau)}{\hbar}\Big[\langle c_{\mathbf{q}\nu}(\tau) c^\dagger_{\mathbf{q}'\nu'}(0)\rangle + \langle c^\dagger_{-\mathbf{q}\nu}(\tau) c_{-\mathbf{q}'\nu'}(0)\rangle\Big] \quad + \quad \frac{-\theta(-\tau)}{\hbar}\Big[\langle c_{-\mathbf{q}'\nu'}(0) c^\dagger_{-\mathbf{q}\nu}(\tau)\rangle + \langle c^\dagger_{\mathbf{q}'\nu'}(0) c_{\mathbf{q}\nu}(\tau)\rangle\Big] \\
&= \dots
\end{aligned}$$

Now we use the identities in Equation (8.27)

$$\begin{aligned}
c_{\mathbf{q}\nu}(\tau) &= c_{\mathbf{q}\nu}(0)\mathrm{e}^{-\tau\omega_{\mathbf{q}\nu}} = c_{\mathbf{q}\nu}\mathrm{e}^{-\tau\omega_{\mathbf{q}\nu}} \qquad & \langle c^\dagger_\alpha c_\beta\rangle &= \delta_{\alpha,\beta}\, \mathrm{B}_{\hbar\beta}(\omega_\alpha) \\
c^\dagger_{\mathbf{q}\nu}(\tau) &= c^\dagger_{\mathbf{q}\nu}(0)\mathrm{e}^{+\tau\omega_{\mathbf{q}\nu}} = c^\dagger_{\mathbf{q}\nu}\mathrm{e}^{+\tau\omega_{\mathbf{q}\nu}} \qquad & \langle c_\beta c^\dagger_\alpha\rangle &= \langle c^\dagger_\alpha c_\beta\rangle + \delta_{\alpha,\beta} \equiv \delta_{\alpha,\beta}\, \mathrm{B}_{\hbar\beta}(\omega_\alpha) + \delta_{\alpha,\beta}
\end{aligned}$$

This gives (together with Remark 12.9.1)

$$\begin{aligned}
\dots &= \frac{-\theta(\tau)}{\hbar}\Big[\mathrm{e}^{-\tau\omega_{\mathbf{q}\nu}}\langle c_{\mathbf{q}\nu} c^\dagger_{\mathbf{q}'\nu'}\rangle + \mathrm{e}^{\tau\omega_{\mathbf{q}\nu}}\langle c^\dagger_{-\mathbf{q}\nu} c_{-\mathbf{q}'\nu'}\rangle\Big] \quad + \quad \frac{-\theta(-\tau)}{\hbar}\Big[\mathrm{e}^{\tau\omega_{\mathbf{q}\nu}}\langle c_{-\mathbf{q}'\nu'} c^\dagger_{-\mathbf{q}\nu}\rangle + \mathrm{e}^{-\tau\omega_{\mathbf{q}\nu}}\langle c^\dagger_{\mathbf{q}'\nu'} c_{\mathbf{q}\nu}\rangle\Big] \\
&= \delta_{\mathbf{q},\mathbf{q}'}\delta_{\nu,\nu'}\frac{-\theta(\tau)}{\hbar}\Big[\mathrm{e}^{-\tau\omega_{\mathbf{q}\nu}}\left(\mathrm{B}_{\hbar\beta}(\omega_\alpha)+1\right) + \mathrm{e}^{+\tau\omega_{\mathbf{q}\nu}}\,\mathrm{B}_{\hbar\beta}(\omega_\alpha)\Big] + \delta_{\mathbf{q},\mathbf{q}'}\delta_{\nu,\nu'}\frac{-\theta(-\tau)}{\hbar}\Big[\mathrm{e}^{+\tau\omega_{\mathbf{q}\nu}}\left(\mathrm{B}_{\hbar\beta}(\omega_\alpha)+1\right) + \mathrm{e}^{-\tau\omega_{\mathbf{q}\nu}}\,\mathrm{B}_{\hbar\beta}(\omega_\alpha)\Big] \\
&= \dots
\end{aligned}$$

which can be summarized as

$$\dots = -\delta_{\alpha,\alpha'}\frac{1}{\hbar}\sum_{\nu\in\{+,-\}}\theta(\nu\tau)\Big[\left(1+\mathrm{B}_{\hbar\beta}(\omega_\alpha)\right)\,\mathrm{e}^{-\nu\,\omega_\alpha\tau} + \mathrm{B}_{\hbar\beta}(\omega_\alpha)\,\mathrm{e}^{\nu\,\omega_\alpha\tau}\Big] \tag{33.134}$$

The Green's function of frequency is

[10] Cf. [32] p. 116-117.

$$\mathscr{D}^{\,0}_{\nu,\nu'}(\mathrm{i}\omega_n,\mathbf{q}) = \frac{1}{\hbar}\int_0^{\hbar\beta} \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\omega_n\tau}\mathscr{D}^{\,0}_{\nu,\nu'}(\tau,\mathbf{q}) \tag{33.135}$$

$$= -\frac{1}{\hbar}\delta_{\nu,\nu'}\left[(\mathrm{B}_{\hbar\beta}(\omega_{\mathbf{q}\nu})+1)\frac{\mathrm{e}^{\beta(\mathrm{i}\omega_n-\omega_{\mathbf{q}\nu})}-1}{\mathrm{i}\omega_n-\omega_{\mathbf{q}\nu}} + \mathrm{B}_{\hbar\beta}(\omega_{\mathbf{q}\nu})\frac{\mathrm{e}^{\beta(\mathrm{i}\omega_n+\omega_{\mathbf{q}\nu})}-1}{\mathrm{i}\omega_n+\omega_{\mathbf{q}\nu}}\right]. \tag{33.136}$$

The terms in the numerators may be simplified by noting that for bosons $\exp(\mathrm{i}\omega_n\beta) = 1$ so that the Green's function is

$$\mathscr{D}^{\,0}_{\nu,\nu'}(\mathrm{i}\omega_n,\mathbf{q}) = -\frac{1}{\hbar}\delta_{\alpha,\alpha'}\left[(\mathrm{B}_{\hbar\beta}(\omega_{\mathbf{q}\nu})+1)\frac{\mathrm{e}^{-\beta\omega_{\mathbf{q}\nu}}-1}{\mathrm{i}\omega_n-\omega_{\mathbf{q}\nu}} + \mathrm{B}_{\hbar\beta}(\omega_{\mathbf{q}\nu})\frac{\mathrm{e}^{\beta\omega_{\mathbf{q}\nu}}-1}{\mathrm{i}\omega_n+\omega_{\mathbf{q}\nu}}\right]. \tag{33.137}$$

Now we compute ...

- for the first numerator

$$\begin{aligned}\mathrm{B}_{\hbar\beta}(\omega_\nu(\mathbf{q}))+1 &= \frac{1}{\mathrm{e}^{\hbar\beta\omega_\nu(\mathbf{q})}-1}+1\\ &= \frac{1}{\mathrm{e}^{\hbar\beta\omega_\nu(\mathbf{q})}-1}+\frac{\mathrm{e}^{\hbar\beta\omega_\nu(\mathbf{q})}-1}{\mathrm{e}^{\hbar\beta\omega_\nu(\mathbf{q})}-1}\\ &= \frac{\mathrm{e}^{\hbar\beta\omega_\nu(\mathbf{q})}}{\mathrm{e}^{\hbar\beta\omega_\nu(\mathbf{q})}-1}\\ &= \frac{1}{1-\mathrm{e}^{-\hbar\beta\omega_\nu(\mathbf{q})}}\end{aligned} \tag{33.138}$$

  such that we obtain

$$(\mathrm{B}_{\hbar\beta}(\omega_{\mathbf{q}\nu})+1)\frac{\mathrm{e}^{-\beta\omega_{\mathbf{q}\nu}}-1}{1} = -1 \tag{33.139}$$

- for the other term we obtain

$$\mathrm{B}_{\hbar\beta}(\omega_\nu(\mathbf{q}))\left(\mathrm{e}^{\hbar\beta\omega_\nu(\mathbf{q})}-1\right) = \frac{1}{\mathrm{e}^{\hbar\beta\omega_\nu(\mathbf{q})}-1}\left(\mathrm{e}^{\hbar\beta\omega_\nu(\mathbf{q})}-1\right) = +1 \tag{33.140}$$

Combining these results yields therefore

$$\begin{aligned}\mathscr{D}^{\,0}_{\nu,\nu'}(\mathrm{i}\omega_n,\mathbf{q}) &= -\frac{1}{\hbar}\left(-\frac{1}{\mathrm{i}\omega_n-\omega_{\mathbf{q}\nu}}+\frac{1}{\mathrm{i}\omega_n+\omega_{\mathbf{q}\nu}}\right)\\ &= \frac{1}{\hbar}\frac{2\omega_{\mathbf{q}\nu}}{(\mathrm{i}\omega_n)^2-\omega_{\mathbf{q}\nu}^2}\\ &= -\frac{1}{\hbar}\frac{2\omega_{\mathbf{q}\nu}}{\omega_n^2+\omega_{\mathbf{q}\nu}^2}.\end{aligned} \tag{33.141}$$

Proof 33.38 of Theorem 13.11

Expanding the time-ordering operator yields the equation

$$\begin{aligned}\mathscr{D}_{\substack{0\\ \alpha\alpha'}}(\tau) &= -\frac{1}{\hbar}\langle T_\tau A_\alpha(\tau) A^\dagger_{\alpha'}(0)\rangle_0 \\ &= -\frac{1}{\hbar}\langle \theta(\tau) A_\alpha(\tau) A^\dagger_{\alpha'}(0) + \theta(-\tau) A^\dagger_{\alpha'}(0) A_\alpha(\tau)\rangle_0\end{aligned}$$

Hence we obtain for the time-derivative

$$\begin{aligned}\partial_\tau \mathscr{D}_{\substack{0\\ \alpha\alpha'}}(\tau) &= -\frac{1}{\hbar}\langle \mathrm{T}_\tau\, \partial_\tau A_\alpha(\tau) A^\dagger_{\alpha'}(0)\rangle_0 - \frac{1}{\hbar}\delta(\tau)\langle A_\alpha(0) A^\dagger_{\alpha'}(0)\rangle_0 + \frac{1}{\hbar}\delta(-\tau)\langle A^\dagger_{\alpha'}(0) A_\alpha(0)\rangle_0 \\ &= \dots\end{aligned}$$

for the first term we have with Heisenbergs equation of motion

$$\partial_\tau A_\alpha(\tau) = -\frac{1}{\hbar}[A_\alpha, H_0]_{\mathrm{H}}(\tau) \tag{33.142}$$

Now we compute the commutators

$$\begin{aligned}[c_\alpha, c^\dagger_\beta c_\beta] &= \delta_{\alpha,\beta} c_\beta \\ [c^\dagger_\alpha, c^\dagger_\beta c_\beta] &= -\delta_{\alpha,\beta} c^\dagger_\beta\end{aligned}$$

and obtain

$$\begin{aligned}[A_\nu(\mathbf{k}), H_0] &= \sum_{\mathbf{k}',\nu'} \hbar\omega_\nu(\mathbf{k}') \left([c_\nu(\mathbf{k}), c^\dagger_{\nu'}(\mathbf{k}') c_{\nu'}(\mathbf{k}')] + [c^\dagger_\nu(-\mathbf{k}), c^\dagger_{\nu'}(\mathbf{k}') c_{\nu'}(\mathbf{k}')] \right) \\ &= \hbar\omega_\nu(\mathbf{k}) \left(c_\nu(\mathbf{k}) - c^\dagger_\nu(-\mathbf{k}) \right) \\ &\equiv \hbar\omega_\nu(\mathbf{k}) P_\nu(\mathbf{k})\end{aligned}$$

hence we obtain, summarizing the terms with delta-functions with the distributivity-law

$$\dots = -\frac{1}{\hbar}\left(\frac{-1}{\hbar}\omega_\nu(\mathbf{k}) \langle \mathrm{T}_\tau\, P_\nu(\mathbf{k}) A^\dagger_{\nu'}(\mathbf{k}')(0)\rangle_0 + \delta(\tau)\Big[\langle A_\nu(\mathbf{k}) A^\dagger_{\nu'}(\mathbf{k}')\rangle_0 - \langle A^\dagger_{\nu'}(\mathbf{k}') A_\nu(\mathbf{k})\rangle_0 \Big] \right)$$

Now we compute the δ-functions

$$\begin{aligned}&\langle A_\nu(\mathbf{k}) A^\dagger_{\nu'}(\mathbf{k}')\rangle_0 - \langle A^\dagger_{\nu'}(\mathbf{k}') A_\nu(\mathbf{k})\rangle_0 \\ &= \delta_{\nu,\nu'}\delta_{\mathbf{k},\mathbf{k}'} \left(1 - \mathrm{B}_{\hbar\beta}(\omega_\nu(\mathbf{k})) + 0 + 0 + \mathrm{B}_{\hbar\beta}(\omega_\nu(-\mathbf{k})) - \left[\mathrm{B}_{\hbar\beta}(\omega_\nu(\mathbf{k})) + 0 + 0 + 1 - \mathrm{B}_{\hbar\beta}(\omega_\nu(-\mathbf{k})) \right] \right) \\ &= 0\end{aligned}$$

in total we obtain thus

$$\partial_\tau \mathscr{D}_{\substack{0\\ \alpha\alpha'}}(\tau) = \frac{+\omega_\nu(\mathbf{k})}{\hbar}\langle \mathrm{T}_\tau\, P_\nu(\mathbf{k},\tau) A^\dagger_{\nu'}(\mathbf{k}',0)\rangle_0 \tag{33.143}$$

Hence we obtain for the second derivative analogously

$$\begin{aligned}\partial_\tau^2 \mathscr{D}_{\substack{0\\ \alpha\alpha'}}(\tau) &= \frac{+\omega_\nu(\mathbf{k})}{\hbar}\left(\langle \mathrm{T}_\tau\, \partial_\tau P_\nu(\mathbf{k},\tau) A^\dagger_{\nu'}(\mathbf{k}',0)\rangle_0 + \delta(\tau)\langle P_\nu(\mathbf{k}) A^\dagger_{\nu'}(\mathbf{k}')\rangle_0 - \delta(-\tau)\langle A^\dagger_{\nu'}(\mathbf{k}') P_\nu(\mathbf{k})\rangle_0\right)\\ &= \dots\end{aligned}$$

The first term becomes a commutator with Heisenbergs equation of motion

$$\partial_\tau P_\nu(\mathbf{k},\tau) = -\frac{1}{\hbar}[P_\nu(\mathbf{k}), H_0]_{\mathrm{H}}(\tau). \tag{33.144}$$

Analogously to the previous computation we obtain

$$[P_\nu(\mathbf{k}), H_0] = \hbar\omega_\nu(\mathbf{k}) A_\nu(\mathbf{k})$$

and for the other term we compute

$$\begin{aligned}&\langle P_\nu(\mathbf{k}) A^\dagger_{\nu'}(\mathbf{k}')\rangle_0 - \langle A^\dagger_{\nu'}(\mathbf{k}') P_\nu(\mathbf{k})\rangle_0\\ &= \delta_{\nu,\nu'}\delta_{\mathbf{k},\mathbf{k}'}\left(1 - \mathrm{B}_{\hbar\beta}(\omega_\nu(\mathbf{k})) + 0 + 0 - \mathrm{B}_{\hbar\beta}(\omega_\nu(-\mathbf{k})) - \left[\mathrm{B}_{\hbar\beta}(\omega_\nu(\mathbf{k})) + 0 + 0 - (1 - \mathrm{B}_{\hbar\beta}(\omega_\nu(-\mathbf{k})))\right]\right)\\ &= 2\delta_{\nu,\nu'}\delta_{\mathbf{k},\mathbf{k}'}\end{aligned}$$

Hence we obtain in total

$$\begin{aligned}\partial_\tau^2 \quad \mathscr{D}_{\substack{0\\ \alpha\alpha'}}(\tau) &= \frac{+\omega_\nu(\mathbf{k})}{\hbar}\left(-\omega_\nu(\mathbf{k})\langle \mathrm{T}_\tau\, A_\nu(\mathbf{k},\tau) A^\dagger_{\nu'}(\mathbf{k}',0)\rangle_0 + 2\delta(\tau)\delta_{\nu,\nu'}\delta_{\mathbf{k},\mathbf{k}'}\right)\\ \iff \left(\partial_\tau^2 - \omega_\nu(\mathbf{k})^2\right) \quad \mathscr{D}_{\substack{0\\ \alpha\alpha'}}(\tau) &= 2\omega_\nu(\mathbf{k})\delta(\tau)\delta_{\nu,\nu'}\delta_{\mathbf{k},\mathbf{k}'}\end{aligned} \tag{33.145}$$

Proof 33.39 of Lemma 13.12

We work within the free phononic gas of Remark 8.28.4, i.e. $a_{\nu,\mathbf{q}} \equiv c_\nu(\mathbf{q})$ with

$$H_0 = \sum_{\nu,\mathbf{q}} \hbar\omega_\nu(\mathbf{q})\, c^\dagger_\nu(\mathbf{q})\, c_\nu(\mathbf{q}),$$

which is a special case of the diagonalized gas of Definition 8.27, and we recall from Definition 12.18 that $A_\nu(\mathbf{q}) = c_\nu(\mathbf{q}) + c^\dagger_\nu(-\mathbf{q})$. We abbreviate $\alpha \equiv (\nu,\mathbf{q})$ and split the proof into the two equality-signs.

First equality sign.

Since H_0 is diagonal in the occupation-number-eigenbasis of Definition 8.27, the thermal state $\propto \mathrm{e}^{-\beta H_0}$ is diagonal in this basis as well. The operators $c_\nu(\mathbf{q})c_\nu(-\mathbf{q})$ and $c^\dagger_\nu(\mathbf{q})c^\dagger_\nu(-\mathbf{q})$ each lower, respectively raise, some occupation-number by a total of two quanta, hence they map every occupation-number-eigenstate onto a state orthogonal to itself. Consequently their diagonal matrix-elements vanish and so do their thermal expectation-values,

$$\langle c_\nu(\mathbf{q})c_\nu(-\mathbf{q})\rangle = 0 = \left\langle c_\nu^\dagger(\mathbf{q})c_\nu^\dagger(-\mathbf{q})\right\rangle .$$

Using this together with the bosonic commutation-relation $\left[c_\nu(-\mathbf{q}),\, c_\nu^\dagger(-\mathbf{q})\right] = 1$ we compute

$$\begin{aligned}\left\langle A_{\nu,\mathbf{q}}^\dagger A_{\nu,\mathbf{q}}\right\rangle &= \left\langle \left(c_\nu^\dagger(\mathbf{q}) + c_\nu(-\mathbf{q})\right)\left(c_\nu(\mathbf{q}) + c_\nu^\dagger(-\mathbf{q})\right)\right\rangle \\ &= \left\langle c_\nu^\dagger(\mathbf{q})c_\nu(\mathbf{q})\right\rangle + \underbrace{\left\langle c_\nu^\dagger(\mathbf{q})c_\nu^\dagger(-\mathbf{q})\right\rangle}_{=0} + \underbrace{\langle c_\nu(-\mathbf{q})c_\nu(\mathbf{q})\rangle}_{=0} + \left\langle c_\nu(-\mathbf{q})c_\nu^\dagger(-\mathbf{q})\right\rangle \\ &= \left\langle c_\nu^\dagger(\mathbf{q})c_\nu(\mathbf{q})\right\rangle + 1 + \left\langle c_\nu^\dagger(-\mathbf{q})c_\nu(-\mathbf{q})\right\rangle .\end{aligned}$$

By Remark 12.9.1, applied to the diagonal gas underlying Remark 8.28.4 (recall $\eta = 0$, $\zeta = +1$ for phonons), both occupation-numbers are given by Bose-functions of the respective mode-energies,

$$\left\langle c_\nu^\dagger(\mathbf{q})c_\nu(\mathbf{q})\right\rangle = \mathrm{B}_{\hbar\beta}\left(\omega_\nu(\mathbf{q})\right), \qquad \left\langle c_\nu^\dagger(-\mathbf{q})c_\nu(-\mathbf{q})\right\rangle = \mathrm{B}_{\hbar\beta}\left(\omega_\nu(-\mathbf{q})\right).$$

Since the crystal is time-reversal-symmetric, Remark 8.28.6 gives $\omega_\nu(\mathbf{q}) = \omega_\nu(-\mathbf{q})$, so the two occupation-numbers above coincide and both equal $\langle a_{\nu,\mathbf{q}}^\dagger a_{\nu,\mathbf{q}}\rangle$. This yields

$$\left\langle A_{\nu,\mathbf{q}}^\dagger A_{\nu,\mathbf{q}}\right\rangle = 2\left\langle a_{\nu,\mathbf{q}}^\dagger a_{\nu,\mathbf{q}}\right\rangle + 1,$$

which is the first equality-sign.

Second equality sign.

From Definition 12.19 (with $\alpha = \alpha'$) we have, using stationarity of the ensemble to place both time-arguments at $t = t' = 0$,

$$D_{\alpha,\alpha}^<(t=0) = -\frac{\mathrm{i}}{\hbar}\left\langle A_\alpha^\dagger A_\alpha\right\rangle \quad \Longleftrightarrow \quad \left\langle A_\alpha^\dagger A_\alpha\right\rangle = \mathrm{i}\hbar\, D_{\alpha,\alpha}^<(t=0).$$

Writing this equal-time value as the Fourier-back-transform of $D_{\alpha,\alpha}^<(\omega)$,

$$D_{\alpha,\alpha}^<(t=0) = \int_{-\infty}^{+\infty}\frac{\mathrm{d}\omega}{2\pi}\, D_{\alpha,\alpha}^<(\omega),$$

and inserting the fluctuation-dissipation-theorem for phonons, Theorem 14.21,

$$D_{\alpha,\alpha}^<(\omega) = 2\mathrm{i}\,\mathrm{B}_{\hbar\beta}(\omega)\,\mathrm{Im}\lim_{\epsilon\to 0} D_{\alpha,\alpha}^{\mathrm{ret}}(\omega + \mathrm{i}\epsilon),$$

we obtain

$$\begin{aligned}\left\langle A_\alpha^\dagger A_\alpha\right\rangle &= \mathrm{i}\hbar\int_{-\infty}^{+\infty}\frac{\mathrm{d}\omega}{2\pi}\, 2\mathrm{i}\,\mathrm{B}_{\hbar\beta}(\omega)\,\mathrm{Im}\lim_{\epsilon\to 0} D_{\alpha,\alpha}^{\mathrm{ret}}(\omega+\mathrm{i}\epsilon) \\ &= -2\hbar\int_{-\infty}^{+\infty}\frac{\mathrm{d}\omega}{2\pi}\,\mathrm{B}_{\hbar\beta}(\omega)\,\mathrm{Im}\lim_{\epsilon\to 0} D_{\alpha,\alpha}^{\mathrm{ret}}(\omega+\mathrm{i}\epsilon) \\ &= \lim_{\epsilon\to 0}\int_{-\infty}^{+\infty}\mathrm{d}\omega\;\mathrm{B}_{\hbar\beta}(\omega)\left(-\frac{\hbar}{\pi}\,\mathrm{Im}\, D_{\alpha,\alpha}^{\mathrm{ret}}(\omega+\mathrm{i}\epsilon)\right),\end{aligned}$$

whereas in the last line we used $\mathrm{i}\cdot 2\mathrm{i} = -2$ and cancelled the resulting factor 2 against the 2π in the denominator. Writing out $\alpha = (\nu, \mathbf{q})$ this is precisely the second equality-sign (with $\nu' \equiv \nu$, $\mathbf{q}' \equiv \mathbf{q}$ in the notation of the Lemma).

Combining both equality-signs concludes the proof.

Remark on the prefactor. One can independently confirm the prefactor obtained above (and thereby rule out an additional factor of 2π) using the explicit free-phonon propagator of Theorem 13.10. Analytically continuing $\mathrm{i}\omega_n \to \omega + \mathrm{i}\epsilon$ and using the Sokhotski-Plemelj-theorem, Equation (14.3), one finds for $\alpha = (\nu, \mathbf{q})$

$$-\frac{\hbar}{\pi}\,\mathrm{Im}\lim_{\epsilon\to 0} D^{\mathrm{ret}}_{\alpha,\alpha}(\omega + \mathrm{i}\epsilon) = \delta\left(\omega - \omega_\nu(\mathbf{q})\right) - \delta\left(\omega + \omega_\nu(\mathbf{q})\right),$$

so that

$$\int_{-\infty}^{+\infty} \mathrm{d}\omega\ \mathrm{B}_{\hbar\beta}(\omega)\left(-\frac{\hbar}{\pi}\,\mathrm{Im}\, D^{\mathrm{ret}}_{\alpha,\alpha}(\omega + \mathrm{i}\epsilon)\right) = \mathrm{B}_{\hbar\beta}\left(\omega_\nu(\mathbf{q})\right) - \mathrm{B}_{\hbar\beta}\left(-\omega_\nu(\mathbf{q})\right) = 2\,\mathrm{B}_{\hbar\beta}\left(\omega_\nu(\mathbf{q})\right) + 1,$$

which reproduces $2\langle a^\dagger_{\nu,\mathbf{q}} a_{\nu,\mathbf{q}}\rangle + 1$ from the first equality-sign, as it must. Had one kept the additional factor of $1/(2\pi)$, this cross-check would fail by exactly that factor.

Proof 33.40 of Lemma 14.4

We complete the proof, by sorting the Green-functions into four groups.

- **Group 1:** Time- and anti-time-ordered Green-function $G^{\mathbb{T}}$, $G^{\overline{\mathbb{T}}}$.
- **Group 2:** Retarded and advanced Green-function G^{ret}, G^{adv}.
- **Group 3:** Lesser and greater Green-function $G^{<}$, $G^{>}$ and the spectral function A.
- **Group 4:** Imaginary time Green-function $\mathscr{G}$.

For each group, we will prove some Lemmata in order to complete the main proof. Ultimately we want to compute the Fourier-expansion coefficients for each Green-function. In each case we set, without loss of generality, the second time argument to zero $t' = \tau' = 0$ in order to simplify the notation.

Lemmata for the first two groups

In the first two groups we are confronted with the obstacle, that the usual Fourier-transform will turn out to be undefined in the functional sense[11]. The Fourier-transform only exists in the distributional sense. We therefore introduce the auxiliary functions

$$G^{\blacksquare}_{\epsilon;\,X,X'}(t) = G^{\blacksquare}_{X,X'}(t)\,\mathrm{e}^{-\epsilon|t|} \qquad \text{for } \blacksquare \in \{\mathbb{T}, \overline{\mathbb{T}}, \mathrm{ret}, \mathrm{adv}\} \tag{33.146}$$

then one has

$$G^{\blacksquare}_{\epsilon;\,X,X'}(\omega) = \int \mathrm{d}t\ \mathrm{e}^{\mathrm{i}\omega t} G^{\blacksquare}_{\epsilon;\,X,X'}(t) = \int \mathrm{d}t\ \mathrm{e}^{\mathrm{i}\omega t} G^{\blacksquare}_{X,X'}(t)\,\mathrm{e}^{-\epsilon|t|} \tag{33.147}$$

In order to compute the regularized Fourier-transformations, we remind the reader of the auxiliary-identities in Lemmata 1.19, 1.19 and Fact 1.21.

[11] Cf. [14].

Group 1

The time-ordered Green-function

For the time-ordered Green-function we obtain

$$\begin{aligned}
G^{\mathbb{T}}_{X,X'}(t) &= G^{\mathbb{T}}_{X,X'}(t, t'=0) \\
&= -\frac{\mathrm{i}}{\hbar}\langle \theta(t)X(t)X'(0) + S_{X,X'}\theta(-t)X'(0)X(t)\rangle \\
&= -\frac{\mathrm{i}}{\hbar}\frac{1}{Z}\sum_{n,m}\theta(t)\langle n|\mathrm{e}^{-\beta\Xi}X(t)|m\rangle\langle m|X'|n\rangle + S_{X,X'}\theta(-t)\langle n|\mathrm{e}^{-\beta\Xi}X'|m\rangle\langle m|X(t)|n\rangle \\
&= -\frac{\mathrm{i}}{\hbar}\frac{1}{Z}\sum_{n,m}\theta(t)\mathrm{e}^{-\beta\xi_n}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar}\langle n|X|m\rangle\langle m|X'|n\rangle + S_{X,X'}\theta(-t)\mathrm{e}^{-\beta\xi_n}\mathrm{e}^{\mathrm{i}t(\xi_m-\xi_n)/\hbar}\langle n|X'|m\rangle\langle m|X|n\rangle \\
&= -\frac{\mathrm{i}}{\hbar}\frac{1}{Z}\sum_{n,m}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar}\langle n|X|m\rangle\langle m|X'|n\rangle\left(\theta(t)\mathrm{e}^{-\beta\xi_n} + S_{X,X'}\theta(-t)\mathrm{e}^{-\beta\xi_m}\right)
\end{aligned}$$

We therefore see, that the Fourier-transform of the time-ordered Green-function is strictly speaking ill defined. We therefore introduce for each "small" $\epsilon > 0$, the regularized time-ordered Green-function

$$\begin{aligned}
G^{\mathbb{T}}_{\substack{\epsilon \\ X,X'}}(t) &= G^{\mathbb{T}}_{X,X'}(t)\,\mathrm{e}^{-\epsilon|t|} \\
&= -\frac{\mathrm{i}}{\hbar}\frac{1}{Z}\sum_{n,m}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar-\epsilon|t|}\langle n|X|m\rangle\langle m|X'|n\rangle\left(\theta(t)\mathrm{e}^{-\beta\xi_n} + S_{X,X'}\theta(-t)\mathrm{e}^{-\beta\xi_m}\right)
\end{aligned}$$

which gives for the Fourier-transform then

$$\begin{aligned}
G^{\mathbb{T}}_{\substack{\epsilon \\ X,X'}}(\omega) &= \int \mathrm{d}t\,\mathrm{e}^{\mathrm{i}\omega t}G^{\mathbb{T}}_{\substack{\epsilon \\ X,X'}}(t) \\
&= -\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\mathrm{e}^{-\beta\xi_n}\frac{\mathrm{i}}{\hbar}\int \mathrm{d}t\,\mathrm{e}^{\mathrm{i}\omega t}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar-\epsilon|t|}\theta(t) \\
&- S_{X,X'}\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\mathrm{e}^{-\beta\xi_m}\frac{\mathrm{i}}{\hbar}\int \mathrm{d}t\,\mathrm{e}^{\mathrm{i}\omega t}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar-\epsilon|t|}\theta(-t) \\
&= -\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\mathrm{e}^{-\beta\xi_n}\frac{-1}{\hbar}\frac{1}{\omega+\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar} \\
&- S_{X,X'}\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\mathrm{e}^{-\beta\xi_m}\frac{1}{\hbar}\frac{1}{\omega-\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar} \\
&= \frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\frac{1}{\hbar}\left(\frac{\mathrm{e}^{-\beta\xi_n}}{\omega+\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar} - S_{X,X'}\frac{\mathrm{e}^{-\beta\xi_m}}{\omega-\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar}\right)
\end{aligned}$$

The anti-time-ordered Green-function

For the anti-time-ordered Green-function we obtain

$$\begin{aligned}
G^{\overline{\mathbb{T}}}_{X,X'}(t) &= G^{\overline{\mathbb{T}}}_{X,X'}(t,t'=0) \\
&= -\frac{\mathrm{i}}{\hbar}\langle\theta(-t)X(t)X'(0) + S_{X,X'}\theta(+t)X'(0)X(t)\rangle \\
&= -\frac{\mathrm{i}}{\hbar}\frac{1}{Z}\sum_{n,m}\theta(-t)\langle n|\mathrm{e}^{-\beta\Xi}X(t)|m\rangle\langle m|X'|n\rangle + S_{X,X'}\theta(+t)\langle n|\mathrm{e}^{-\beta\Xi}X'|m\rangle\langle m|X(t)|n\rangle \\
&= -\frac{\mathrm{i}}{\hbar}\frac{1}{Z}\sum_{n,m}\theta(-t)\mathrm{e}^{-\beta\xi_n}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar}\langle n|X|m\rangle\langle m|X'|n\rangle + S_{X,X'}\theta(+t)\mathrm{e}^{-\beta\xi_n}\mathrm{e}^{\mathrm{i}t(\xi_m-\xi_n)/\hbar}\langle n|X'|m\rangle\langle m|X|n\rangle \\
&= -\frac{\mathrm{i}}{\hbar}\frac{1}{Z}\sum_{n,m}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar}\langle n|X|m\rangle\langle m|X'|n\rangle\left(\theta(-t)\mathrm{e}^{-\beta\xi_n} + S_{X,X'}\theta(+t)\mathrm{e}^{-\beta\xi_m}\right)
\end{aligned}$$

We therefore see, that the Fourier-transform of the anti-time-ordered Green-function is strictly speaking ill defined. We therefore introduce for each „small“ $\epsilon > 0$, the regularized anti time-ordered Green-function

$$\begin{aligned}
G^{\overline{\mathbb{T}}}_{\substack{\epsilon\\X,X'}}(t) &= G^{\overline{\mathbb{T}}}_{X,X'}(t)\,\mathrm{e}^{-\epsilon|t|} \\
&= -\frac{\mathrm{i}}{\hbar}\frac{1}{Z}\sum_{n,m}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar-\epsilon|t|}\langle n|X|m\rangle\langle m|X'|n\rangle\left(\theta(-t)\mathrm{e}^{-\beta\xi_n} + S_{X,X'}\theta(+t)\mathrm{e}^{-\beta\xi_m}\right)
\end{aligned}$$

which gives for the Fourier-transform then

$$\begin{aligned}
G^{\overline{\mathbb{T}}}_{\substack{\epsilon\\X,X'}}(\omega) &= \int \mathrm{d}t\,\mathrm{e}^{\mathrm{i}\omega t}G^{\overline{\mathbb{T}}}_{\substack{\epsilon\\X,X'}}(t) \\
&= -\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\mathrm{e}^{-\beta\xi_n}\frac{\mathrm{i}}{\hbar}\int \mathrm{d}t\,\mathrm{e}^{\mathrm{i}\omega t}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar-\epsilon|t|}\theta(-t) \\
&- S_{X,X'}\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\mathrm{e}^{-\beta\xi_m}\frac{\mathrm{i}}{\hbar}\int \mathrm{d}t\,\mathrm{e}^{\mathrm{i}\omega t}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar-\epsilon|t|}\theta(+t) \\
&= -\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\mathrm{e}^{-\beta\xi_n}\frac{+1}{\hbar}\frac{1}{\omega-\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar} \\
&- S_{X,X'}\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\mathrm{e}^{-\beta\xi_m}\frac{-1}{\hbar}\frac{1}{\omega+\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar} \\
&= \frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\frac{1}{\hbar}\left(\frac{-\mathrm{e}^{-\beta\xi_n}}{\omega-\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar} + S_{X,X'}\frac{\mathrm{e}^{-\beta\xi_m}}{\omega+\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar}\right)
\end{aligned}$$

Group 2

The retarded Green-function

For the retarded Green-function we obtain

$$
\begin{aligned}
G^{\mathrm{ret}}_{X,X'}(t) &= G^{\mathrm{ret}}_{X,X'}(t, t' = 0) \\
&= -\frac{\mathrm{i}}{\hbar}\theta(t)\langle X(t)X'(0) - S_{X,X'}X'(0)X(t)\rangle \\
&= -\frac{\mathrm{i}}{\hbar}\theta(t)\frac{1}{Z}\sum_{n,m}\langle n|\mathrm{e}^{-\beta\Xi}X(t)|m\rangle\langle m|X'|n\rangle - S_{X,X'}\langle n|\mathrm{e}^{-\beta\Xi}X'|m\rangle\langle m|X(t)|n\rangle \\
&= -\frac{\mathrm{i}}{\hbar}\theta(t)\frac{1}{Z}\sum_{n,m}\mathrm{e}^{-\beta\xi_n}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar}\langle n|X|m\rangle\langle m|X'|n\rangle - S_{X,X'}\mathrm{e}^{-\beta\xi_n}\mathrm{e}^{\mathrm{i}t(\xi_m-\xi_n)/\hbar}\langle n|X'|m\rangle\langle m|X|n\rangle \\
&= -\frac{\mathrm{i}}{\hbar}\frac{1}{Z}\theta(t)\sum_{n,m}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar}\langle n|X|m\rangle\langle m|X'|n\rangle\left(\mathrm{e}^{-\beta\xi_n} - S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)
\end{aligned}
$$

We therefore see, that the Fourier-transform of the retarded Green-function is strictly speaking ill defined. We therefore introduce for each „small“ $\epsilon > 0$, the regularized retarded Green-function

$$
\begin{aligned}
G^{\mathrm{ret}}_{\substack{\epsilon\\X,X'}}(t) &= G^{\mathrm{ret}}_{X,X'}(t)\,\mathrm{e}^{-\epsilon|t|} \\
&= -\frac{\mathrm{i}}{\hbar}\frac{1}{Z}\theta(t)\sum_{n,m}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar-\epsilon|t|}\langle n|X|m\rangle\langle m|X'|n\rangle\left(\mathrm{e}^{-\beta\xi_n} - S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)
\end{aligned}
$$

which gives for the Fourier-transform then

$$
\begin{aligned}
G^{\mathrm{ret}}_{\substack{\epsilon\\X,X'}}(\omega) &= \int \mathrm{d}t\,\mathrm{e}^{\mathrm{i}\omega t}G^{\mathrm{ret}}_{\substack{\epsilon\\X,X'}}(t) \\
&= -\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\left(\mathrm{e}^{-\beta\xi_n} - S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\frac{\mathrm{i}}{\hbar}\int \mathrm{d}t\,\mathrm{e}^{\mathrm{i}\omega t}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar-\epsilon|t|}\theta(t) \\
&= -\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\left(\mathrm{e}^{-\beta\xi_n} - S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\frac{-1}{\hbar}\frac{1}{\omega + \mathrm{i}\epsilon + (\xi_n-\xi_m)/\hbar} \\
&= \frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\left(\mathrm{e}^{-\beta\xi_n} - S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\frac{1}{\hbar}\frac{1}{\omega + \mathrm{i}\epsilon + (\xi_n-\xi_m)/\hbar}
\end{aligned}
$$

Lastly we switch to the usual notation found in physics-textbooks and note the formal identity

$$
\begin{aligned}
G^{\mathrm{ret}}_{\substack{\epsilon\\X,X'}}(\omega) &= \int \mathrm{d}t\,\mathrm{e}^{\mathrm{i}\omega t}G^{\mathrm{ret}}_{\substack{\epsilon\\X,X'}}(t) \\
&= -\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\left(\mathrm{e}^{-\beta\xi_n} - S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\frac{\mathrm{i}}{\hbar}\int \mathrm{d}t\,\mathrm{e}^{\mathrm{i}\omega t}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar-\epsilon|t|}\theta(t) \\
&= -\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\left(\mathrm{e}^{-\beta\xi_n} - S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\frac{\mathrm{i}}{\hbar}\int_0^\infty \mathrm{d}t\,\mathrm{e}^{\mathrm{i}\omega t}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar-\epsilon t}
\end{aligned}
$$

$$
\begin{aligned}
&= -\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\left(\mathrm{e}^{-\beta\xi_n} - S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\frac{\mathrm{i}}{\hbar}\int_0^\infty \mathrm{d}t\,\mathrm{e}^{\mathrm{i}(\omega+\mathrm{i}\epsilon)t}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar}\\
&= -\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\left(\mathrm{e}^{-\beta\xi_n} - S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\frac{\mathrm{i}}{\hbar}\int \mathrm{d}t\,\mathrm{e}^{\mathrm{i}(\omega+\mathrm{i}\epsilon)t}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar}\theta(t)\\
&= \int \mathrm{d}t\,\mathrm{e}^{\mathrm{i}(\omega+\mathrm{i}\epsilon)t}G^{\mathrm{ret}}_{X,X'}(t)\\
&= G^{\mathrm{ret}}_{X,X'}(\omega+\mathrm{i}\epsilon)
\end{aligned}
$$

Hence, for future reference, we have

$$
G^{\mathrm{ret}}_{X,X'}(\omega+\mathrm{i}\epsilon) = \frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\left(\mathrm{e}^{-\beta\xi_n} - S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\frac{1}{\hbar}\frac{1}{\omega+\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar}
$$

The advanced Green-function

For the advanced Green-function we obtain

$$
\begin{aligned}
G^{\mathrm{adv}}_{X,X'}(t) &= G^{\mathrm{adv}}_{X,X'}(t,t'=0)\\
&= +\frac{\mathrm{i}}{\hbar}\theta(-t)\langle X(t)X'(0) - S_{X,X'}X'(0)X(t)\rangle\\
&= +\frac{\mathrm{i}}{\hbar}\theta(-t)\frac{1}{Z}\sum_{n,m}\langle n|\mathrm{e}^{-\beta\Xi}X(t)|m\rangle\langle m|X'|n\rangle - S_{X,X'}\langle n|\mathrm{e}^{-\beta\Xi}X'|m\rangle\langle m|X(t)|n\rangle\\
&= +\frac{\mathrm{i}}{\hbar}\theta(-t)\frac{1}{Z}\sum_{n,m}\mathrm{e}^{-\beta\xi_n}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar}\langle n|X|m\rangle\langle m|X'|n\rangle - S_{X,X'}\mathrm{e}^{-\beta\xi_n}\mathrm{e}^{\mathrm{i}t(\xi_m-\xi_n)/\hbar}\langle n|X'|m\rangle\langle m|X|n\rangle\\
&= +\frac{\mathrm{i}}{\hbar}\frac{1}{Z}\theta(-t)\sum_{n,m}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar}\langle n|X|m\rangle\langle m|X'|n\rangle\left(\mathrm{e}^{-\beta\xi_n} - S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)
\end{aligned}
$$

We therefore see, that the Fourier-transform of the advanced Green-function is strictly speaking ill defined. We therefore introduce for each „small“ $\epsilon > 0$, the regularized advanced Green-function

$$
\begin{aligned}
G^{\mathrm{adv}}_{\substack{\epsilon\\X,X'}}(t) &= G^{\mathrm{adv}}_{X,X'}(t)\,\mathrm{e}^{-\epsilon|t|}\\
&= +\frac{\mathrm{i}}{\hbar}\frac{1}{Z}\theta(-t)\sum_{n,m}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar-\epsilon|t|}\langle n|X|m\rangle\langle m|X'|n\rangle\left(\mathrm{e}^{-\beta\xi_n} - S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)
\end{aligned}
$$

which gives for the Fourier-transform then

$$
\begin{aligned}
G^{\mathrm{adv}}_{\substack{\epsilon\\X,X'}}(\omega) &= \int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t} G^{\mathrm{adv}}_{\substack{\epsilon\\X,X'}}(t) \\
&= +\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle \left(\mathrm{e}^{-\beta\xi_n} - S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\frac{\mathrm{i}}{\hbar}\int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar-\epsilon|t|}\theta(-t) \\
&= +\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle \left(\mathrm{e}^{-\beta\xi_n} - S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\frac{1}{\hbar}\frac{1}{\omega - \mathrm{i}\epsilon + (\xi_n-\xi_m)/\hbar} \\
&= \frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle \left(\mathrm{e}^{-\beta\xi_n} - S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\frac{1}{\hbar}\frac{1}{\omega - \mathrm{i}\epsilon + (\xi_n-\xi_m)/\hbar}
\end{aligned}
$$

Lastly we switch to the usual notation found in physics-textbooks and note the formal identity

$$
\begin{aligned}
G^{\mathrm{adv}}_{\substack{\epsilon\\X,X'}}(\omega) &= \int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t} G^{\mathrm{adv}}_{\substack{\epsilon\\X,X'}}(t) \\
&= +\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle \left(\mathrm{e}^{-\beta\xi_n} - S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\frac{\mathrm{i}}{\hbar}\int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar-\epsilon|t|}\theta(-t) \\
&= +\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle \left(\mathrm{e}^{-\beta\xi_n} - S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\frac{\mathrm{i}}{\hbar}\int_{-\infty}^{0} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar+\epsilon t} \\
&= +\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle \left(\mathrm{e}^{-\beta\xi_n} - S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\frac{\mathrm{i}}{\hbar}\int_{-\infty}^{0} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}(\omega-\mathrm{i}\epsilon)t}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar} \\
&= +\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle \left(\mathrm{e}^{-\beta\xi_n} - S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\frac{\mathrm{i}}{\hbar}\int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}(\omega-\mathrm{i}\epsilon)t}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar}\theta(-t) \\
&= \int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}(\omega-\mathrm{i}\epsilon)t} G^{\mathrm{adv}}_{X,X'}(t) \\
&= G^{\mathrm{adv}}_{X,X'}(\omega - \mathrm{i}\epsilon)
\end{aligned}
$$

Hence, for future reference, we have

$$
G^{\mathrm{adv}}_{X,X'}(\omega - \mathrm{i}\epsilon) = \frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle \left(\mathrm{e}^{-\beta\xi_n} - S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\frac{1}{\hbar}\frac{1}{\omega - \mathrm{i}\epsilon + (\xi_n-\xi_m)/\hbar}
$$

Group 3

Lemmata for the third group

In the third group we are in the comfortable situation that we can refer to standard-theorems about distribution-theory, such as Theorem 1.22. Notice also that we can reformulate Fact 14.2 equivalently (in wise foresight) as

$$
\frac{1}{\omega + \mathrm{i}\epsilon + (\xi_n-\xi_m)/\hbar} = \mathrm{P}\,\frac{1}{\omega + (\xi_n-\xi_m)/\hbar} - \mathrm{i}\pi\delta(\omega + (\xi_n-\xi_m)/\hbar) \tag{33.148}
$$

The lesser Green-function

For the lesser Green-function we obtain

$$\begin{aligned}
G^<_{X,X'}(t) &= G^<_{X,X'}(t, t' = 0) \\
&= -\frac{\mathrm{i}}{\hbar} S_{X,X'} \langle X'(0) X(t) \rangle \\
&= -\frac{\mathrm{i}}{\hbar} S_{X,X'} \frac{1}{Z} \sum_{n,m} \langle n | \mathrm{e}^{-\beta \Xi} X' | m \rangle \langle m | X(t) | n \rangle \\
&= -\frac{\mathrm{i}}{\hbar} S_{X,X'} \frac{1}{Z} \sum_{n,m} \mathrm{e}^{-\beta \xi_n} \mathrm{e}^{\mathrm{i}t(\xi_m - \xi_n)/\hbar} \langle n | X' | m \rangle \langle m | X | n \rangle \\
&= \frac{1}{Z} \sum_{n,m} \langle n | X | m \rangle \langle m | X' | n \rangle \mathrm{e}^{-\beta \xi_m} \left(-\frac{\mathrm{i}}{\hbar} S_{X,X'} \right) \mathrm{e}^{\mathrm{i}t(\xi_n - \xi_m)/\hbar}
\end{aligned}$$

We therefore see, that the Fourier-transform of the lesser Green-function is simply the usual delta-distribution. This gives for the Fourier-transform then

$$\begin{aligned}
G^<_{X,X'}(\omega) &= \int \mathrm{d}t \, \mathrm{e}^{\mathrm{i}\omega t} G^<_{X,X'}(t) \\
&= \frac{1}{Z} \sum_{n,m} \langle n | X | m \rangle \langle m | X' | n \rangle \left(-\frac{\mathrm{i}}{\hbar} S_{X,X'} \right) \mathrm{e}^{-\beta \xi_m} \int \mathrm{d}t \, \mathrm{e}^{\mathrm{i}\omega t} \mathrm{e}^{\mathrm{i}t(\xi_n - \xi_m)/\hbar} \\
&= -\frac{1}{Z} \sum_{n,m} \langle n | X | m \rangle \langle m | X' | n \rangle \left(-2\pi \frac{\mathrm{i}}{\hbar} S_{X,X'} \right) \mathrm{e}^{-\beta \xi_m} \delta(\omega + (\xi_n - \xi_m)/\hbar)
\end{aligned}$$

The greater Green-function

For the greater Green-function we obtain

$$\begin{aligned}
G^>_{X,X'}(t) &= G^>_{X,X'}(t, t' = 0) \\
&= -\frac{\mathrm{i}}{\hbar} \langle X(t) X'(0) \rangle \\
&= -\frac{\mathrm{i}}{\hbar} \frac{1}{Z} \sum_{n,m} \langle n | \mathrm{e}^{-\beta \Xi} X(t) | m \rangle \langle m | X' | n \rangle \\
&= -\frac{\mathrm{i}}{\hbar} \frac{1}{Z} \sum_{n,m} \mathrm{e}^{-\beta \xi_n} \mathrm{e}^{\mathrm{i}t(\xi_n - \xi_m)/\hbar} \langle n | X | m \rangle \langle m | X' | n \rangle \\
&= \frac{1}{Z} \sum_{n,m} \langle n | X | m \rangle \langle m | X' | n \rangle \mathrm{e}^{-\beta \xi_n} \left(-\frac{\mathrm{i}}{\hbar} \right) \mathrm{e}^{\mathrm{i}t(\xi_n - \xi_m)/\hbar}
\end{aligned}$$

We therefore see, that the Fourier-transform of the greater Green-function is simply the usual delta-distribution. This gives for the Fourier-transform then

$$
\begin{aligned}
G^{>}_{X,X'}(\omega) &= \int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t} G^{>}_{X,X'}(t) \\
&= \frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle \left(-\frac{\mathrm{i}}{\hbar}\right)\mathrm{e}^{-\beta\xi_n}\int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t}\mathrm{e}^{\mathrm{i}t(\xi_n-\xi_m)/\hbar} \\
&= \frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle \left(-2\pi\frac{\mathrm{i}}{\hbar}\right)\mathrm{e}^{-\beta\xi_n}\delta(\omega+(\xi_n-\xi_m)/\hbar)
\end{aligned}
$$

The spectral function

We have for the spectral function

$$
\begin{aligned}
A_{X,X'}(\omega) &= -\frac{\hbar}{\pi}\,\mathrm{Im}\lim_{\epsilon\to 0} G^{\mathrm{ret}}_{X,X'}(\omega+\mathrm{i}\epsilon) \\
&= -\frac{\hbar}{\pi}\,\mathrm{Im}\lim_{\epsilon\to 0}\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\left(\mathrm{e}^{-\beta\xi_n}-S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\frac{1}{\hbar}\frac{1}{\omega+\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar} \\
&= -\frac{\hbar}{\pi}\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\left(\mathrm{e}^{-\beta\xi_n}-S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\frac{1}{\hbar}\,\mathrm{Im}\left[\mathrm{P}\frac{1}{\omega+(\xi_n-\xi_m)/\hbar}-\mathrm{i}\pi\delta(\omega+(\xi_n-\xi_m)/\hbar)\right] \\
&= \frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\left(\mathrm{e}^{-\beta\xi_n}-S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\delta(\omega+(\xi_n-\xi_m)/\hbar) \\
&= \dots
\end{aligned}
$$

Notice, for later reference, that this can be simplified further as[12]

$$
\begin{aligned}
A_{X,X'}(\omega) &= \dots \\
&= \frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\mathrm{e}^{-\beta\xi_n}\left(1-S_{X,X'}\mathrm{e}^{-\beta(\xi_m-\xi_n)}\right)\delta(\omega+(\xi_n-\xi_m)/\hbar) \\
&= \frac{1}{Z}\left(1-S_{X,X'}\mathrm{e}^{-\hbar\beta\omega}\right)\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\mathrm{e}^{-\beta\xi_n}\delta(\omega+(\xi_n-\xi_m)/\hbar)
\end{aligned}
\tag{33.149}
$$

Group 4 (The imaginary-time Green-function)

Lemma for the four group

In the third group we are in the comfortable situation that we are dealing with a periodic functions, which are particularly simple to handle due to the vast literature about them. We only need Lemma 1.13.

The imaginary-time-ordered Green-function

For the imaginary-time-ordered Green-function we obtain

[12] It is just a simple use of the delta-distribution, but yet smart to do it like this. Cf. [32] page 122.

$$
\begin{aligned}
\mathscr{G}_{X,X'}(\tau) &= \mathscr{G}_{X,X'}(\tau,\tau'=0)\\
&= -\frac{1}{\hbar}\langle\theta(\tau)X(\tau)X'(0) + S_{X,X'}\theta(-\tau)X'(0)X(\tau)\rangle\\
&= -\frac{1}{\hbar}\frac{1}{Z}\sum_{n,m}\theta(\tau)\langle n|\mathrm{e}^{-\beta\Xi}X(\tau)|m\rangle\langle m|X'|n\rangle + S_{X,X'}\theta(-\tau)\langle n|\mathrm{e}^{-\beta\Xi}X'|m\rangle\langle m|X(\tau)|n\rangle\\
&= -\frac{1}{\hbar}\frac{1}{Z}\sum_{n,m}\theta(\tau)\mathrm{e}^{-\beta\xi_n}\mathrm{e}^{\tau(\xi_n-\xi_m)/\hbar}\langle n|X|m\rangle\langle m|X'|n\rangle + S_{X,X'}\theta(-\tau)\mathrm{e}^{-\beta\xi_n}\mathrm{e}^{\tau(\xi_m-\xi_n)/\hbar}\langle n|X'|m\rangle\langle m|X|n\rangle\\
&= -\frac{1}{\hbar}\frac{1}{Z}\sum_{n,m}\mathrm{e}^{\tau(\xi_n-\xi_m)/\hbar}\langle n|X|m\rangle\langle m|X'|n\rangle\left(\theta(\tau)\mathrm{e}^{-\beta\xi_n} + S_{X,X'}\theta(-\tau)\mathrm{e}^{-\beta\xi_m}\right)
\end{aligned}
$$

We now compute the Matsubara-coefficients of these functions.

$$
\begin{aligned}
\mathscr{G}_{X,X'}(\mathrm{i}\omega_n) &= \int_0^{\hbar\beta}\mathrm{d}\tau\,\mathrm{e}^{\mathrm{i}\omega_\tau}\mathscr{G}_{X,X'}(\tau)\\
&= -\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\mathrm{e}^{-\beta\xi_n}\frac{1}{\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau\,\mathrm{e}^{\mathrm{i}\omega_n\tau}\mathrm{e}^{\tau(\xi_n-\xi_m)/\hbar}\\
&= -\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\mathrm{e}^{-\beta\xi_n}\frac{1}{\hbar}\frac{S_{X,X'}\mathrm{e}^{\beta\left(\xi_n-\xi_m\right)}-1}{\mathrm{i}\omega_n+\left(\xi_n-\xi_m\right)/\hbar}\\
&= \frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\frac{1}{\hbar}\frac{\mathrm{e}^{-\beta\xi_n}-S_{X,X'}\mathrm{e}^{-\beta\xi_m}}{\mathrm{i}\omega_n+\left(\xi_n-\xi_m\right)/\hbar}
\end{aligned}
$$

Summarizing the results, one finds for the different Green-functions (and the spectral function)

$$
G^{\mathbb{T}}_{\substack{\epsilon\\X,X'}}(\omega) = \frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\frac{1}{\hbar}\left(\frac{\mathrm{e}^{-\beta\xi_n}}{\omega+\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar} - S_{X,X'}\frac{\mathrm{e}^{-\beta\xi_m}}{\omega-\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar}\right) \tag{33.150}
$$

$$
G^{<}_{X,X'}(\omega) = \frac{1}{Z}\sum_{(n,m)\in\mathbb{N}^2}\langle n|X|m\rangle\langle m|X'|n\rangle\frac{-2\pi\mathrm{i}S_{X,X'}e^{-\beta\xi_m}}{\hbar}\delta(\omega+(\xi_n-\xi_m)/\hbar) \tag{33.151}
$$

$$
G^{>}_{X,X'}(\omega) = \frac{1}{Z}\sum_{(n,m)\in\mathbb{N}^2}\langle n|X|m\rangle\langle m|X'|n\rangle\frac{2\pi\mathrm{i}e^{-\beta\xi_n}}{\hbar}\delta(\omega+(\xi_n-\xi_m)/\hbar) \tag{33.152}
$$

$$
G^{\overline{\mathbb{T}}}_{\substack{\epsilon\\X,X'}}(\omega) = \frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\frac{1}{\hbar}\left(\frac{-\mathrm{e}^{-\beta\xi_n}}{\omega-\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar} + S_{X,X'}\frac{\mathrm{e}^{-\beta\xi_m}}{\omega+\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar}\right) \tag{33.153}
$$

$$
G^{\mathrm{ret}}_{X,X'}(\omega+\mathrm{i}\epsilon) = \frac{1}{Z}\sum_{(n,m)\in\mathbb{N}^2}\langle n|X|m\rangle\langle m|X'|n\rangle\frac{e^{-\beta\xi_n}-S_{X,X'}e^{-\beta\xi_m}}{\hbar}\frac{1}{\omega+\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar} \tag{33.154}
$$

$$G^{\mathrm{adv}}_{X,X'}(\omega - \mathrm{i}\epsilon) = \frac{1}{Z}\sum_{(n,m)\in\mathbb{N}^2}\langle n|X|m\rangle\langle m|X'|n\rangle\,\frac{e^{-\beta\xi_n} - S_{X,X'}e^{-\beta\xi_m}}{\hbar}\,\frac{1}{\omega - \mathrm{i}\epsilon + (\xi_n - \xi_m)/\hbar} \tag{33.155}$$

$$\mathscr{G}_{X,X'}(\mathrm{i}\omega_l) = \frac{1}{Z}\sum_{(n,m)\in\mathbb{N}^2}\langle n|X|m\rangle\langle m|X'|n\rangle\,\frac{e^{-\beta\xi_n} - S_{X,X'}e^{-\beta\xi_m}}{\hbar}\,\frac{1}{\mathrm{i}\omega_l + (\xi_n - \xi_m)/\hbar} \tag{33.156}$$

$$A_{X,X'}(\omega) = \frac{1}{Z}\sum_{(n,m)\in\mathbb{N}^2}\langle n|X|m\rangle\langle m|X'|n\rangle\left(e^{-\beta\xi_n} - S_{X,X'}e^{-\beta\xi_m}\right)\delta(\omega + (\xi_n - \xi_m)/\hbar) \tag{33.157}$$

Proof 33.41 of Theorem 14.6 We divide the proof into the two equation signs.

The spectral function for the lesser Green-function

We recall from Equation (33.157) that the spectral function

$$\begin{aligned}
A_{X,X'}(\omega) &= \frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\left(\mathrm{e}^{-\beta\xi_n} - S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\delta(\omega + (\xi_n - \xi_m)/\hbar)\\
&= \frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\mathrm{e}^{-\beta\xi_m}\left(\mathrm{e}^{\beta(\xi_m - \xi_n)} - S_{X,X'}\right)\delta(\omega + (\xi_n - \xi_m)/\hbar)\\
&= \frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\mathrm{e}^{-\beta\xi_m}\left(\mathrm{e}^{\beta\hbar\omega} - S_{X,X'}\right)\delta(\omega + (\xi_n - \xi_m)/\hbar)\\
&= \frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\mathrm{e}^{-\beta\xi_m}\left(\mathrm{n}^{S_{X,X'}}_{\hbar\beta}(\omega)\right)^{-1}\delta(\omega + (\xi_n - \xi_m)/\hbar)
\end{aligned}$$

With the the ζ-distribution from Equation (TBReferenced). Now comparing the Lehmann-representation of the spectral-function (with a proper prefactor) with the one for the lesser-Green-function gives

$$\begin{aligned}
-2\pi\frac{\mathrm{i}}{\hbar}S_{X,X'}\,\mathrm{n}^{S_{X,X'}}_{\hbar\beta}(\omega)A_{X,X'}(\omega) &= 2\mathrm{i}S_{X,X'}\,\mathrm{n}^{S_{X,X'}}_{\hbar\beta}(\omega)\,\mathrm{Im}\lim_{\epsilon\to 0}G^{\mathrm{ret}}_{X,X'}(\omega + \mathrm{i}\epsilon)\\
&= -2\pi\frac{\mathrm{i}}{\hbar}S_{X,X'}\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\mathrm{e}^{-\beta\xi_m}\delta(\omega + (\xi_n - \xi_m)/\hbar)\\
&= G^{<}_{X,X'}(\omega)
\end{aligned}$$

whereas in the last equation we used Equation (33.151).

The spectral function for the greater Green-function

We recall from Equation (33.157) that the spectral function

$$\begin{aligned}
A_{X,X'}(\omega) &= \frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\left(\mathrm{e}^{-\beta\xi_n} - S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\delta(\omega+(\xi_n-\xi_m)/\hbar)\\
&= \frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\mathrm{e}^{-\beta\xi_n}\left(1 - S_{X,X'}\mathrm{e}^{-\beta(\xi_m-\xi_n)}\right)\delta(\omega+(\xi_n-\xi_m)/\hbar)\\
&= \frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\mathrm{e}^{-\beta\xi_n}\left(1 - S_{X,X'}\mathrm{e}^{-\beta\hbar\omega}\right)\delta(\omega+(\xi_n-\xi_m)/\hbar)\\
&= \dots
\end{aligned}$$

Now we compute with the ζ-distribution

$$1 + S_{X,X'}\,\mathrm{n}_{\hbar\beta}^{S_{X,X'}}(\omega) = 1 + \frac{S_{X,X'}}{\mathrm{e}^{\hbar\beta\omega} - S_{X,X'}} = \frac{\mathrm{e}^{\hbar\beta\omega} - S_{X,X'} + S_{X,X'}}{\mathrm{e}^{\hbar\beta\omega} - S_{X,X'}} = \frac{1}{1 - S_{X,X'}\mathrm{e}^{-\hbar\beta\omega}} = \left(1 - S_{X,X'}\mathrm{e}^{-\hbar\beta\omega}\right)^{-1}$$

$$\iff \left(1 + S_{X,X'}\,\mathrm{n}_{\hbar\beta}^{S_{X,X'}}(\omega)\right)^{-1} = 1 - S_{X,X'}\mathrm{e}^{-\hbar\beta\omega}$$

and inserting this above allows us to rewrite the expression above to the form

$$A_{X,X'}(\omega) = \dots = \frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\mathrm{e}^{-\beta\xi_n}\left(1 + S_{X,X'}\,\mathrm{n}_{\hbar\beta}^{S_{X,X'}}(\omega)\right)^{-1}\delta(\omega+(\xi_n-\xi_m)/\hbar)$$

This yields then

$$\begin{aligned}
-\frac{\mathrm{i}}{\hbar}2\pi\left(1 + S_{X,X'}\,\mathrm{n}_{\hbar\beta}^{S_{X,X'}}(\omega)\right)A_{X,X'}(\omega) &= 2\mathrm{i}\left(1 + S_{X,X'}\,\mathrm{n}_{\hbar\beta}^{S_{X,X'}}(\omega)\right)\mathrm{Im}\lim_{\epsilon\to 0}G^{\mathrm{ret}}_{X,X'}(\omega+\mathrm{i}\epsilon)\\
&= \frac{-\mathrm{i}}{\hbar}2\pi\frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\mathrm{e}^{-\beta\xi_n}\delta(\omega+(\xi_n-\xi_m)/\hbar)\\
&= G^{>}_{X,X'}(\omega)
\end{aligned}$$

whereas we used Equation (33.152) in the last step.

Proof 33.42 of Theorem 14.7

We first prove the identities relating the time-ordered and the retarded Green-function. For this we recall Equations (33.150), (33.154) and the Sokhotski-Plemelj-theorem in Equation (14.3)

$$\frac{1}{\omega + \mathrm{i}\epsilon + \text{const.}} = \mathrm{P}\frac{1}{\omega + \text{const.}} - \mathrm{i}\pi\delta(\omega + \text{const.}), \tag{33.158}$$

$$\frac{1}{\omega - \mathrm{i}\epsilon + \text{const.}} = \mathrm{P}\frac{1}{\omega + \text{const.}} + \mathrm{i}\pi\delta(\omega + \text{const.}), \tag{33.159}$$

such that we obtain the identities

$$G^{\mathbb{T}}_{\substack{\epsilon \\ X,X'}}(\omega) = \frac{1}{Z}\sum_{n,m}\langle n|X|m\rangle\langle m|X'|n\rangle\frac{1}{\hbar}\left(\frac{\mathrm{e}^{-\beta\xi_n}}{\omega+\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar} - S_{X,X'}\frac{\mathrm{e}^{-\beta\xi_m}}{\omega-\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar}\right) \tag{33.160}$$

$$G^{\mathrm{ret}}_{X,X'}(\omega+\mathrm{i}\epsilon) = \frac{1}{Z}\sum_{(n,m)\in\mathbb{N}^2}\langle n|X|m\rangle\langle m|X'|n\rangle\,\frac{e^{-\beta\xi_n}-S_{X,X'}e^{-\beta\xi_m}}{\hbar}\,\frac{1}{\omega+\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar} \tag{33.161}$$

We will prove the identity for each term in the individual summations, which will hence prove the theorem.

The time-ordered Green-function $G^{\mathbb{T}}$

For the time-ordered Green-function we obtain on the one hand

$$\begin{aligned}\frac{\mathrm{e}^{-\beta\xi_n}}{\omega+\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar} - S_{X,X'}\frac{\mathrm{e}^{-\beta\xi_m}}{\omega-\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar} &= \left(\mathrm{e}^{-\beta\xi_n}-S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\mathrm{P}\,\frac{1}{\omega+(\xi_n-\xi_m)/\hbar}\\ &\quad+\left(-\mathrm{e}^{-\beta\xi_n}-S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\mathrm{i}\pi\delta(\omega+(\xi_n-\xi_m)/\hbar)\end{aligned}$$

and hence we obtain

$$\mathrm{Re}\left(\frac{\mathrm{e}^{-\beta\xi_n}}{\omega+\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar} - S_{X,X'}\frac{\mathrm{e}^{-\beta\xi_m}}{\omega-\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar}\right) = \left(\mathrm{e}^{-\beta\xi_n}-S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\mathrm{P}\,\frac{1}{\omega+(\xi_n-\xi_m)/\hbar}$$

$$\mathrm{Im}\left(\frac{\mathrm{e}^{-\beta\xi_n}}{\omega+\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar} - S_{X,X'}\frac{\mathrm{e}^{-\beta\xi_m}}{\omega-\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar}\right) = \left(-\mathrm{e}^{-\beta\xi_n}-S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\pi\delta(\omega+(\xi_n-\xi_m)/\hbar)$$

The retarded Green-function G^{ret}

For the retarded Green-function we obtain on the other hand

$$\left(e^{-\beta\xi_n}-S_{X,X'}e^{-\beta\xi_m}\right)\frac{1}{\omega+\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar} = \left(e^{-\beta\xi_n}-S_{X,X'}e^{-\beta\xi_m}\right)\left(\mathrm{P}\,\frac{1}{\omega+(\xi_n-\xi_m)/\hbar} - \mathrm{i}\pi\delta(\omega+(\xi_n-\xi_m)/\hbar)\right)$$

and hence

$$\mathrm{Re}\left(e^{-\beta\xi_n}-S_{X,X'}e^{-\beta\xi_m}\right)\frac{1}{\omega+\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar} = \left(e^{-\beta\xi_n}-S_{X,X'}e^{-\beta\xi_m}\right)\mathrm{P}\,\frac{1}{\omega+(\xi_n-\xi_m)/\hbar}$$

$$\mathrm{Im}\left(e^{-\beta\xi_n}-S_{X,X'}e^{-\beta\xi_m}\right)\frac{1}{\omega+\mathrm{i}\epsilon+(\xi_n-\xi_m)/\hbar} = -\left(e^{-\beta\xi_n}-S_{X,X'}e^{-\beta\xi_m}\right)\pi\delta(\omega+(\xi_n-\xi_m)/\hbar)$$

Comparing the Results

The real parts obviously coincide. For the imaginary part we obtain, using the delta-distribution

$$
\begin{aligned}
&-\left(e^{-\beta\xi_n} - S_{X,X'}e^{-\beta\xi_m}\right)\cdot\left(\coth\frac{\beta\hbar\omega}{2}\right)^{S_{X,X'}} \overset{!}{=} -\left(\mathrm{e}^{-\beta\xi_n} + S_{X,X'}\mathrm{e}^{-\beta\xi_m}\right)\\
\Longleftrightarrow\ &\left(\coth\frac{\beta\hbar\omega}{2}\right)^{S_{X,X'}} \overset{!}{=} \frac{\mathrm{e}^{-\beta\xi_n} + S_{X,X'}\mathrm{e}^{-\beta\xi_m}}{e^{-\beta\xi_n} - S_{X,X'}e^{-\beta\xi_m}} \equiv \frac{\mathrm{e}^{-\beta\xi_n} + S_{X,X'}\mathrm{e}^{-\beta(\xi_n+\hbar\omega)}}{e^{-\beta\xi_n} - S_{X,X'}e^{-\beta(\xi_n+\hbar\omega)}} = \frac{1 + S_{X,X'}\mathrm{e}^{-\beta\hbar\omega}}{1 - S_{X,X'}e^{-\beta\hbar\omega}} = \frac{\mathrm{e}^{\beta\hbar\omega/2} + S_{X,X'}\mathrm{e}^{-\beta\hbar\omega/2}}{\mathrm{e}^{\beta\hbar\omega/2} - S_{X,X'}e^{-\beta\hbar\omega/2}}
\end{aligned}
$$

Recalling now the definition of the cotangens-hyperbolicus we have proven the theorem. For the advanced Green-function the theorem is proven analogously.

Proof 33.43 of Lemma 14.14

We re-express the average particle number as lesser Green-functions and then use the fluctuation-dissipation-theorem

$$
\begin{aligned}
\langle N\rangle &= \sum_{\alpha\in\mathscr{A}}\langle c_\alpha^\dagger c_\alpha\rangle\\
&= -\zeta\frac{\hbar}{\mathrm{i}}\sum_{\alpha\in\mathscr{A}} G^<_{\alpha,\alpha}(t=0)\\
&= -\zeta\frac{1}{2\pi\mathrm{i}}\oint\!\!\!\!\!\!\sum_{\substack{\alpha\in\mathscr{A}\\ E\in(-\infty,+\infty)}} G^<_{\alpha,\alpha}(E)\\
&= \frac{-1}{\pi}\lim_{\eta\to 0}\oint\!\!\!\!\!\!\sum_{\substack{\alpha\in\mathscr{A}\\ E\in(-\infty,+\infty)}} \mathrm{n}^\zeta_\beta(E)\ \mathrm{Im}\ G^{\mathrm{ret}}_{\alpha,\alpha}(E+\mathrm{i}\eta)
\end{aligned}
\tag{33.162}
$$

Proof 33.44 of Lemma 14.15

For the first identity we compute

$$
\begin{aligned}
\delta_{\alpha,\alpha'} &= \langle\delta_{\alpha,\alpha'}\rangle\\
&= \langle[c_\alpha, c^\dagger_{\alpha'}]_\zeta\rangle\\
&= \langle c_\alpha c^\dagger_{\alpha'}\rangle - \zeta\langle c^\dagger_{\alpha'}c_\alpha\rangle\\
&= -\frac{\hbar}{\mathrm{i}}\left(G^>_{\alpha,\alpha'}(t=0) - G^<_{\alpha,\alpha'}(t=0)\right)\\
&= -\frac{\hbar}{\mathrm{i}}\int\frac{\mathrm{d}\omega}{2\pi}\left(G^>_{\alpha,\alpha'}(\omega) - G^<_{\alpha,\alpha'}(\omega)\right)\\
&= -\frac{\hbar}{\mathrm{i}}\lim_{\eta\to 0}\int\frac{\mathrm{d}\omega}{2\pi}2\mathrm{i}\,\mathrm{Im}\,G^{\mathrm{ret}}_{\alpha,\alpha'}(\omega+\mathrm{i}\eta)\\
&= \lim_{\eta\to 0} -\frac{\hbar}{\pi}\int\mathrm{d}\omega\ \mathrm{Im}\,G^{\mathrm{ret}}_{\alpha,\alpha'}(\omega+\mathrm{i}\eta)\\
&\equiv \int\mathrm{d}\omega\, A_{\alpha,\alpha'}(\omega)
\end{aligned}
$$

The second identity follows from the first identity with

$$\mathrm{d} = \sum_{\alpha \in \mathscr{A}} \delta_{\alpha,\alpha} = \ldots = \int \mathrm{d}\omega \sum_{\alpha \in \mathscr{A}} \delta_{\alpha,\alpha}\, A_{\alpha,\alpha}(\omega) \tag{33.163}$$

The third identity follows immediately from Equation (33.157).

Proof 33.45 of Lemma 15.2

We compute straight forwardly

$$\begin{aligned} \partial_\tau U_{\mathrm{int}}(\tau) &= \mathrm{e}^{\tau \Xi_0/\hbar} \frac{\Xi_0 - \Xi}{\hbar} \mathrm{e}^{-\tau \Xi/\hbar} \\ &= -\frac{1}{\hbar} \mathrm{e}^{\tau \Xi_0/\hbar} V \mathrm{e}^{-\tau \Xi/\hbar} \\ &= -\frac{1}{\hbar} \mathrm{e}^{\tau \Xi_0/\hbar} V \mathrm{e}^{-\tau \Xi_0/\hbar} \mathrm{e}^{+\tau \Xi_0/\hbar} \mathrm{e}^{-\tau \Xi/\hbar} \\ &= -\frac{1}{\hbar} V_{\mathrm{H}_{\Xi_0}}(\tau) U_{\mathrm{int}}(\tau). \end{aligned} \tag{33.164}$$

Proof 33.46 of Corollary 15.3

By using repeated integrations on both sides, demanding $U(0) = 1$, we obtain

$$\begin{aligned} U_{\mathrm{int}} &= 1 \quad - \quad \frac{1}{\hbar} \int_0^\tau \mathrm{d}\tau_1\, V_{\mathrm{H}_{\Xi_0}}(\tau_1) U_{\mathrm{int}}(\tau_1) \\ &= 1 \quad + \quad \left(-\frac{1}{\hbar}\right) \int_0^\tau \mathrm{d}\tau_1\, V_{\mathrm{H}_{\Xi_0}}(\tau_1) U_{\mathrm{int}}(\tau_1) \quad + \quad \left(-\frac{1}{\hbar}\right)^2 \int_0^\tau \mathrm{d}\tau_1 \int_0^{\tau_1} \mathrm{d}\tau_2\, V_{\mathrm{H}_{\Xi_0}}(\tau_1) V_{\mathrm{H}_{\Xi_0}}(\tau_2) U_{\mathrm{int}}(\tau_1) \\ &= \ldots \\ &= \sum_{n=0}^{\infty} \left(-\frac{1}{\hbar}\right)^n \int_0^\tau \mathrm{d}\tau_1 \cdots \int_0^{\tau_{n-1}} \mathrm{d}\tau_n\, V_{\mathrm{H}_{\Xi_0}}(\tau_1) \ldots V_{\mathrm{H}_{\Xi_0}}(\tau_n) \\ &= \sum_{n=0}^{\infty} \left(-\frac{1}{\hbar}\right)^n \frac{1}{n!} \int_0^\tau \mathrm{d}\tau_1 \cdots \int_0^\tau \mathrm{d}\tau_n\, \mathrm{T}_\tau \left[V_{\mathrm{H}_{\Xi_0}}(\tau_1) \ldots V_{\mathrm{H}_{\Xi_0}}(\tau_n) \right] \\ &\equiv \mathrm{T}_\tau \exp\left[-\frac{1}{\hbar} \int_0^\tau \mathrm{d}\tilde{\tau}\, V_{\mathrm{H}_{\Xi_0}}(\tilde{\tau}) \right] \end{aligned} \tag{33.165}$$

whereas in the last steps we regrouped the summation as an ordered product.

Proof 33.47 of Lemma 15.4

We compute straight forwardly

$$
\begin{aligned}
\mathscr{G}_{X,X'}(\tau) &\equiv -\frac{1}{\hbar}\left\langle X(\tau)\,X'(0)\right\rangle \\
&\equiv -\frac{1}{\hbar}\frac{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta\Xi}X(\tau)\,X'(0)}{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta\Xi}} \\
&\equiv -\frac{1}{\hbar}\frac{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta\Xi}\mathrm{e}^{+\tau\Xi/\hbar}X(\tau)\,\mathrm{e}^{-\tau\Xi/\hbar}X'(0)}{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta\Xi}} \\
&\equiv -\frac{1}{\hbar}\frac{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta\Xi_0}\mathrm{e}^{+\beta\Xi_0}\mathrm{e}^{-\beta\Xi}\mathrm{e}^{+\tau\Xi/\hbar}\mathrm{e}^{-\beta\Xi_0}\mathrm{e}^{+\beta\Xi_0}X\,\mathrm{e}^{-\beta\Xi_0}\mathrm{e}^{+\beta\Xi_0}\mathrm{e}^{-\tau\Xi/\hbar}X'(0)}{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta\Xi_0}\mathrm{e}^{+\beta\Xi_0}\mathrm{e}^{-\beta\Xi}} \\
&\equiv -\frac{1}{\hbar}\frac{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta\Xi_0}U_{\mathrm{int}}(\beta)U_{\mathrm{int}}^{-1}(\tau)X_{\mathrm{H}_{\Xi_0}}(\tau)\,U_{\mathrm{int}}(\tau)X'(0)}{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta\Xi_0}U(\beta)}
\end{aligned}
\tag{33.166}
$$

proving the Lemma.

Proof 33.48 of Theorem 15.7

We combine the prior results as

$$
\begin{aligned}
\mathscr{G}_{X,X'}(\tau) &\equiv -\frac{1}{\hbar}\left\langle \mathrm{T}_\tau\,X(\tau)\,X'(0)\right\rangle \\
&= -\frac{1}{\hbar}\left\langle X(\tau)\,X'(0)\right\rangle \\
&= -\frac{1}{\hbar}\frac{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta\Xi_0}U_{\mathrm{int}}(\beta)U_{\mathrm{int}}^{-1}(\tau)X_{\mathrm{H}_{\Xi_0}}(\tau)\,U_{\mathrm{int}}(\tau)X'(0)}{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta\Xi_0}U(\beta)} \\
&= -\frac{1}{\hbar}\frac{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta\Xi_0}S(\beta,\tau)X_{\mathrm{H}_{\Xi_0}}(\tau)\,S(\tau)X'_{\mathrm{H}_{\Xi_0}}(0)}{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta\Xi_0}S(\beta)} \\
&= -\frac{1}{\hbar}\frac{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta\Xi_0}\,\mathrm{T}_\tau\,S(\beta,\tau)X_{\mathrm{H}_{\Xi_0}}(\tau)\,S(\tau)X'_{\mathrm{H}_{\Xi_0}}(0)}{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta\Xi_0}S(\beta)} \\
&= -\frac{1}{\hbar}\frac{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta\Xi_0}S(\beta)X_{\mathrm{H}_{\Xi_0}}(\tau)\,X'_{\mathrm{H}_{\Xi_0}}(0)}{\mathrm{Tr}_{\mathscr{H}}\,\mathrm{e}^{-\beta\Xi_0}S(\beta)} \\
&= -\frac{1}{\hbar}\frac{\langle S(\beta)X_{\mathrm{H}_{\Xi_0}}(\tau)\,X'_{\mathrm{H}_{\Xi_0}}(0)\rangle_0}{\langle S(\beta)\rangle_0}
\end{aligned}
\tag{33.167}
$$

whereas we used that we had a time-ordered product, such that we could re-introduce the time-ordering operator, and we subsequently used that inside the time-ordering operator we could re-arrange terms at the cost of potential minus signs, and that the time-ordering operator is even in the creation- and annihilation-operators.

Proof 33.49 of Lemma 15.14 Notice that for typical phononic systems that one encounters in crystals, one obtains with Theorem 13.10 the identity

$$
\mathscr{D}^{-1}_{\substack{0\\ \nu,\nu'}}(\mathbf{q},\mathrm{i}\omega_n) = -\hbar\,\frac{\omega_n^2+\omega_\nu^2(\mathbf{q})}{2\omega_\nu(\mathbf{q})}\,\delta_{\nu,\nu'},
\tag{33.168}
$$

The correct procedure is to keep (33.168) in matrix form and invert the *full* matrix. Introduce the diagonal matrices (both of size $rd_{\mathbf{x}}\times rd_{\mathbf{x}}$, at fixed $\mathbf{q}$)

$$2\boldsymbol{\omega}(\mathbf{q}) := 2\,\mathrm{diag}_{rd_{\mathrm{x}}\times rd_{\mathrm{x}}}\left(\omega_1(\mathbf{q}),\omega_2(\mathbf{q}),\dots,\omega_{rd_{\mathrm{x}}}(\mathbf{q})\right), \qquad \boldsymbol{\omega}^2(\mathbf{q}) := \mathrm{diag}_{rd_{\mathrm{x}}\times rd_{\mathrm{x}}}\left(\omega_1^2(\mathbf{q}),\omega_2^2(\mathbf{q}),\dots,\omega_{rd_{\mathrm{x}}}^2(\mathbf{q})\right), \tag{33.169}$$

so that (33.168) reads, as a matrix equation,

$$\mathscr{D}_0^{-1}(\mathbf{q},\mathrm{i}\omega_n) = -\hbar\ (2\boldsymbol{\omega}(\mathbf{q}))^{-1}\left[\left(\omega_n^2 1_{rd_{\mathrm{x}}\times rd_{\mathrm{x}}} + \boldsymbol{\omega}^2(\mathbf{q})\right)\right]. \tag{33.170}$$

Using the fact that $\boldsymbol{\omega}^{-1}(\mathbf{q})\cdot\boldsymbol{\omega}(\mathbf{q}) = \mathbb{1}$ we can factor

$$\begin{aligned}\mathscr{D}^{-1}(\mathbf{q},\mathrm{i}\omega_n) &= \mathscr{D}_0^{-1}(\mathbf{q},\mathrm{i}\omega_n) - \Pi(\mathbf{q},\mathrm{i}\omega_n)\\ &= -\hbar\ (2\boldsymbol{\omega}(\mathbf{q}))^{-1}\left[\left(\omega_n^2\mathbb{1} + \Omega^2(\mathbf{q})\right) + \frac{2}{\hbar}\boldsymbol{\omega}(\mathbf{q})\,\Pi(\mathbf{q},\mathrm{i}\omega_n)\right],\end{aligned} \tag{33.171}$$

Inverting both sides gives then

$$\begin{aligned}\mathscr{D}(\mathbf{q},\mathrm{i}\omega_n) &= -\frac{1}{\hbar}\left[\left(\omega_n^2\mathbb{1}_{rd_{\mathrm{x}}\times rd_{\mathrm{x}}} + \boldsymbol{\omega}^2(\mathbf{q})\right) + \frac{2}{\hbar}\boldsymbol{\omega}(\mathbf{q})\,\Pi(\mathbf{q},\mathrm{i}\omega_n)\right]^{-1} 2\boldsymbol{\omega}(\mathbf{q}),\\ &= -\frac{1}{\hbar}\frac{2\boldsymbol{\omega}(\mathbf{q})}{\left(\omega_n^2\mathbb{1}_{rd_{\mathrm{x}}\times rd_{\mathrm{x}}} + \boldsymbol{\omega}^2(\mathbf{q})\right) + \frac{2}{\hbar}\boldsymbol{\omega}(\mathbf{q})\,\Pi(\mathbf{q},\mathrm{i}\omega_n)}\end{aligned} \tag{33.172}$$

Proof 33.50 of Lemma 15.18 We write $z = \mathrm{i}\omega_n + \Delta z$ and consider

$$\begin{aligned}\lim_{\Delta z\to 0}\Delta z\, g_\zeta(\mathrm{i}\omega_n+\Delta z) &= \lim_{\Delta z\to 0}\Delta z\frac{\hbar\beta}{\mathrm{e}^{\mathrm{i}\omega_n\hbar\beta}\mathrm{e}^{\hbar\beta\Delta z}-\zeta}\\ &= \lim_{\Delta z\to 0}\Delta z\frac{\hbar\beta}{\mathrm{e}^{\hbar\beta\Delta z}-1}\zeta\\ &= \lim_{\Delta z\to 0}\frac{\hbar\beta\Delta z}{\hbar\beta\Delta z+\frac{1}{2}(\hbar\beta\Delta z)^2+\dots}\zeta\\ &= \zeta.\end{aligned}$$

Proof 33.51 of Theorem 15.20

We compute

$$\mathrm{Res}\left(f_\zeta(z),\ z=\mathrm{i}\omega_n\right) = \lim_{z\to\mathrm{i}\omega_n}(z-\mathrm{i}\omega_n)g_\zeta(z)h(-\mathrm{i}z) = \zeta h(\omega_n)$$

and obtain therefore

$$
\begin{aligned}
0 = \frac{1}{2\pi \mathrm{i}} \oint_\gamma \mathrm{d}z\, f_\zeta(z) \quad &\Longleftrightarrow \quad 0 = \sum_{z_\star \in \mathrm{P}} \mathrm{Res}\left(f(z),\, z = z_\star\right) \\
&\Longleftrightarrow \quad 0 = \sum_{z_\star \in \mathrm{Z}} \mathrm{Res}\left(f(z),\, z = z_\star\right) + \sum_{\mathrm{i}\omega_n \in \Omega_\zeta} \mathrm{Res}\left(f(z),\, z = \mathrm{i}\omega_n\right) \\
&\Longleftrightarrow S = -\zeta \sum_{z_\star \in \mathrm{Z}} \mathrm{Res}\left(f(z),\, z = z_\star\right)
\end{aligned}
$$

Proof 33.52 of Corollary 15.22

One obtains the function

$$
\mathbb{C} - \{\mathrm{C}\} \ni z \mapsto h(-\mathrm{i}z) \equiv \frac{1}{\hbar\beta} \frac{1}{(z - C)} \in \mathbb{C} \tag{33.173}
$$

Therefore, with the Lemma above, we obtain

$$
\sum_{\omega_n \in \Omega_\zeta} \frac{1}{\hbar} \frac{1}{\mathrm{i}\omega_n - C} = -\frac{\zeta}{\hbar\beta} g_\zeta(C) = -\zeta \mathrm{n}^\zeta_{\hbar\beta}(C) = -\zeta \mathrm{n}^\zeta_{\hbar\beta}(C) \tag{33.174}
$$

Proof 33.53 of Corollary 15.23

One obtains the function

$$
\mathbb{C} - \{z_1, z_2, z_3\} \ni z \mapsto h(-\mathrm{i}z) \equiv \frac{1}{\hbar^2\beta} \frac{1}{\left(z - C_1\right)} \frac{-2C_2}{\left(\omega_m + \mathrm{i}z\right)^2 + C_2^2} \in \mathbb{C} \tag{33.175}
$$

The first pole of this function is $z_1 = C_1$. The other two poles are determined by the equation

$$
\begin{aligned}
0 = \left(\omega_m + \mathrm{i}z\right)^2 + C_2^2 &\Longleftrightarrow \pm \mathrm{i}C_2 = \omega_m + \mathrm{i}z_\pm \\
&\Longleftrightarrow \mathrm{i}z_\pm = \pm \mathrm{i}C_2 - \omega_m \\
&\Longleftrightarrow z_\pm \equiv z_{2,3} = \mp C_2 + \mathrm{i}\omega_m
\end{aligned}
$$

Hence

$$
z_1 = C_1, \qquad z_2 = -C_2 + \mathrm{i}\omega_m, \qquad z_3 = +C_2 + \mathrm{i}\omega_m \tag{33.176}
$$

and since

$$
\begin{aligned}
(z - z_2)(z - z_3) &= (z + C_2 - \mathrm{i}\omega_m)(z - C_2 - \mathrm{i}\omega_m) \\
&= (z - \mathrm{i}\omega_m)^2 - C_2^2 \\
&= -\mathrm{i}^2 \left((z - \mathrm{i}\omega_m)^2 - C_2^2\right) \\
&= -\left((\omega_m + \mathrm{i}z)^2 + C_2^2\right)
\end{aligned}
$$

we conclude that

$$\text{const.} \equiv \frac{2C_2}{\hbar^2\beta} \tag{33.177}$$

Therefore we can now write down the products appearing in Equation (15.29) to evaluate the Matsubara-summation

$$k=1: \qquad \mathrm{n}^{\zeta}_{\hbar\beta}(z_1) = \mathrm{F}_{\hbar\beta}(C_1), \qquad z_1 - z_2 = C_1 + C_2 - \mathrm{i}\omega_m, \quad z_1 - z_3 = C_1 - C_2 - \mathrm{i}\omega_m$$

$$k=2: \qquad \mathrm{n}^{\zeta}_{\hbar\beta}(z_1) = \mathrm{F}_{\hbar\beta}(-C_2+\mathrm{i}\omega_m), \qquad z_2-z_1 = -C_2+\mathrm{i}\omega_m-C_1, \quad z_2-z_3 = -C_2+\mathrm{i}\omega_m-C_2-\mathrm{i}\omega_m = -2C_2$$

$$k=3: \qquad \mathrm{n}^{\zeta}_{\hbar\beta}(z_1) = \mathrm{F}_{\hbar\beta}(+C_2+\mathrm{i}\omega_m), \qquad z_3 - z_1 = C_2 + \mathrm{i}\omega_m - C_1, \quad z_3 - z_2 = C_2 + \mathrm{i}\omega_m + C_2 - \mathrm{i}\omega_m = 2C_2$$

Using the identities in Lemma 9.65 we obtain therefore

$$k=1: \qquad \mathrm{n}^{\zeta}_{\hbar\beta}(z_1) = \mathrm{F}_{\hbar\beta}(C_1), \qquad z_1 - z_2 = C_1 + C_2 - \mathrm{i}\omega_m, \quad z_1 - z_3 = C_1 - C_2 - \mathrm{i}\omega_m$$

$$k=2: \qquad \mathrm{n}^{\zeta}_{\hbar\beta}(z_1) = \mathrm{B}_{\hbar\beta}(C_2) + 1, \qquad z_2 - z_1 = -C_2 + \mathrm{i}\omega_m - C_1, \quad z_2 - z_3 = -2C_2$$

$$k=3: \qquad \mathrm{n}^{\zeta}_{\hbar\beta}(z_1) = -\mathrm{B}_{\hbar\beta}(C_2), \qquad z_3 - z_1 = C_2 + \mathrm{i}\omega_m - C_1, \quad z_3 - z_2 = 2C_2$$

This gives with Equation (15.29) the intermediate result

$$\begin{aligned}
S_{-1} &= \sum_{\omega_n \in \Omega_{-1}} h(\omega_n) \\
&= +1\hbar\beta\,\text{const}\sum_{k=1}^{N} \mathrm{n}^{\zeta}_{\hbar\beta}(z_k) \prod_{\substack{l=1 \\ l\neq k}}^{N} \frac{1}{z_k - z_l} \\
&= \frac{2C_2}{\hbar}\left[\frac{\mathrm{F}_{\hbar\beta}(C_1)}{(C_1+C_2-\mathrm{i}\omega_m)(C_1-C_2-\mathrm{i}\omega_m)} + \frac{\mathrm{B}_{\hbar\beta}(C_2)+1}{(-C_2+\mathrm{i}\omega_m-C_1)(-2C_2)} + \frac{-\mathrm{B}_{\hbar\beta}(C_2)}{(C_2+\mathrm{i}\omega_m-C_1)(2C_2)}\right] \\
&= \frac{1}{\hbar}\left[\frac{2C_2\mathrm{F}_{\hbar\beta}(C_1)}{(\mathrm{i}\omega_m-C_1-C_2)(\mathrm{i}\omega_m-C_1+C_2)} - \frac{\mathrm{B}_{\hbar\beta}(C_2)+1}{-C_2+\mathrm{i}\omega_m-C_1} - \frac{\mathrm{B}_{\hbar\beta}(C_2)}{C_2+\mathrm{i}\omega_m-C_1}\right] \\
&= \star\star\star
\end{aligned}$$

We now use the partial fraction expansion (cf. WolframAlpha)

$$\frac{2C_2}{(x+C_2)(x-C_2)} = -\frac{1}{x+C_2} + \frac{1}{x-C_2} \tag{33.178}$$

and obtain

$$\begin{aligned}\star\star\star &= \frac{1}{\hbar}\left[\frac{-\mathrm{F}_{\hbar\beta}(C_1)}{\mathrm{i}\omega_m - C_1 + C_2} + \frac{\mathrm{F}_{\hbar\beta}(C_1)}{\mathrm{i}\omega_m - C_1 - C_2} - \frac{\mathrm{B}_{\hbar\beta}(C_2)+1}{-C_2 + \mathrm{i}\omega_m - C_1} - \frac{\mathrm{B}_{\hbar\beta}(C_2)}{C_2 + \mathrm{i}\omega_m - C_1}\right] \\ &= \frac{-1}{\hbar}\left[\frac{\mathrm{B}_{\hbar\beta}(C_2)+\mathrm{F}_{\hbar\beta}(C_1)}{\mathrm{i}\omega_m - C_1 + C_2} + \frac{\mathrm{B}_{\hbar\beta}(C_2)+1-\mathrm{F}_{\hbar\beta}(C_1)}{\mathrm{i}\omega_m - C_1 - C_2}\right]\end{aligned}$$

34. Appendix - Proofs for Part III

Proof 34.1 of Lemma 16.6 For $\zeta = +1$ the invertibility follows from basic algebraic ruels. $\zeta = -1$, we prove that Equation (16.7) is indeed the inverse element of f. For this, we compute

$$\begin{aligned} f^{-1}(\psi,\overline{\psi})f(\psi,\overline{\psi}) &= \frac{1}{f_0}\sum_{n=0}^{N_f-1}\left(-\frac{f_{\text{nil}}(\psi,\overline{\psi})}{f_0}\right)^n\left(f_0+f_{\text{nil}}\right) \\ &= \sum_{n=0}^{N_f-1}\left(-\frac{f_{\text{nil}}(\psi,\overline{\psi})}{f_0}\right)^n \quad + \quad \frac{f_{\text{nil}}}{f_0}\sum_{n=0}^{N_f-1}\left(-\frac{f_{\text{nil}}(\psi,\overline{\psi})}{f_0}\right)^n \\ &= \sum_{n=0}^{N_f-1}\left(-\frac{f_{\text{nil}}(\psi,\overline{\psi})}{f_0}\right)^n \quad - \quad \sum_{n=1}^{N_f}\left(-\frac{f_{\text{nil}}(\psi,\overline{\psi})}{f_0}\right)^n \\ &= 1+0+0 \end{aligned} \tag{34.1}$$

Proof 34.2 of Lemma 16.14 The bosonic case is trivial. In the fermionic case we obtain by direct computation for the first identity

$$\exp\sum_k \bar{j}_k\psi_k = \prod_k \exp\bar{j}_k\psi_k = \exp\bar{j}_i\psi_i\prod_{\substack{k\\k\neq i}}\exp\bar{j}_k\psi_k \tag{34.2}$$

which can be combined with

$$\frac{\partial}{\partial\bar{j}_i}\exp\bar{j}_i\psi_i = \frac{\partial}{\partial\bar{j}_i}\left(1+\bar{j}_i\psi_i\right) = \psi_i = \psi_i\left(1+\bar{j}_i\psi_i\right) \tag{34.3}$$

and

$$\frac{\partial}{\partial j_{i'}}\exp\overline{\psi}_{i'}j_{i'} = \frac{\partial}{\partial j_{i'}}\left(1+\overline{\psi}_{i'}j_{i'}\right) = -\overline{\psi}_{i'} = -\overline{\psi}_{i'}\left(1+\overline{\psi}_{i'}j_{i'}\right) \tag{34.4}$$

Proof 34.3 of Lemma 16.32

We will provide two proofs of this identity. One direct proof (presented here), and another proof based on symmetry-principles, presented in Chapter 18. We simply compute

$$\begin{aligned} W[j,\bar{j}] &= \log\left\langle \mathrm{e}^{-\left(j^\dagger\psi+\psi^\dagger j\right)}\right\rangle \\ &= \log\left\langle \exp-\sum_\alpha\left(j^\dagger\psi+\psi^\dagger j\right)\right\rangle \\ &= \log\left\langle\left(\prod_\alpha \exp -j^\dagger\psi\right)\left(\prod_\alpha \exp -\psi^\dagger j\right)\right\rangle \end{aligned} \tag{34.5}$$

Now taking the expectation-value we see that W is *even* in the fields j and $\bar{j}$ and therefore ϕ and $\overline{\phi}$ are odd in the fields.

Proof 34.4 of Lemma 16.33

Setting and Assumptions.

As in the remainder of this section, we assume that the action S contains only monomials with equally many variables ψ and $\overline{\psi}$ („U(1)-invariance“; for $\zeta=-1$ this is already demanded in Notation 16.24) and that there is no spontaneous symmetry breaking. Moreover, we assume that the matrix $\left(\mathscr{G}_{\mathrm{c}}(i\,|\,i')\right)_{i,i'}$ of the connected one-body Green-function (which equals $\mathscr{G}(i\,|\,i')$ by Corollary 16.43) is invertible. This assumption is tacitly contained in the Lemma, and it is also *necessary*: The linear part of an invertible power-series is an invertible matrix (see below). All expansions are understood as formal power-series (for $\zeta=-1$ they terminate, since there are only finitely many Graßmann-generators), and all sums run over the generalized indices $\{1,\dots,\mathrm{D}\}$. As in the Lemma, we denote the prescribed fields by ϕ', $\overline{\phi'}$, with components $\phi'(i)$, $\overline{\phi'}(i)$.

The Expansion of W.

For $\alpha\in\mathbb{R}$ the U(1)-invariance makes $M=\mathrm{e}^{\mathrm{i}\alpha}\mathbb{1}$ (with $\overline{M}=\mathrm{e}^{-\mathrm{i}\alpha}\mathbb{1}$) a symmetry-transformation (Definition 18.1), and Lemma 18.2 gives $W[j,\bar{j}]=W[\mathrm{e}^{-\mathrm{i}\alpha}j,\mathrm{e}^{\mathrm{i}\alpha}\bar{j}]$. A monomial with n factors $\bar{j}$ and m factors j picks up the phase $\mathrm{e}^{\mathrm{i}\alpha(n-m)}$, such that only the coefficients with $n=m$ survive in the series-expansion of Notation 16.36 (with coefficients w, cf. Table 16.1):

$$\begin{aligned} W[\bar{j},j] = \log Z \quad &+ \sum_{i,i'}\bar{j}(i)\,w(i\,|\,i')\,j(i') \\ &+\frac{1}{(2!)^2}\sum_{i_1,i_2,i'_1,i'_2}\bar{j}(i_1)\,\bar{j}(i_2)\,w(i_1,i_2\,|\,i'_1,i'_2)\,j(i'_2)\,j(i'_1) \\ &+\sum_{n=3}^{\infty}\frac{1}{(n!)^2}\sum_{\substack{i_1,\dots,i_n\\ i'_1,\dots,i'_n}}\bar{j}(i_1)\cdots\bar{j}(i_n)\,w(i_1,\dots,i_n\,|\,i'_1,\dots,i'_n)\,j(i'_n)\cdots j(i'_1). \end{aligned} \tag{34.6}$$

Here $\log Z=W[0,0]$ drops out of all derivatives, the coefficients are (anti)symmetric,

$$w(i_2,i_1\,|\,i'_1,i'_2)=\zeta\,w(i_1,i_2\,|\,i'_1,i'_2)=w(i_1,i_2\,|\,i'_2,i'_1),$$

and by Definition 16.41 and the subsequent Remark (with the convention $c\equiv\hbar$)

$$w(i\,|\,i')=-\hbar\,\mathscr{G}_{\mathrm{c}}(i\,|\,i'),\qquad w(i_1,i_2\,|\,i'_1,i'_2)=\hbar^2\,\mathscr{G}_{\mathrm{c}}(i_1,i_2\,|\,i'_1,i'_2). \tag{34.7}$$

We denote by $w^{-1}(i\,|\,i')$ the matrix-elements of the inverse of the matrix $\left(w(i\,|\,i')\right)_{i,i'}$, i.e.

$$\sum_k w^{-1}(i \mid k)\, w(k \mid i') = \delta_{i,i'} = \sum_k w(i \mid k)\, w^{-1}(k \mid i'), \qquad w^{-1}(i \mid i') = -\frac{1}{\hbar}\, \mathscr{G}_{\mathrm{c}}^{-1}(i \mid i'). \tag{34.8}$$

All coefficients w, w^{-1} are complex numbers and therefore commute with all sources and fields.

The Field-Expectation-Values as Power-Series in the Sources.

We use $\phi = \partial W / \partial \bar{j}$ and $\bar{\phi} = \zeta\, \partial W / \partial j$ (Notation 16.31). The statistics neutral commutation relations (Lemma 16.11, applied to the sources) give

$$\begin{aligned} \frac{\partial}{\partial \bar{j}(k)}\, \bar{j}(i_1)\, \bar{j}(i_2) &= \delta_{k,i_1}\, \bar{j}(i_2) + \zeta\, \bar{j}(i_1)\, \delta_{k,i_2}, \\ \frac{\partial}{\partial j(k)}\, \bar{j}(i_1)\, \bar{j}(i_2)\, j(i_2')\, j(i_1') &= \bar{j}(i_1)\, \bar{j}(i_2) \Big(\delta_{k,i_2'}\, j(i_1') + \zeta\, j(i_2')\, \delta_{k,i_1'} \Big), \end{aligned}$$

where in the second line the derivative has been moved past the two factors $\bar{j}$ (sign $\zeta^2 = 1$). For the quartic part of W we therefore obtain

$$\begin{aligned} \frac{\partial}{\partial \bar{j}(k)}\, \frac{1}{4} \sum_{i_1,i_2,i_1',i_2'} \bar{j}(i_1)\, \bar{j}(i_2)\, w(i_1,i_2 \mid i_1',i_2')\, j(i_2')\, j(i_1') &= \frac{1}{4} \sum_{i_2,i_1',i_2'} \bar{j}(i_2)\, w(k,i_2 \mid i_1',i_2')\, j(i_2')\, j(i_1') \\ &\quad + \frac{\zeta}{4} \sum_{i_1,i_1',i_2'} \bar{j}(i_1)\, w(i_1,k \mid i_1',i_2')\, j(i_2')\, j(i_1') \\ &= \frac{1}{2} \sum_{l,l_1',l_2'} \bar{j}(l)\, w(k,l \mid l_1',l_2')\, j(l_2')\, j(l_1') \end{aligned}$$

and

$$\begin{aligned} \zeta\, \frac{\partial}{\partial j(k)}\, \frac{1}{4} \sum_{i_1,i_2,i_1',i_2'} \bar{j}(i_1)\, \bar{j}(i_2)\, w(i_1,i_2 \mid i_1',i_2')\, j(i_2')\, j(i_1') &= \frac{\zeta}{4} \sum_{i_1,i_2,i_1'} \bar{j}(i_1)\, \bar{j}(i_2)\, w(i_1,i_2 \mid i_1',k)\, j(i_1') \\ &\quad + \frac{\zeta^2}{4} \sum_{i_1,i_2,i_2'} \bar{j}(i_1)\, \bar{j}(i_2)\, w(i_1,i_2 \mid k,i_2')\, j(i_2') \\ &= \frac{1}{2} \sum_{l_1,l_2,l'} \bar{j}(l_1)\, \bar{j}(l_2)\, w(l_1,l_2 \mid k,l')\, j(l'), \end{aligned}$$

where in both cases we renamed the summation-indices and used the (anti)symmetry of w (e.g. $\zeta\, w(l,k \mid l_1',l_2') = w(k,l \mid l_1',l_2')$), such that the two contributions coincide. The quadratic part of W is treated analogously (with $\zeta \cdot \zeta = 1$ for $\bar{\phi}$). For the monomials of order $2n$ the derivative hits each of the n factors $\bar{j}$ (resp. j); the sign for moving the derivative to this factor (together with the prefactor ζ in the case of $\bar{\phi}$) is compensated by the sign for moving the corresponding index into the first (unprimed resp. primed) slot of w, such that all n contributions coincide and the prefactor becomes $\frac{n}{(n!)^2} = \frac{1}{n!\,(n-1)!}$. Altogether

$$\phi[k,j,\bar{j}] = \sum_{i'} w(k \mid i')\, j(i') \quad + \quad \frac{1}{2} \sum_{l,l_1',l_2'} \bar{j}(l)\, w(k,l \mid l_1',l_2')\, j(l_2')\, j(l_1') \quad + \quad R(k), \tag{34.9}$$

$$\bar{\phi}[k,j,\bar{j}] = \sum_{i} \bar{j}(i)\, w(i \mid k) \quad + \quad \frac{1}{2} \sum_{l_1,l_2,l'} \bar{j}(l_1)\, \bar{j}(l_2)\, w(l_1,l_2 \mid k,l')\, j(l') \quad + \quad \bar{R}(k), \tag{34.10}$$

with the remainders (all monomials of order ≥ 5 in the sources)

$$R(k) = \sum_{n=3}^{\infty} \frac{1}{n!\,(n-1)!} \sum_{\substack{l_2,\dots,l_n \\ l'_1,\dots,l'_n}} \bar{j}(l_2)\cdots\bar{j}(l_n)\, w(k,l_2,\dots,l_n \mid l'_1,\dots,l'_n)\, j(l'_1)\cdots j(l'_n),$$

$$\overline{R}(k) = \sum_{n=3}^{\infty} \frac{1}{n!\,(n-1)!} \sum_{\substack{l_1,\dots,l_n \\ l'_2,\dots,l'_n}} \bar{j}(l_1)\cdots\bar{j}(l_n)\, w(l_1,\dots,l_n \mid k,l'_2,\dots,l'_n)\, j(l'_1)\cdots j(l'_n).$$

This makes Lemma 16.32 explicit: ϕ and $\overline{\phi}$ are odd in the sources (each monomial of $\phi(k)$ contains one factor j more than $\bar{j}$, each monomial of $\overline{\phi}(k)$ one factor $\bar{j}$ more than j), and in particular $\phi[\bullet,0,0] = \overline{\phi}[\bullet,0,0] = 0$. We therefore have to solve the coupled nonlinear system

$$\phi[k,j,\bar{j}] = \phi'(k), \qquad \overline{\phi}[k,j,\bar{j}] = \overline{\phi'}(k) \qquad \text{for all } k.$$

Unlike in the case of a real scalar field theory that one knows from textbooks, both equations must be inverted *simultaneously*: From the cubic order on, $\bar{j}$ enters the equation for ϕ and j enters the equation for $\overline{\phi}$. The clue (that is missing from every book that the author opened so far) is to understand this as the inversion of a *power-series*.

Ansatz and Recursion.

Since $\phi[\bullet,0,0] = \overline{\phi}[\bullet,0,0] = 0$, we make the ansatz of power-series without constant term

$$j(i) \equiv j[i,\phi',\overline{\phi'}] = \sum_{d=1}^{\infty} j^{(d)}(i), \qquad \bar{j}(i) \equiv \bar{j}[i,\phi',\overline{\phi'}] = \sum_{d=1}^{\infty} \bar{j}^{(d)}(i), \tag{34.11}$$

where $j^{(d)}(i)$ and $\bar{j}^{(d)}(i)$ are homogeneous polynomials of degree d in the fields ϕ', $\overline{\phi'}$ with complex coefficients. We multiply Equation (34.9) (with $\phi[k,j,\bar{j}] = \phi'(k)$) from the left by $w^{-1}(i \mid k)$ and Equation (34.10) (with $\overline{\phi}[k,j,\bar{j}] = \overline{\phi'}(k)$) from the right by $w^{-1}(k \mid i)$, and sum over k. With Equation (34.8) we obtain the equivalent system

$$\begin{aligned} j(i) &= \sum_k w^{-1}(i \mid k)\,\phi'(k) \quad - \quad \sum_k w^{-1}(i \mid k) \left[\frac{1}{2} \sum_{l,l'_1,l'_2} \bar{j}(l)\, w(k,l \mid l'_1,l'_2)\, j(l'_2)\, j(l'_1) + R(k) \right], \\ \bar{j}(i) &= \sum_k \overline{\phi'}(k)\, w^{-1}(k \mid i) \quad - \quad \sum_k \left[\frac{1}{2} \sum_{l_1,l_2,l'} \bar{j}(l_1)\,\bar{j}(l_2)\, w(l_1,l_2 \mid k,l')\, j(l') + \overline{R}(k) \right] w^{-1}(k \mid i). \end{aligned} \tag{34.12}$$

The square brackets consist of products of $2n-1 \geq 3$ factors $j(\cdot)$, $\bar{j}(\cdot)$, each of which is of degree ≥ 1 in the fields. Hence the degree-d part $[\dots]_d$ of the square brackets contains only the $j^{(d')}$, $\bar{j}^{(d')}$ with $d' \leq d-2$. Taking the degree-d part of Equation (34.12) gives

$$\begin{aligned} j^{(1)}(i) &= \sum_k w^{-1}(i \mid k)\,\phi'(k), \qquad \bar{j}^{(1)}(i) = \sum_k \overline{\phi'}(k)\, w^{-1}(k \mid i), \\ j^{(d)}(i) &= -\sum_k w^{-1}(i \mid k) \left[\dots\right]_d, \quad \bar{j}^{(d)}(i) = -\sum_k \left[\dots\right]_d w^{-1}(k \mid i) \qquad (d \geq 2), \end{aligned} \tag{34.13}$$

where $[\dots]_d$ denotes the degree-d part of the respective square bracket in Equation (34.12). Since $[\dots]_d$ only contains lower orders, all $j^{(d)}$, $\bar{j}^{(d)}$ are *uniquely* determined recursively, order by order. Moreover:

- The even orders vanish: For $d = 2$ the square brackets have no degree-2 part. If $j^{(d')} = \overline{j}^{(d')} = 0$ for all even $d' < d$ (d even), all factors in the square brackets are of odd degree, and a product of an odd number $2n-1$ of them is of odd degree, such that $[\dots]_d = 0$ and $j^{(d)} = \overline{j}^{(d)} = 0$. Thus j and $\overline{j}$ are *odd* in the fields ϕ', $\overline{\phi'}$ (cf. the Remark after the Lemma).
- Counting the factors in the recursion (each monomial in the first square bracket contains one factor j more than $\overline{j}$, in the second one factor $\overline{j}$ more than j) one sees inductively that each monomial of $j^{(2N+1)}(i)$ contains N factors $\overline{\phi'}$ and $N+1$ factors ϕ', and each monomial of $\overline{j}^{(2N+1)}(i)$ contains $N+1$ factors $\overline{\phi'}$ and N factors ϕ'.
- The series (34.11) constructed in this way fulfill Equation (34.12), and thus the coupled system, in every degree. For $\zeta = -1$ one uses here that $j(i)$, $\overline{j}(i)$ are odd elements of the Graßmann-algebra, such that they obey the same (anti)commutation-relations as the sources themselves and can consistently be inserted into $\phi[\bullet, j, \overline{j}]$, $\overline{\phi}[\bullet, j, \overline{j}]$. Hence $\phi[\bullet, j[\bullet, \phi', \overline{\phi'}], \overline{j}[\bullet, \phi', \overline{\phi'}]] = \phi'$ and $\overline{\phi}[\bullet, j[\bullet, \phi', \overline{\phi'}], \overline{j}[\bullet, \phi', \overline{\phi'}]] = \overline{\phi'}$, which proves the Lemma.
- Conversely, the degree-1 part of these equations states that the linear parts of the two maps are inverse matrices of each other, which shows the necessity of the invertibility of $w(\cdot \mid \cdot)$, i.e. of $\mathscr{G}_{\mathrm{c}}(\cdot \mid \cdot)$.

The Linear Order.

By Equations (34.13) and (34.8) one has

$$\begin{aligned} j^{(1)}(i) &= \sum_k w^{-1}(i \mid k)\, \phi'(k) = -\frac{1}{\hbar} \sum_k \mathscr{G}_{\mathrm{c}}^{-1}(i \mid k)\, \phi'(k), \\ \overline{j}^{(1)}(i) &= \sum_k \overline{\phi'}(k)\, w^{-1}(k \mid i) = -\frac{1}{\hbar} \sum_k \overline{\phi'}(k)\, \mathscr{G}_{\mathrm{c}}^{-1}(k \mid i). \end{aligned} \tag{34.14}$$

The inversion of the linear part therefore requires exactly the invertibility of the connected one-body Green-function. Once the linear part is inverted, the nonlinear corrections follow *order by order*.

The Cubic Order.

The remainders R, $\overline{R}$ start at degree 5, so only the quartic part of W contributes to $[\dots]_3$, with all three factors taken in linear order. For j this gives

$$\begin{aligned} j^{(3)}(i) &= -\frac{1}{2} \sum_{k,l,l'_1,l'_2} w^{-1}(i \mid k)\, \overline{j}^{(1)}(l)\, w(k, l \mid l'_1, l'_2)\, j^{(1)}(l'_2)\, j^{(1)}(l'_1) \\ &= -\frac{1}{2} \sum_{k,l,l'_1,l'_2} \sum_{m,m'_1,m'_2} w^{-1}(i \mid k)\, \overline{\phi'}(m)\, w^{-1}(m \mid l)\, w(k, l \mid l'_1, l'_2) \\ &\qquad \times w^{-1}(l'_2 \mid m'_2)\, \phi'(m'_2)\, w^{-1}(l'_1 \mid m'_1)\, \phi'(m'_1) \\ &= -\frac{1}{2} \sum_{m,m'_1,m'_2} \overline{\phi'}(m)\, \hat{w}(i, m \mid m'_1, m'_2)\, \phi'(m'_2)\, \phi'(m'_1), \end{aligned}$$

where we collected the (commuting) complex coefficients between the fields and introduced the *amputated* coefficients

$$\begin{aligned}\widehat{w}(i_1,i_2\mid i_1',i_2') &:= \sum_{k_1,k_2,k_1',k_2'} w^{-1}(i_1\mid k_1)\,w^{-1}(i_2\mid k_2)\,w(k_1,k_2\mid k_1',k_2')\,w^{-1}(k_1'\mid i_1')\,w^{-1}(k_2'\mid i_2')\\ &= \frac{1}{\hbar^2}\sum_{k_1,k_2,k_1',k_2'} \mathscr{G}_{\mathrm{c}}^{-1}(i_1\mid k_1)\,\mathscr{G}_{\mathrm{c}}^{-1}(i_2\mid k_2)\,\mathscr{G}_{\mathrm{c}}(k_1,k_2\mid k_1',k_2')\,\mathscr{G}_{\mathrm{c}}^{-1}(k_1'\mid i_1')\,\mathscr{G}_{\mathrm{c}}^{-1}(k_2'\mid i_2')\end{aligned} \tag{34.15}$$

(the second line follows from Equations (34.7) and (34.8) with $(-1/\hbar)^4\hbar^2 = 1/\hbar^2$). They inherit the (anti)symmetry of $w(k_1,k_2\mid k_1',k_2')$. Analogously, one finds for $\overline{j}$

$$\begin{aligned}\overline{j}^{(3)}(i) &= -\frac{1}{2}\sum_{k,l_1,l_2,l'} \overline{j}^{(1)}(l_1)\,\overline{j}^{(1)}(l_2)\,w(l_1,l_2\mid k,l')\,j^{(1)}(l')\,w^{-1}(k\mid i)\\ &= -\frac{1}{2}\sum_{k,l_1,l_2,l'}\sum_{m_1,m_2,m'} \overline{\phi}'(m_1)\,w^{-1}(m_1\mid l_1)\,\overline{\phi}'(m_2)\,w^{-1}(m_2\mid l_2)\,w(l_1,l_2\mid k,l')\\ &\qquad\times w^{-1}(l'\mid m')\,\phi'(m')\,w^{-1}(k\mid i)\\ &= -\frac{1}{2}\sum_{m_1,m_2,m'} \overline{\phi}'(m_1)\,\overline{\phi}'(m_2)\,\widehat{w}(m_1,m_2\mid i,m')\,\phi'(m').\end{aligned}$$

Result.

Up to (and including) the cubic order, the inverse mapping reads

$$\begin{aligned} j[i,\phi',\overline{\phi}'] &= \sum_k w^{-1}(i\mid k)\,\phi'(k) \;-\; \frac{1}{2}\sum_{m,m_1',m_2'} \overline{\phi}'(m)\,\widehat{w}(i,m\mid m_1',m_2')\,\phi'(m_2')\,\phi'(m_1') \;+\; \mathcal{O}\big((\phi')^5\big),\\ \overline{j}[i,\phi',\overline{\phi}'] &= \sum_k \overline{\phi}'(k)\,w^{-1}(k\mid i) \;-\; \frac{1}{2}\sum_{m_1,m_2,m'} \overline{\phi}'(m_1)\,\overline{\phi}'(m_2)\,\widehat{w}(m_1,m_2\mid i,m')\,\phi'(m') \;+\; \mathcal{O}\big((\phi')^5\big),\end{aligned} \tag{34.16}$$

where $\mathcal{O}\big((\phi')^5\big)$ denotes terms of degree ≥ 5 in ϕ', $\overline{\phi}'$, and w^{-1}, $\widehat{w}$ are given in Equations (34.8) and (34.15).

Consistency Check.

By Lemma 16.35 one has $j = \partial\Gamma/\partial\overline{\phi}$ and $\overline{j} = \zeta\,\partial\Gamma/\partial\phi$. The same computation that led to Equations (34.9) and (34.10) (with $W \to \Gamma$, $\overline{j}, j \to \overline{\phi}', \phi'$ and $w \to \gamma$) gives

$$j[i,\phi',\overline{\phi}'] = \sum_k \gamma(i\mid k)\,\phi'(k) \;+\; \frac{1}{2}\sum_{m,m_1',m_2'} \overline{\phi}'(m)\,\gamma(i,m\mid m_1',m_2')\,\phi'(m_2')\,\phi'(m_1') \;+\; \mathcal{O}\big((\phi')^5\big),$$

and comparing coefficients with Equation (34.16) (both coefficients are (anti)symmetric in m_1', m_2') yields

$$\gamma(i\mid i') = w^{-1}(i\mid i'), \qquad \gamma(i_1,i_2\mid i_1',i_2') = -\widehat{w}(i_1,i_2\mid i_1',i_2').$$

The expansion of $\overline{j}$ gives the same identifications. With $\mathrm{Vert} = (-\hbar)^n\gamma$ (Remark after the definition of the vertex-functions), the first identity is $\mathrm{Vert}(:,:) = \mathscr{G}_{\mathrm{c}}^{-1}(:,:)$ (Lemma after Corollary 16.45), and the second one is, by Equation (34.15), equivalent to Theorem 16.47. The expansions (34.9), (34.10) and (34.16), as well as these identifications, have been checked numerically with random coefficients (including a sextic term in W), for $\zeta = -1$ with an exact implementation of the Graßmann-algebra and for $\zeta = +1$, both with $\mathrm{D} = 2$ and $\mathrm{D} = 3$.

Remark. Without the U(1)-invariance (but for W even in the sources), W also contains monomials with $n \neq m$ (e.g. $\overline{j}\,\overline{j}$ and jj). Then the linear part of the map $(j, \overline{j}) \mapsto (\phi, \overline{\phi})$ is given by the 2×2-block-matrix of second derivatives of W in Corollary 16.45, and the above recursion goes through unchanged as long as this block-matrix is invertible.

Proof 34.5 of Lemma 16.37

We use Equation (16.46) and simplify the notation as

$$F[\pi, \overline{\pi}] \equiv \sum_{\substack{i_1, i_2 \\ i'_1, i'_2}} \overline{\pi}(i_1)\overline{\pi}(i_2)\widetilde{f}(i_1, i_2, i'_1, i'_2)\,\pi(i'_2)\pi(i'_1) \equiv \sum_{\substack{1,2 \\ 1',2'}} \overline{\pi}(1)\overline{\pi}(2)\widetilde{f}(1, 2, 1', 2')\,\pi(2')\pi(1') = \dots \tag{34.17}$$

now we decompose the interaction f as

$$f \equiv f^{\text{ sym, sym}} + f^{\text{ sym, as}} + f^{\text{ as, sym}} + f^{\text{ as, as}} \tag{34.18}$$

with

$$\begin{aligned}
&\bullet \quad f^{\text{ sym, sym}}(1,2,3,4) \quad \equiv \frac{1}{4}\Big(\widetilde{f}(1,2,3,4) + \widetilde{f}(2,1,3,4) + \widetilde{f}(1,2,4,3) + \widetilde{f}(2,1,4,3)\Big) \\
&\bullet \quad f^{\text{ as, sym}}(1,2,3,4) \quad \equiv \frac{1}{4}\Big(\widetilde{f}(1,2,3,4) - \widetilde{f}(2,1,3,4) + \widetilde{f}(1,2,4,3) - \widetilde{f}(2,1,4,3)\Big) \\
&\bullet \quad f^{\text{ sym, as}}(1,2,3,4) \quad \equiv \frac{1}{4}\Big(\widetilde{f}(1,2,3,4) + \widetilde{f}(2,1,3,4) - \widetilde{f}(1,2,4,3) - \widetilde{f}(2,1,4,3)\Big) \\
&\bullet \quad f^{\text{ as, as}}(1,2,3,4) \quad \equiv \frac{1}{4}\Big(\widetilde{f}(1,2,3,4) - \widetilde{f}(2,1,3,4) - \widetilde{f}(1,2,4,3) + \widetilde{f}(2,1,4,3)\Big)
\end{aligned} \tag{34.19}$$

such that we have

$$f^{\bullet,\bullet'}(\sigma(1), \sigma(2), \sigma'(3), \sigma'(4)) = (\operatorname{sgn}(\sigma))^{\mathrm{n}(\bullet)} \left(\operatorname{sgn}(\sigma')\right)^{\mathrm{n}(\bullet')} f(1,2,3,4) \tag{34.20}$$

with

$$\mathrm{n}(\bullet) = \begin{cases} 1, & \bullet = \text{as} \\ 0, & \bullet = \text{sym} \end{cases} \tag{34.21}$$

whereas we obtain

$$f = \sum_{\bullet,\bullet' \in \text{ as, sym}} f^{\bullet,\bullet'} \tag{34.22}$$

This gives, for example for $\zeta = -1$

$$\sum_{1,2,3,4} \overline{\pi}_1\overline{\pi}_2 f^{\text{ sym, as}}(1,2,3,4)\psi_4\psi_3 \overset{\substack{1\to 2,\\ 2\to 1}}{=} \sum_{1,2,3,4} \underbrace{\overline{\pi}_2\overline{\pi}_1}_{-\overline{\pi}_1\overline{\pi}_2} \underbrace{f^{\text{ sym, as}}(2,1,3,4)}_{f^{\text{ sym, as}}(1,2,3,4)} \psi_4\psi_3 = -\sum_{1,2,3,4} \overline{\pi}_1\overline{\pi}_2 f^{\text{ sym, as}}(1,2,3,4)\psi_4\psi_3 = 0 \tag{34.23}$$

and similar for $\zeta = +1$ (except that one needs to use the (anti)-symmetry of the respective other part of the coupling-function).

Proof 34.6 of Lemma 16.39.

We compute the derivatives explicitly and find the identity

$$\begin{aligned}
&\frac{\partial^{n+m}}{\partial\overline{\pi}(i_1)\cdots\partial\overline{\pi}(i_n)\partial\pi(i'_m)\cdots\partial\pi(i'_1)}F[\overline{\pi},\pi]\Big|_{\overline{\pi}=\pi=0}\\
&=\frac{\partial^{n+m}}{\partial\overline{\pi}(i_1)\cdots\partial\overline{\pi}(i_n)\partial\pi(i'_m)\cdots\partial\pi(i'_1)}\sum_{n,m=0}^{\infty}\sum_{\substack{i_1<\ldots<i_n\\ i'_1<i'_2<\ldots<i'_m}}\overline{\pi}(i_1)\cdots\overline{\pi}(i_n)f(i_1,\ldots,i_n,i'_1,\ldots i'_m)\,\pi(i'_m)\cdots\pi(i'_1)\\
&=\zeta^{nm}\sum_{n,m=0}^{\infty}\sum_{\substack{i_1<\ldots<i_n\\ i'_1<i'_2<\ldots<i'_n}}\frac{\partial^n}{\partial\overline{\pi}(i_1)\cdots\partial\overline{\pi}(i_n)}\overline{\pi}(i_1)\cdots\overline{\pi}(i_n)f(i_1,\ldots,i_n,i'_1,\ldots i'_m)\,\frac{\partial^n}{\partial\pi(i'_m)\cdots\partial\pi(i'_1)}\pi(i'_m)\cdots\pi(i'_1)\\
&=\zeta^{nm+n(n-1)/2+m(m-1)/2}f(i_1,\ldots,i_n,i'_1,\ldots i'_m)
\end{aligned}\tag{34.24}$$

Proof 34.7 of Lemma 16.35. One has[1]

$$\begin{aligned}
\frac{\partial}{\partial\phi(\bullet)}\Gamma[\phi,\overline{\phi}] &= -\sum_x\left(\frac{\partial j(x)}{\partial\phi(\bullet)},\frac{\partial\overline{j}(x)}{\partial\phi(\bullet)}\right)\cdot\begin{pmatrix}\frac{\partial}{\partial j(x)}W[j,\overline{j}]\\ \frac{\partial}{\partial\overline{j}(x)}W[j,\overline{j}]\end{pmatrix}+\zeta\overline{j}(\bullet)+\sum_x\left(\frac{\partial\overline{j}(x)}{\partial\phi(\bullet)}\phi(x)+\zeta\overline{\phi}(x)\frac{\partial j(x)}{\partial\phi(\bullet)}\right)\\
&=-\sum_x\left(\frac{\partial j(x)}{\partial\phi(\bullet)},\frac{\partial\overline{j}(x)}{\partial\phi(\bullet)}\right)\cdot\begin{pmatrix}\zeta\overline{\phi}(x)\\ \phi(x)\end{pmatrix}+\zeta\overline{j}(\bullet)+\sum_x\left(\frac{\partial\overline{j}(x)}{\partial\phi(\bullet)}\phi(x)+\zeta\overline{\phi}(x)\frac{\partial j(x)}{\partial\phi(\bullet)}\right)\\
&=-\sum_x\left(\frac{\partial j(x)}{\partial\phi(\bullet)}\zeta\overline{\phi}(x)+\frac{\partial\overline{j}(x)}{\partial\phi(\bullet)}\phi(x)\right)+\zeta\overline{j}(\bullet)+\sum_x\left(\frac{\partial\overline{j}(x)}{\partial\phi(\bullet)}\phi(x)+\zeta\overline{\phi}(x)\frac{\partial j(x)}{\partial\phi(\bullet)}\right)\\
&=-\sum_x\left(\frac{\partial j(x)}{\partial\phi(\bullet)}\zeta\overline{\phi}(x)\right)+\zeta\overline{j}(\bullet)+\sum_x\left(\zeta\overline{\phi}(x)\frac{\partial j(x)}{\partial\phi(\bullet)}\right)\\
&=\zeta\overline{j}(\bullet),
\end{aligned}$$

and

$$\begin{aligned}
\frac{\partial}{\partial\overline{\phi}(\bullet)}\Gamma[\phi,\overline{\phi}] &= -\sum_x\left(\frac{\partial j(x)}{\partial\overline{\phi}(\bullet)},\frac{\partial\overline{j}(x)}{\partial\overline{\phi}(\bullet)}\right)\cdot\begin{pmatrix}\frac{\partial}{\partial j(x)}W[j,\overline{j}]\\ \frac{\partial}{\partial\overline{j}(x)}W[j,\overline{j}]\end{pmatrix}+j(\bullet)+\sum_x\left(\frac{\partial\overline{j}(x)}{\partial\overline{\phi}(\bullet)}\phi(x)+\zeta\overline{\phi}(x)\frac{\partial j(x)}{\partial\overline{\phi}(\bullet)}\right)\\
&=-\sum_x\left(\frac{\partial j(x)}{\partial\overline{\phi}(\bullet)},\frac{\partial\overline{j}(x)}{\partial\overline{\phi}(\bullet)}\right)\cdot\begin{pmatrix}\zeta\overline{\phi}(x)\\ \phi(x)\end{pmatrix}+j(\bullet)+\sum_x\left(\frac{\partial\overline{j}(x)}{\partial\overline{\phi}(\bullet)}\phi(x)+\zeta\overline{\phi}(x)\frac{\partial j(x)}{\partial\overline{\phi}(\bullet)}\right)\\
&=+j(\bullet).
\end{aligned}$$

[1] Cf. the derivative-rule for Grassmann-vector-valued functions. Cf. the differentiation-rule from Zinn-Justin on page 8!

Proof 34.8 of Lemma 16.40

We use Corollary 16.15 and find

$$\begin{aligned}\frac{\partial^n}{\partial\bar{j}(i_1)\cdots\partial\bar{j}(i_n)}\frac{\partial^n}{\partial j(i'_n)\cdots\partial j(i'_1)}\frac{Z[\bar{j},j]}{Z} &= \frac{\partial^n}{\partial\bar{j}(i_1)\cdots\partial\bar{j}(i_n)}\zeta^n\left\langle\overline{\psi}(i'_n)\cdots\overline{\psi}(i'_1)\exp\left[j^\dagger\psi+\psi^\dagger j\right]\right\rangle\\ &= \pm\zeta^n\left\langle\overline{\psi}(i'_n)\cdots\overline{\psi}(i'_1)\frac{\partial^n}{\partial\bar{j}(i_1)\cdots\partial\bar{j}(i_n)}\exp\left[j^\dagger\psi+\psi^\dagger j\right]\right\rangle\\ &= \pm\zeta^n\left\langle\overline{\psi}(i'_n)\cdots\overline{\psi}(i'_1)\psi(i_1)\cdots\psi(i_n)\exp\left[j^\dagger\psi+\psi^\dagger j\right]\right\rangle\\ &= +\zeta^n\left\langle\psi(i_1)\cdots\psi(i_n)\overline{\psi}(i'_n)\cdots\overline{\psi}(i'_1)\exp\left[j^\dagger\psi+\psi^\dagger j\right]\right\rangle\end{aligned}$$

Therefore we obtain

$$\begin{aligned}(-\zeta/c)^n\frac{\partial^n}{\partial\bar{j}(i_1)\cdots\partial\bar{j}(i_n)}\frac{\partial^n}{\partial j(i'_n)\cdots\partial j(i'_1)}\frac{Z[\bar{j},j]}{Z} &= +(-1/c)^n\left\langle\psi(i_1)\cdots\psi(i_n)\overline{\psi}(i'_n)\cdots\overline{\psi}(i'_1)\exp\left[j^\dagger\psi+\psi^\dagger j\right]\right\rangle\\ &= \ldots\end{aligned}$$

comparing this now with Equation (16.33) proves the Lemma

$$\ldots = \mathscr{G}(i_1,\ldots,i_n\,|\,i'_1,\ldots,i'_n). \tag{34.25}$$

Proof 34.9 of Corollary 16.43

We compute

$$\begin{aligned}
\mathscr{G}_{\mathrm{c}}(i_1|i_1') &= -\left(\frac{\zeta}{c}\right)\left(\frac{\partial^2}{\partial\bar{j}(i_1)\partial j(i_1')}W\right)[j,\bar{j}]_{|j=\bar{j}=0} \\
&= -\left(\frac{\zeta}{c}\right)\partial_{\bar{j}(i_1)}\partial_{j(i_1')}\log\left\langle\exp\left[j^\dagger\psi+\psi^\dagger j\right]\right\rangle_{|j=\bar{j}=0} \\
&= -\left(\frac{\zeta}{c}\right)\partial_{\bar{j}(i_1)}\left\langle\exp\left[j^\dagger\psi+\psi^\dagger j\right]\right\rangle^{-1}\left\langle\zeta\overline{\psi}(i_1')\exp\left[j^\dagger\psi+\psi^\dagger j\right]\right\rangle_{|j=\bar{j}=0} \\
&= -\left(\frac{1}{c}\right)\partial_{\bar{j}(i_1)}\left\langle\exp\left[j^\dagger\psi+\psi^\dagger j\right]\right\rangle^{-1}\left\langle\overline{\psi}(i_1')\exp\left[j^\dagger\psi+\psi^\dagger j\right]\right\rangle_{|j=\bar{j}=0} \\
&= -\left(\frac{1}{c}\right)\Big[\left\langle\exp\left[j^\dagger\psi+\psi^\dagger j\right]\right\rangle^{-2}\left\langle\psi(i_1)\exp\left[j^\dagger\psi+\psi^\dagger j\right]\right\rangle\left\langle\overline{\psi}(i_1')\exp\left[j^\dagger\psi+\psi^\dagger j\right]\right\rangle \\
&\qquad + \left\langle\exp\left[j^\dagger\psi+\psi^\dagger j\right]\right\rangle^{-2}\left\langle\zeta\overline{\psi}(i_1')\psi(i_1)\exp\left[j^\dagger\psi+\psi^\dagger j\right]\right\rangle\Big]_{|j=\bar{j}=0} \\
&= -\frac{\zeta}{c}\langle\overline{\psi}(i_1')\psi(i_1)\rangle \\
&= -\frac{1}{c}\langle\psi(i_1)\overline{\psi}(i_1')\rangle \\
&= \mathscr{G}(i_1|i_1')
\end{aligned} \tag{34.26}$$

For the other formula: Cf. Negele and Orland somewhere around page 107, 108.

Proof 34.10 of Lemma 16.44 We compute straight-forwardly

$$\begin{aligned}
\frac{\partial}{\partial\phi(\bullet)}F[\bar{j},j] &= \sum_x\left(\frac{\partial F}{\partial\bar{j}(x)},\frac{\partial F}{\partial j(x)},\right)\cdot\begin{pmatrix}\frac{\partial\bar{j}(x)}{\partial\phi(\bullet)}\\ \frac{\partial j(x)}{\partial\phi(\bullet)}\end{pmatrix} \\
&= \sum_x\frac{\partial F}{\partial\bar{j}(x)}\frac{\partial\bar{j}(x)}{\partial\phi(\bullet)}+\frac{\partial F}{\partial j(x)}\frac{\partial j(x)}{\partial\phi(\bullet)} \\
&= \sum_x\zeta\frac{\partial F}{\partial\bar{j}(x)}\frac{\partial^2\Gamma}{\partial\phi(\bullet)\partial\phi(x)}+\frac{\partial F}{\partial j(x)}\frac{\partial^2\Gamma}{\partial\phi(\bullet)\partial\overline{\phi}(x)}
\end{aligned} \tag{34.27}$$

and

$$\begin{aligned}
\frac{\partial}{\partial\overline{\phi}(\bullet)}F[\bar{j},j] &= \sum_x\left(\frac{\partial F}{\partial\bar{j}(x)},\frac{\partial F}{\partial j(x)},\right)\cdot\begin{pmatrix}\frac{\partial\bar{j}(x)}{\partial\overline{\phi}(\bullet)}\\ \frac{\partial j(x)}{\partial\overline{\phi}(\bullet)}\end{pmatrix} \\
&= \sum_x\frac{\partial F}{\partial\bar{j}(x)}\frac{\partial\bar{j}(x)}{\partial\overline{\phi}(\bullet)}+\frac{\partial F}{\partial j(x)}\frac{\partial j(x)}{\partial\overline{\phi}(\bullet)} \\
&= \sum_x\zeta\frac{\partial F}{\partial\bar{j}(x)}\frac{\partial^2\Gamma}{\partial\overline{\phi}(\bullet)\partial\phi(x)}+\frac{\partial F}{\partial j(x)}\frac{\partial^2\Gamma}{\partial\overline{\phi}(\bullet)\partial\overline{\phi}(x)}
\end{aligned} \tag{34.28}$$

Proof 34.11 of Corollary 16.45 We use the Lemma and compute ...

The first equation:

$$\begin{aligned}\delta_{1,3} = \frac{\partial\phi(3)}{\partial\phi(1)} &= \frac{\partial}{\partial\phi(1)}\frac{\partial W}{\partial\bar{j}(3)} \\ &= \sum_2 \zeta \left(\frac{\partial^2 W}{\partial\bar{j}(2)\partial\bar{j}(3)}\right)\left(\frac{\partial^2\Gamma}{\partial\phi(1)\partial\phi(2)}\right) + \left(\frac{\partial^2 W}{\partial j(2)\partial\bar{j}(3)}\right)\left(\frac{\partial^2\Gamma}{\partial\phi(1)\partial\bar{\phi}(2)}\right)\end{aligned} \tag{34.29}$$

The second equation:

$$\begin{aligned}\delta_{1,3} = \frac{\partial\bar{\phi}(3)}{\partial\bar{\phi}(1)} &= \zeta\frac{\partial}{\partial\phi(1)}\frac{\partial W}{\partial j(3)} \\ &= \zeta\sum_2 \zeta \left(\frac{\partial^2 W}{\partial\bar{j}(2)\partial j(3)}\right)\left(\frac{\partial^2\Gamma}{\partial\bar{\phi}(1)\partial\phi(2)}\right) + \left(\frac{\partial^2 W}{\partial j(2)\partial j(3)}\right)\left(\frac{\partial^2\Gamma}{\partial\bar{\phi}(1)\partial\bar{\phi}(2)}\right) \\ &= \sum_2 \left(\frac{\partial^2 W}{\partial\bar{j}(2)\partial j(3)}\right)\left(\frac{\partial^2\Gamma}{\partial\bar{\phi}(1)\partial\phi(2)}\right) + \zeta\left(\frac{\partial^2 W}{\partial j(2)\partial j(3)}\right)\left(\frac{\partial^2\Gamma}{\partial\bar{\phi}(1)\partial\bar{\phi}(2)}\right)\end{aligned} \tag{34.30}$$

Correction note. In the first line of this equation the derivative has to be taken w.r.t. $\bar{\phi}(1)$ instead of $\phi(1)$, i.e.

$$\delta_{1,3} = \frac{\partial\bar{\phi}(3)}{\partial\bar{\phi}(1)} = \zeta\frac{\partial}{\partial\bar{\phi}(1)}\frac{\partial W}{\partial j(3)}.$$

The second and third line are already written for $\partial/\partial\bar{\phi}(1)$ and are correct (Lemma 16.44 with $F = \zeta\,\partial W/\partial j(3)$).

The third equation:

$$\begin{aligned}0 = \frac{\partial\phi(3)}{\partial\bar{\phi}(1)} &= \frac{\partial}{\partial\bar{\phi}(1)}\frac{\partial W}{\partial\bar{j}(3)} \\ &= \sum_2 \zeta \left(\frac{\partial^2 W}{\partial\bar{j}(2)\partial\bar{j}(3)}\right)\left(\frac{\partial^2\Gamma}{\partial\bar{\phi}(1)\partial\phi(2)}\right) + \left(\frac{\partial^2 W}{\partial j(2)\partial\bar{j}(3)}\right)\left(\frac{\partial^2\Gamma}{\partial\bar{\phi}(1)\partial\bar{\phi}(2)}\right)\end{aligned} \tag{34.31}$$

The fourth equation:

$$\begin{aligned}0 = \frac{\partial\bar{\phi}(3)}{\partial\phi(1)} &= \zeta\frac{\partial}{\partial\phi(1)}\frac{\partial W}{\partial j(3)} \\ &= \sum_2 \left(\frac{\partial^2 W}{\partial\bar{j}(2)\partial j(3)}\right)\left(\frac{\partial^2\Gamma}{\partial\phi(1)\partial\phi(2)}\right) + \zeta\left(\frac{\partial^2 W}{\partial j(2)\partial j(3)}\right)\left(\frac{\partial^2\Gamma}{\partial\phi(1)\partial\bar{\phi}(2)}\right)\end{aligned} \tag{34.32}$$

Now summarizing[2] the equations we find

[2] The first equation gives the 1,1 component, the second to the 2,2 component, the third for the 1,2 and the fourth to the 2,1 component.

$$\sum_{i_2}\begin{pmatrix} \frac{\partial^2 W}{\partial \bar{j}(i_3)\partial j(i_2)} & \zeta\frac{\partial^2 W}{\partial \bar{j}(i_3)\partial \bar{j}(i_2)} \\ \zeta\frac{\partial^2 W}{\partial j(i_3)\partial j(i_2)} & \frac{\partial^2 W}{\partial j(i_3)\partial \bar{j}(i_2)} \end{pmatrix}\begin{pmatrix} \frac{\partial^2 \Gamma}{\partial \bar{\phi}(i_2)\partial \phi(i_1)} & \frac{\partial^2 \Gamma}{\partial \bar{\phi}(i_2)\partial \bar{\phi}(i_1)} \\ \frac{\partial^2 \Gamma}{\partial \phi(i_2)\partial \phi(i_1)} & \frac{\partial^2 \Gamma}{\partial \phi(i_2)\partial \bar{\phi}(i_1)} \end{pmatrix} = \delta_{i_1,i_3}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{34.33}$$

Note. The four equations are not literally the entries of this matrix product (with $i_1 = 1$, $i_2 = 2$, $i_3 = 3$). To bring them into this form, one has to reorder the second derivatives with the statistics neutral Schwartz-rule (Lemma 16.12), $\frac{\partial^2 F}{\partial \pi_x \partial \pi'_y} = \zeta\frac{\partial^2 F}{\partial \pi'_y \partial \pi_x}$. For the first equation, for example,

$$\zeta\frac{\partial^2 W}{\partial \bar{j}(2)\,\partial \bar{j}(3)}\frac{\partial^2 \Gamma}{\partial \phi(1)\,\partial \phi(2)} = \zeta\frac{\partial^2 W}{\partial \bar{j}(3)\,\partial \bar{j}(2)}\frac{\partial^2 \Gamma}{\partial \phi(2)\,\partial \phi(1)}, \qquad \frac{\partial^2 W}{\partial j(2)\,\partial \bar{j}(3)}\frac{\partial^2 \Gamma}{\partial \phi(1)\,\partial \bar{\phi}(2)} = \frac{\partial^2 W}{\partial \bar{j}(3)\,\partial j(2)}\frac{\partial^2 \Gamma}{\partial \bar{\phi}(2)\,\partial \phi(1)},$$

which are the products of the $(1,2)$- and $(2,1)$-blocks and of the $(1,1)$-blocks, respectively. A compact proof that directly produces the matrix form is given in Lemma 19.10; the matrix identity itself has been checked numerically (Remark 19.27.3).

Proof 34.12 of Theorem 16.47

We start with Equation (34.30)

$$\delta_{1,3} = \sum_2 \left(\frac{\partial^2 W}{\partial \bar{j}(2)\partial j(3)}\right)\left(\frac{\partial^2 \Gamma}{\partial \bar{\phi}(1)\partial \phi(2)}\right) + \zeta\left(\frac{\partial^2 W}{\partial j(2)\partial j(3)}\right)\left(\frac{\partial^2 \Gamma}{\partial \bar{\phi}(1)\partial \bar{\phi}(2)}\right) \tag{34.34}$$

and now we take the derivative w.r.t. $\phi(4)$ on both sides

$$\begin{aligned} 0 = \partial_{\phi(4)}\delta_{1,3} = &\sum_2 \left(\partial_{\phi(4)}\frac{\partial^2 W}{\partial \bar{j}(2)\partial j(3)}\right)\left(\frac{\partial^2 \Gamma}{\partial \bar{\phi}(1)\partial \phi(2)}\right) + \left(\frac{\partial^2 W}{\partial \bar{j}(2)\partial j(3)}\right)\left(\partial_{\phi(4)}\frac{\partial^2 \Gamma}{\partial \bar{\phi}(1)\partial \phi(2)}\right) \\ &+ \zeta\left(\partial_{\phi(4)}\frac{\partial^2 W}{\partial j(2)\partial j(3)}\right)\left(\frac{\partial^2 \Gamma}{\partial \bar{\phi}(1)\partial \bar{\phi}(2)}\right) + \zeta\left(\frac{\partial^2 W}{\partial j(2)\partial j(3)}\right)\left(\partial_{\phi(4)}\frac{\partial^2 \Gamma}{\partial \bar{\phi}(1)\partial \bar{\phi}(2)}\right) \\ &= \dots \end{aligned} \tag{34.35}$$

now we consider the following two terms individually:

$$\partial_{\phi(4)}\frac{\partial^2 W}{\partial \bar{j}(2)\partial j(3)} = \sum_5 \zeta\left(\frac{\partial^3 W}{\partial \bar{j}(5)\partial \bar{j}(2)\partial j(3)}\right)\left(\frac{\partial^2 \Gamma}{\partial \phi(4)\partial \phi(5)}\right) + \left(\frac{\partial^3 W}{\partial j(5)\partial \bar{j}(2)\partial j(3)}\right)\left(\frac{\partial^2 \Gamma}{\partial \phi(4)\partial \bar{\phi}(5)}\right) \tag{34.36}$$

and

$$\partial_{\phi(4)}\frac{\partial^2 W}{\partial j(2)\partial j(3)} = \sum_5 \zeta\left(\frac{\partial^3 W}{\partial \bar{j}(5)\partial j(2)\partial j(3)}\right)\left(\frac{\partial^2 \Gamma}{\partial \phi(4)\partial \phi(5)}\right) + \left(\frac{\partial^3 W}{\partial j(5)\partial j(2)\partial j(3)}\right)\left(\frac{\partial^2 \Gamma}{\partial \phi(4)\partial \bar{\phi}(5)}\right) \tag{34.37}$$

inserting this above yields

$$
\begin{aligned}
0 = \ldots = \sum_2 \Bigg[& \left(\frac{\partial^2 W}{\partial \bar{j}(2)\partial j(3)}\right)\left(\frac{\partial^3 \Gamma}{\partial\phi(4)\partial\bar{\phi}(1)\partial\bar{\phi}(2)}\right) + \zeta\left(\frac{\partial^2 W}{\partial j(2)\partial j(3)}\right)\left(\frac{\partial^3 \Gamma}{\partial\phi(4)\partial\bar{\phi}(1)\partial\bar{\phi}(2)}\right) \\
& + \sum_5 \left[\zeta \frac{\partial^3 W}{\partial \bar{j}(5)\partial \bar{j}(2)\partial j(3)} \cdot \frac{\partial^2\Gamma}{\partial\phi(4)\partial\bar{\phi}(5)} + \frac{\partial^3 W}{\partial j(5)\partial \bar{j}(2)\partial j(3)} \cdot \frac{\partial^2\Gamma}{\partial\phi(4)\partial\bar{\phi}(5)}\right] \cdot \frac{\partial^2\Gamma}{\partial\bar{\phi}(1)\partial\phi(2)} \\
& + \sum_2 \left[\frac{\partial^3 W}{\partial \bar{j}(5)\partial j(2)\partial j(3)} \frac{\partial^2\Gamma}{\partial\phi(4)\partial\phi(5)} + \zeta \frac{\partial^3 W}{\partial j(5)\partial j(2)\partial j(3)} \frac{\partial^2\Gamma}{\partial\phi(4)\partial\bar{\phi}(5)}\right] \cdot \frac{\partial^2\Gamma}{\partial\bar{\phi}(1)\partial\bar{\phi}(2)}\Bigg]
\end{aligned} \tag{34.38}
$$

Now we take the derivative w.r.t. $\bar{\phi}(6)$. We consider each of the six terms (seperated by plus-symbols respectively) separately:

1. We compute

$$
\begin{aligned}
& \partial_{\bar{\phi}(6)} \sum_2 \left(\frac{\partial^2 W}{\partial \bar{j}(2)\partial j(3)}\right)\left(\frac{\partial^3 \Gamma}{\partial\phi(4)\partial\bar{\phi}(1)\partial\phi(2)}\right) \\
= & \sum_2 \left(\partial_{\bar{\phi}(6)} \frac{\partial^2 W}{\partial \bar{j}(2)\partial j(3)}\right)\left(\frac{\partial^3 \Gamma}{\partial\phi(4)\partial\bar{\phi}(1)\partial\phi(2)}\right) + \left(\frac{\partial^2 W}{\partial \bar{j}(2)\partial j(3)}\right)\left(\frac{\partial^4 \Gamma}{\partial\bar{\phi}(6)\partial\phi(4)\partial\bar{\phi}(1)\partial\phi(2)}\right) \\
\equiv & \sum_2 0 + \left(\frac{\partial^2 W}{\partial \bar{j}(2)\partial j(3)}\right)\left(\frac{\partial^4 \Gamma}{\partial\bar{\phi}(6)\partial\phi(4)\partial\bar{\phi}(1)\partial\phi(2)}\right)
\end{aligned} \tag{34.39}
$$

2. This term doesn't contribute because of $\partial_{j(2)}\partial_{j(3)}$
3. This term doesn't contribute because of $\partial_{\phi(4)}\partial_{\phi(5)}$
4. We compute straight-forwardly

$$
\begin{aligned}
& \partial_{\bar{\phi}(6)} \sum_{2,5} \left(\frac{\partial^3 W}{\partial j(5)\partial \bar{j}(2)\partial j(3)}\right)\left(\frac{\partial^2 \Gamma}{\partial\phi(4)\partial\bar{\phi}(5)}\right)\left(\frac{\partial^2 \Gamma}{\partial\bar{\phi}(1)\partial\phi(2)}\right) \\
= & \sum_{2,5} \left(\partial_{\bar{\phi}(6)} \frac{\partial^3 W}{\partial j(5)\partial \bar{j}(2)\partial j(3)}\right)\left(\frac{\partial^2 \Gamma}{\partial\phi(4)\partial\bar{\phi}(5)}\right)\left(\frac{\partial^2 \Gamma}{\partial\bar{\phi}(1)\partial\phi(2)}\right) \\
& + \left(\frac{\partial^3 W}{\partial j(5)\partial \bar{j}(2)\partial j(3)}\right)\left[\frac{\partial^3 \Gamma}{\partial\bar{\phi}(6)\partial\phi(4)\partial\bar{\phi}(5)} \cdot \frac{\partial^2\Gamma}{\partial\bar{\phi}(1)\partial\phi(2)} + \frac{\partial^2\Gamma}{\partial\phi(4)\partial\bar{\phi}(5)} \cdot \frac{\partial^3 \Gamma}{\partial\bar{\phi}(6)\partial\bar{\phi}(1)\partial\phi(2)}\right] \\
\equiv & \ldots
\end{aligned} \tag{34.40}
$$

   now we will simplify this, using that the terms in the second line dont contribute in the absence of external sources and spontaneous symmetry breaking, implying that one obtains

$$
\ldots = \sum_{2,5,7} \left[\zeta \frac{\partial^4 W}{\partial \bar{j}(7)\partial j(5)\partial \bar{j}(2)\partial j(3)} \cdot \frac{\partial^2\Gamma}{\partial\bar{\phi}(6)\partial\phi(7)} + \cdots\right] \cdot \frac{\partial^2\Gamma}{\partial\phi(4)\partial\bar{\phi}(5)} \cdot \frac{\partial^2\Gamma}{\partial\bar{\phi}(1)\partial\phi(2)} \tag{34.41}
$$

5. This term doesn't contribute because of $\partial_{\bar{\phi}(1)}\partial_{\bar{\phi}(2)}$
6. This term doesn't contribute because of $\partial_{\bar{\phi}(1)}\partial_{\bar{\phi}(2)}$

Now we collect the individual (non-vanishing) contributions and obtain

$$
\begin{aligned}
0 &= \sum_{2} \left(\frac{\partial^2 W}{\partial \bar{j}(2) \partial j(3)} \right) \left(\frac{\partial^4 \Gamma}{\partial \bar{\phi}(6) \partial \phi(4) \partial \bar{\phi}(1) \partial \phi(2)} \right) \\
&+ \zeta \sum_{2,5,7} \left(\frac{\partial^4 W}{\partial \bar{j}(7) \partial j(5) \partial \bar{j}(2) \partial j(3)} \right) \left(\frac{\partial^2 \Gamma}{\partial \phi(4) \partial \bar{\phi}(5)} \right) \left(\frac{\partial^2 \Gamma}{\partial \bar{\phi}(1) \partial \phi(2)} \right) \left(\frac{\partial^2 \Gamma}{\partial \bar{\phi}(6) \partial \phi(7)} \right) \\
&= \sum_{2} \left(\frac{\partial^2 W}{\partial \bar{j}(2) \partial j(3)} \right) \left(\frac{\zeta \partial^4 \Gamma}{\partial \bar{\phi}(6) \partial \bar{\phi}(1) \partial \phi(4) \partial \phi(2)} \right) \\
&+ \zeta \sum_{2,5,7} \left(\frac{\zeta \partial^4 W}{\partial \bar{j}(7) \partial \bar{j}(2) \partial j(5) \partial j(3)} \right) \left(\frac{\zeta \partial^2 \Gamma}{\partial \bar{\phi}(5) \partial \phi(4)} \right) \left(\frac{\partial^2 \Gamma}{\partial \bar{\phi}(1) \partial \phi(2)} \right) \left(\frac{\partial^2 \Gamma}{\partial \bar{\phi}(6) \partial \phi(7)} \right) \\
&= \sum_{2} \left(-\frac{\hbar}{\zeta} \mathcal{G}_c(2,3) \right) \zeta \left(-\frac{\zeta}{\hbar} \right)^2 V(6,1|2,4) \\
&+ \zeta \sum_{2,5,7} \zeta \left(-\frac{\hbar}{\zeta} \right)^2 \mathcal{G}_c(7,2|3,5) \zeta \left(-\frac{\zeta}{\hbar} V(5,4) \right) \left(-\frac{\zeta}{\hbar} V(1,2) \right) \left(-\frac{\zeta}{\hbar} V(6,7) \right) \\
&= -\frac{1}{\hbar} \sum_{2} \mathcal{G}_c(2,3) V(6,1|2,4) \\
&- \frac{1}{\hbar} \sum_{2,5,7} \mathcal{G}_c(7,2|3,5) V(5,4) V(1,2) V(6,7)
\end{aligned}
\tag{34.42}
$$

rearranging terms and multiplying both sides with $\hbar$ gives therefore

$$
\sum_{2} \mathcal{G}_c(2,3) V(6,1|2,4) = - \sum_{2,5,7} \mathcal{G}_c(7,2|3,5) V(5,4) V(1,2) V(6,7) \tag{34.43}
$$

Notice that this equation holds for all 1, 3, 4, 6. Now we make the replacements

- $1 \mapsto \tilde{1}$
- $3 \mapsto \tilde{2}$
- $4 \mapsto \tilde{3}$
- $6 \mapsto \tilde{4}$

and obtain therefore

$$
\sum_{2} \mathcal{G}_c(2,\tilde{2}) V(\tilde{4},\tilde{1}|2,\tilde{3}) = - \sum_{2,5,7} \mathcal{G}_c(7,2|\tilde{2},5) V(5,\tilde{3}) V(\tilde{1},2) V(\tilde{4},7) \tag{34.44}
$$

or, equivalently

$$
\sum_{2} \mathcal{G}_c(2,i_2) V(i_4,i_1|2,i_3) = - \sum_{2,5,7} \mathcal{G}_c(7,2|i_2,5) V(5,i_3) V(i_1,2) V(i_4,7) \tag{34.45}
$$

Now we multiply both sides with $\mathcal{G}_c(i_3|x_1)$ and sum over i_3, whereas x_1 still has to be determined, and we obtain

$$\begin{aligned}\sum_{2,i_3} \mathcal{G}_c(2,i_2)V(i_4,i_1|2,i_3)\mathcal{G}_c(i_3|x_1) &= -\sum_{2,5,7} \mathcal{G}_c(7,2|i_2,5)V(i_1,2)V(i_4,7)\sum_{i_3} V(5,i_3)\mathcal{G}_c(i_3|x_1) \\ &= -\sum_{2,5,7} \mathcal{G}_c(7,2|i_2,5)V(i_1,2)V(i_4,7)\delta_{5,x_1} \\ &= -\sum_{2,7} \mathcal{G}_c(7,2|i_2,x_1)V(i_1,2)V(i_4,7)\end{aligned} \tag{34.46}$$

Now we multiply both sides with $\mathcal{G}_c(x_2|i_1)\mathcal{G}_c(x_3|i_4)$ and sum over i_1, whereas i_4 still has to be determined, and we obtain

$$\begin{aligned}\sum_{2,i_1,i_3,i_4} \mathcal{G}_c(2,i_2)V(i_4,i_1|2,i_3)\mathcal{G}_c(i_3|x_1)\mathcal{G}_c(x_2|i_1)\mathcal{G}_c(x_3|i_4) &= -\sum_{2,7} \mathcal{G}_c(7,2|i_2,x_1)\sum_{i_1} \mathcal{G}_c(x_2|i_1)V(i_1,2)\sum_{i_4} \mathcal{G}_c(x_3|i_4)V(i_4,7) \\ &= -\sum_{2,7} \mathcal{G}_c(7,2|i_2,x_1)\delta_{x_2,2}\delta_{x_3,7} \\ &= -\mathcal{G}_c(x_3,x_2|i_2,x_1)\end{aligned} \tag{34.47}$$

Now we replace

1. $x_3 \mapsto y_1$
2. $x_2 \mapsto y_2$
3. $i_2 \mapsto y_3$
4. $x_1 \mapsto y_4$

and we obtain

$$\begin{aligned}\mathcal{G}_c(y_1,y_2|y_3,y_4) &= -\sum_{2,i_1,i_3,i_4} \mathcal{G}_c(2,y_3)V(i_4,i_1|2,i_3)\mathcal{G}_c(i_3|y_4)\mathcal{G}_c(y_2|i_1)\mathcal{G}_c(y_1|i_4) \\ &= -\sum_{2,i_1,i_3,i_4} \mathcal{G}_c(y_1|i_4)\mathcal{G}_c(y_2|i_1)V(i_4,i_1|2,i_3)\mathcal{G}_c(2,y_3)\mathcal{G}_c(i_3|y_4) \\ &= \dots\end{aligned} \tag{34.48}$$

and now, we replace finally

1. $i_4 \mapsto l_1$
2. $i_1 \mapsto l_2$
3. $2 \mapsto l'_1$
4. $i_3 \mapsto l'_2$

and obtain

$$\mathcal{G}_c(y_1,y_2|y_3,y_4) = -\sum_{l_1,l_2,l'_1,l'_2} \mathcal{G}_c(y_1|l_1)\mathcal{G}_c(y_2|l_2)V(l_1,l_2|l'_1,l'_2)\mathcal{G}_c(l'_1,y_3)\mathcal{G}_c(l'_2|y_4) \tag{34.49}$$

proving the theorem.

Proof 34.13 of Approximation 16.55.

The problem is here, that we need a very clean definition of the left right derivative in the series-expansion

Starting with eq. (16.44) and lightening the notation, we obtain

$$\begin{aligned}\Gamma[\phi,\overline{\phi}] &= -W[j,\overline{j}] + \sum \overline{j}\phi + \overline{\phi}j \\ &= -\log Z[j,\overline{j}] + \sum \overline{j}\phi + \overline{\phi}j,\end{aligned}$$

We do the following things:

1. We multiply this equation by -1 and apply the exponential-function to both sides,
2. we insert the definition of the source-dependent partition function $Z[j,\overline{j}]$ from eq. (16.37),
3. we use the invariance of the functional integral by translations (Graßmann-valued *and* complex) $\psi - \phi \to \Delta$, etc.

This gives in equations

$$\begin{aligned}\exp\left(-\Gamma[\phi,\overline{\phi}]\right) &= Z[j,\overline{j}]\exp\left(-\sum \overline{j}\phi + \overline{\phi}j\right) \\ &= \int \mathscr{D}(\psi,\overline{\psi})\exp\left(-S[\psi,\overline{\psi}] + \sum \overline{j}(\psi-\phi) + (\overline{\psi}-\overline{\phi})j\right) \\ &= \int \mathscr{D}(\Delta,\overline{\Delta})\exp\left(-S[\phi+\Delta,\overline{\phi}+\overline{\Delta}] + \sum \overline{j}\Delta + \overline{\Delta}j\right).\end{aligned}$$

The action S can now be expanded in the variation analogously to Notation 16.36, whereas here we use schematic notation and we emphasize that the left-right-derivative carries non-trivial signs, giving us the equation

$$\begin{aligned}S[\phi+\Delta,\overline{\phi}+\overline{\Delta}] = \quad & S[\phi,\overline{\phi}] \\ & + \sum\left(\frac{\partial}{\partial\phi}S[\phi,\overline{\phi}],\frac{\partial}{\partial\overline{\phi}}S[\phi,\overline{\phi}]\right)\cdot\begin{pmatrix}\Delta\\ \overline{\Delta}\end{pmatrix} \\ & + \frac{1}{2!}\sum\sum\begin{pmatrix}\Delta\\ \overline{\Delta}\end{pmatrix}^{\mathrm{T}}\cdot\begin{pmatrix}\frac{\partial^2}{\partial\phi\,\partial\phi}S[\phi,\overline{\phi}] & \frac{\partial^2}{\partial\phi\,\partial\overline{\phi}}S[\phi,\overline{\phi}]\\ \frac{\partial^2}{\partial\overline{\phi}\,\partial\phi}S[\phi,\overline{\phi}] & \frac{\partial^2}{\partial\overline{\phi}\,\partial\overline{\phi}}S[\phi,\overline{\phi}]\end{pmatrix}\cdot\begin{pmatrix}\Delta\\ \overline{\Delta}\end{pmatrix} \\ & + \mathcal{O}\left(\Delta^3,\Delta^2\overline{\Delta}^1,\Delta^1\overline{\Delta}^2,\overline{\Delta}^3\right).\end{aligned}$$

With this we get

$$\exp\left(-\Gamma[\phi,\overline{\phi}]\right) = \exp\left(-S[\phi,\overline{\phi}]\right)\int \mathscr{D}(\Delta,\overline{\Delta})\,\exp \mathrm{P}(\Delta,\overline{\Delta},\phi,\overline{\phi}) \tag{34.50}$$

with a polynomial P in the integration-variables and in the fields. In the so-called *Tree-Level-approximation* one now approximates[3]

[3]The meaning of the symbol "≈" is always referring to "closeness" (in some sense that needs to be specified) to experimental data.

$$\int \mathscr{D}(\Delta, \overline{\Delta}) \, \exp \mathrm{P}(\Delta, \overline{\Delta}, \phi, \overline{\phi}) \quad \approx \quad \mathcal{O}(1).$$

So, one assumes that the functional integral (which, when evaluated, is again a polynomial expression in the classical fields) gives essentially ϕ-independent contributions. After applying the logarithm and using the inverse property (also for Graßmann-valued polynomial expressions?!) we thus obtain

$$\Gamma[\phi, \overline{\phi}] \quad \approx \quad S[\phi, \overline{\phi}] + \text{const}.$$

Remembering now that the physically relevant part of the effective action is in the numerical values of the non-trivial correlators (and thus in the coefficients of the non-constant monomials in Γ (cf. the series-expansion in Equation (16.45))), then, one usually simply notes for convenience:

$$\Gamma[\phi, \overline{\phi}] \quad \approx \quad S[\phi, \overline{\phi}].$$

Proof 34.14 of Approximation 16.57.

The *One-Loop-approximation* builds on the Tree-Level-approximation. If we use Corollary 16.56, then (in the context of the Tree-Level-approximation) in eq. (34.50) the terms linear in Δ and $\overline{\Delta}$ cancel out. Then we can use this to connect to eq. (34.50), by neglecting the contributions to the polynomial P of order $\Delta^n \overline{\Delta}^m$ with $n+m \geq 3$:

$$\begin{aligned}
\exp\left(-\Gamma[\phi,\overline{\phi}]\right) &\approx \exp\left(-S[\phi,\overline{\phi}]\right) \int \mathscr{D}(\Delta,\overline{\Delta}) \exp\, -\frac{1}{2} \sum\sum \begin{pmatrix} \Delta \\ \overline{\Delta} \end{pmatrix}^{\mathrm{T}} \cdot \begin{pmatrix} \frac{\partial^2}{\partial\phi\,\partial\phi} S[\phi,\overline{\phi}] & \frac{\partial^2}{\partial\phi\,\partial\overline{\phi}} S[\phi,\overline{\phi}] \\ \frac{\partial^2}{\partial\overline{\phi}\,\partial\phi} S[\phi,\overline{\phi}] & \frac{\partial^2}{\partial\overline{\phi}\,\partial\overline{\phi}} S[\phi,\overline{\phi}] \end{pmatrix} \cdot \begin{pmatrix} \Delta \\ \overline{\Delta} \end{pmatrix} \\
&= \exp\left(-S[\phi,\overline{\phi}]\right) \mathrm{Pf} \begin{pmatrix} \frac{\partial^2}{\partial\phi\,\partial\phi} S[\phi,\overline{\phi}] & \frac{\partial^2}{\partial\phi\,\partial\overline{\phi}} S[\phi,\overline{\phi}] \\ \frac{\partial^2}{\partial\overline{\phi}\,\partial\phi} S[\phi,\overline{\phi}] & \frac{\partial^2}{\partial\overline{\phi}\,\partial\overline{\phi}} S[\phi,\overline{\phi}] \end{pmatrix}.
\end{aligned}$$

If we now take the logarithm on both sides and use the inversion-property between exponential-function and logarithm (?!) and fundamental identities for the matrix logarithm (also for Graßmann-valued matrices?!), we get

$$\begin{aligned}
-\Gamma[\phi,\overline{\phi}] &\approx -S[\phi,\overline{\phi}] + \log \mathrm{Pf} \begin{pmatrix} \frac{\partial^2}{\partial\phi\,\partial\phi} S[\phi,\overline{\phi}] & \frac{\partial^2}{\partial\phi\,\partial\overline{\phi}} S[\phi,\overline{\phi}] \\ \frac{\partial^2}{\partial\overline{\phi}\,\partial\phi} S[\phi,\overline{\phi}] & \frac{\partial^2}{\partial\overline{\phi}\,\partial\overline{\phi}} S[\phi,\overline{\phi}] \end{pmatrix} \\
&\overset{?!}{=} -S[\phi,\overline{\phi}] + \frac{1}{2} \log \mathrm{Det} \begin{pmatrix} \frac{\partial^2}{\partial\phi\,\partial\phi} S[\phi,\overline{\phi}] & \frac{\partial^2}{\partial\phi\,\partial\overline{\phi}} S[\phi,\overline{\phi}] \\ \frac{\partial^2}{\partial\overline{\phi}\,\partial\phi} S[\phi,\overline{\phi}] & \frac{\partial^2}{\partial\overline{\phi}\,\partial\overline{\phi}} S[\phi,\overline{\phi}] \end{pmatrix} \\
&\overset{?!}{=} -S[\phi,\overline{\phi}] + \frac{1}{2} \mathrm{Tr} \log \begin{pmatrix} \frac{\partial^2}{\partial\phi\,\partial\phi} S[\phi,\overline{\phi}] & \frac{\partial^2}{\partial\phi\,\partial\overline{\phi}} S[\phi,\overline{\phi}] \\ \frac{\partial^2}{\partial\overline{\phi}\,\partial\phi} S[\phi,\overline{\phi}] & \frac{\partial^2}{\partial\overline{\phi}\,\partial\overline{\phi}} S[\phi,\overline{\phi}] \end{pmatrix} \\
\Longleftrightarrow +\Gamma[\phi,\overline{\phi}] &\approx +S[\phi,\overline{\phi}] - \frac{1}{2} \mathrm{Tr} \log \begin{pmatrix} \frac{\partial^2}{\partial\phi\,\partial\phi} S[\phi,\overline{\phi}] & \frac{\partial^2}{\partial\phi\,\partial\overline{\phi}} S[\phi,\overline{\phi}] \\ \frac{\partial^2}{\partial\overline{\phi}\,\partial\phi} S[\phi,\overline{\phi}] & \frac{\partial^2}{\partial\overline{\phi}\,\partial\overline{\phi}} S[\phi,\overline{\phi}] \end{pmatrix}.
\end{aligned}$$

Proof 34.15 of Approximation 16.58.

One separates the second variation according to

$$\begin{pmatrix} \frac{\partial^2}{\partial\phi\,\partial\phi}S[\phi,\overline{\phi}] & \frac{\partial^2}{\partial\phi\,\partial\overline{\phi}}S[\phi,\overline{\phi}] \\ \frac{\partial^2}{\partial\overline{\phi}\,\partial\phi}S[\phi,\overline{\phi}] & \frac{\partial^2}{\partial\overline{\phi}\,\partial\overline{\phi}}S[\phi,\overline{\phi}] \end{pmatrix} = \begin{pmatrix} 0 & -x\mathscr{G}_0^{-\mathrm{T}} \\ x\mathscr{G}_0^{-1} & 0 \end{pmatrix} + \begin{pmatrix} \frac{\partial^2}{\partial\phi\,\partial\phi}S_{\mathrm{int}}[\phi,\overline{\phi}] & \frac{\partial^2}{\partial\phi\,\partial\overline{\phi}}S_{\mathrm{int}}[\phi,\overline{\phi}] \\ \frac{\partial^2}{\partial\overline{\phi}\,\partial\phi}S_{\mathrm{int}}[\phi,\overline{\phi}] & \frac{\delta^2}{\partial\overline{\phi}\,\partial\overline{\phi}}S_{\mathrm{int}}[\phi,\overline{\phi}] \end{pmatrix}$$
$$\equiv \quad x\widehat{\mathscr{G}}_0^{-1} \quad + \quad \widehat{V}[\phi,\overline{\phi}].$$

Using now that

$$x\widehat{\mathscr{G}}_0 = \begin{pmatrix} 0 & -x\mathscr{G}_0^{-\mathrm{T}} \\ x\mathscr{G}_0^{-1} & 0 \end{pmatrix}^{-1} = \begin{pmatrix} 0 & x\mathscr{G}_0 \\ -x\mathscr{G}_0^{\mathrm{T}} & 0 \end{pmatrix},$$

it follows, after simplifying the notation $\widehat{V}[\phi,\overline{\phi}] \equiv \widehat{V}$, that

$$\begin{aligned} \mathrm{Tr}\log\left[x\widehat{\mathscr{G}}_0^{-1} + \widehat{V}\right] &= \mathrm{Tr}\log\left[x\widehat{\mathscr{G}}_0^{-1}\cdot\left(1 + x\widehat{\mathscr{G}}_0\widehat{V}\right)\right] \\ &\overset{?!}{=} \mathrm{Tr}\log\left[x\widehat{\mathscr{G}}_0^{-1}\right] + \mathrm{Tr}\log\left[1 + x\widehat{\mathscr{G}}_0\cdot\widehat{V}\right] \\ &= \mathcal{O}(1) + \mathrm{Tr}\log\left[1 + x\widehat{\mathscr{G}}_0\cdot\widehat{V}\right]. \end{aligned}$$

The first term again provides a (in ϕ and $\overline{\phi}$) constant (and thus physically irrelevant) contribution. The second term provides (physically relevant) corrections. Therefore, we focus on the second term and expand the logarithm in its series representation for "small" corrections to the identity:

$$\begin{aligned} \mathrm{Tr}\log\left[1 + x\widehat{\mathscr{G}}_0\cdot\widehat{V}\right] &\approx \mathrm{Tr}\left[x\widehat{\mathscr{G}}_0\cdot\widehat{V} - \frac{\left(x\widehat{\mathscr{G}}_0\cdot\widehat{V}\right)^2}{2} \overset{+}{-} \cdots\right] \\ &= \mathrm{Tr}\left[x\widehat{\mathscr{G}}_0\cdot\widehat{V}\right] - \frac{1}{2}\mathrm{Tr}\left[x^2\widehat{\mathscr{G}}_0\cdot\widehat{V}\cdot\widehat{\mathscr{G}}_0\cdot\widehat{V}\right] \overset{+}{-} \cdots \end{aligned}$$

First summand. One computes

$$\begin{aligned} x\widehat{\mathscr{G}}_0\widehat{V} &= \begin{pmatrix} 0 & x\mathscr{G}_0 \\ -x\mathscr{G}_0^{\mathrm{T}} & 0 \end{pmatrix}\cdot\begin{pmatrix} \frac{\partial^2}{\partial\phi\,\partial\phi}S_{\mathrm{int}}[\phi,\overline{\phi}] & \frac{\partial^2}{\partial\phi\,\partial\overline{\phi}}S_{\mathrm{int}}[\phi,\overline{\phi}] \\ \frac{\partial^2}{\partial\overline{\phi}\,\partial\phi}S_{\mathrm{int}}[\phi,\overline{\phi}] & \frac{\partial^2}{\partial\overline{\phi}\,\partial\overline{\phi}}S_{\mathrm{int}}[\phi,\overline{\phi}] \end{pmatrix} \\ &= \begin{pmatrix} x\mathscr{G}_0\cdot\frac{\partial^2}{\partial\overline{\phi}\,\partial\phi}S_{\mathrm{int}}[\phi,\overline{\phi}] & x\mathscr{G}_0\cdot\frac{\partial^2}{\partial\overline{\phi}\,\partial\overline{\phi}}S_{\mathrm{int}}[\phi,\overline{\phi}] \\ -x\mathscr{G}_0^{\mathrm{T}}\cdot\frac{\partial^2}{\partial\phi\,\partial\phi}S_{\mathrm{int}}[\phi,\overline{\phi}] & -x\mathscr{G}_0^{\mathrm{T}}\cdot\frac{\partial^2}{\partial\phi\,\partial\overline{\phi}}S_{\mathrm{int}}[\phi,\overline{\phi}] \end{pmatrix}, \end{aligned}$$

where the formal products are to be evaluated by insertion of corresponding "unities".

Because of the symmetry of the statistical derivatives, one easily concludes that

$$\frac{\partial^2}{\partial\phi\,\partial\overline{\phi}} S_{\text{int}}[\phi,\overline{\phi}] = x \left(\frac{\partial^2}{\partial\overline{\phi}\,\partial\phi} S_{\text{int}}[\phi,\overline{\phi}] \right)^{\mathrm{T}}, \qquad \text{and} \qquad B^{\mathrm{T}} A^{\mathrm{T}} = (AB)^{\mathrm{T}}. \tag{34.51}$$

Due to the cyclicity of the trace we arrive at the first term in eq. (16.79).

Second summand. We write

$$\begin{aligned}
\widehat{\mathscr{G}_0}\widehat{V}\,\widehat{\mathscr{G}_0}\widehat{V} &= \begin{pmatrix} \mathscr{G}_0 \cdot \frac{\partial^2}{\partial\overline{\phi}\,\partial\phi} S_{\text{int}}[\phi,\overline{\phi}] & \mathscr{G}_0 \cdot \frac{\partial^2}{\partial\overline{\phi}\,\partial\overline{\phi}} S_{\text{int}}[\phi,\overline{\phi}] \\ -\mathscr{G}_0^{\mathrm{T}} \cdot \frac{\partial^2}{\partial\phi\,\partial\phi} S_{\text{int}}[\phi,\overline{\phi}] & -\mathscr{G}_0^{\mathrm{T}} \cdot \frac{\partial^2}{\partial\phi\,\partial\overline{\phi}} S_{\text{int}}[\phi,\overline{\phi}] \end{pmatrix} \cdot \begin{pmatrix} \mathscr{G}_0 \cdot \frac{\partial^2}{\partial\overline{\phi}\partial\phi} S_{\text{int}}[\phi,\overline{\phi}] & \mathscr{G}_0 \cdot \frac{\partial^2}{\partial\overline{\phi}\,\partial\overline{\phi}} S_{\text{int}}[\phi,\overline{\phi}] \\ -\mathscr{G}_0^{\mathrm{T}} \cdot \frac{\partial^2}{\partial\phi\,\partial\phi} S_{\text{int}}[\phi,\overline{\phi}] & -\mathscr{G}_0^{\mathrm{T}} \cdot \frac{\delta^2}{\partial\phi\,\partial\overline{\phi}} S_{\text{int}}[\phi,\overline{\phi}] \end{pmatrix} \\
&\equiv \begin{pmatrix} A+B & \cdots \\ \cdots & C+D \end{pmatrix},
\end{aligned}$$

(the secondary diagonals are irrelevant if one takes the trace and only provide corrections on higher orders of perturbation theory) with

$$\begin{aligned}
A &= \mathscr{G}_0 \cdot \frac{\partial^2}{\partial\overline{\phi}\,\partial\phi} S_{\text{int}}[\phi,\overline{\phi}] \cdot \mathscr{G}_0 \cdot \frac{\partial^2}{\partial\overline{\phi}\,\partial\phi} S_{\text{int}}[\phi,\overline{\phi}], \\
B &= -\mathscr{G}_0 \cdot \frac{\partial^2}{\partial\overline{\phi}\,\partial\overline{\phi}} S_{\text{int}}[\phi,\overline{\phi}] \cdot \mathscr{G}_0^{\mathrm{T}} \cdot \frac{\partial^2}{\partial\phi\,\partial\phi} S_{\text{int}}[\phi,\overline{\phi}], \\
C &= -\mathscr{G}_0^{\mathrm{T}} \cdot \frac{\partial^2}{\partial\phi\,\partial\phi} S_{\text{int}}[\phi,\overline{\phi}] \cdot \mathscr{G}_0 \cdot \frac{\partial^2}{\partial\overline{\phi}\,\partial\overline{\phi}} S_{\text{int}}[\phi,\overline{\phi}], \\
D &= \mathscr{G}_0^{\mathrm{T}} \cdot \frac{\partial^2}{\partial\phi\,\partial\overline{\phi}} S_{\text{int}}[\phi,\overline{\phi}] \cdot \mathscr{G}_0^{\mathrm{T}} \cdot \frac{\partial^2}{\partial\phi\,\partial\overline{\phi}} S_{\text{int}}[\phi,\overline{\phi}].
\end{aligned}$$

Now, one has $\mathrm{Tr}\, B = \mathrm{Tr}\, C$. Due to the cyclicity of the trace and $\mathrm{Tr}\, A = \mathrm{Tr}\, D$ because of eq. (34.51). Eq. (16.79) is now proven.

Proof 34.16 of Lemma 17.5 We complete the square around $\Delta_0 \equiv Vj$. Using $V^\dagger = V$ we have

$$V^{-1}\Delta_0 = j, \qquad \Delta_0^\dagger = j^\dagger V^\dagger = j^\dagger V, \qquad \Delta_0^\dagger V^{-1} = j^\dagger, \qquad \Delta_0^\dagger V^{-1}\Delta_0 = j^\dagger V j.$$

Expanding the shifted quadratic form and inserting these four relations,

$$\begin{aligned}(\Delta-\Delta_0)^\dagger V^{-1}(\Delta-\Delta_0) &= \Delta^\dagger V^{-1}\Delta - \Delta^\dagger V^{-1}\Delta_0 - \Delta_0^\dagger V^{-1}\Delta + \Delta_0^\dagger V^{-1}\Delta_0 \\ &= \Delta^\dagger V^{-1}\Delta - \Delta^\dagger j - j^\dagger\Delta + j^\dagger V j.\end{aligned}$$

Solving for the exponent of the integrand,

$$-\Delta^\dagger V^{-1}\Delta + \Delta^\dagger j + j^\dagger\Delta = -(\Delta-\Delta_0)^\dagger V^{-1}(\Delta-\Delta_0) + j^\dagger V j.$$

The factor $\exp(j^\dagger V j)$ does not depend on Δ and can be pulled out of the integral. In the remaining integral we substitute $\Delta = \Delta' + \Delta_0$. This is a translation of $\mathbb{R}^{2N}$ by the fixed vector $(\operatorname{Re}\Delta_0, \operatorname{Im}\Delta_0)$, under which the Lebesgue measure is invariant. Hence

$$\int \mathrm{d}\mu_V(\Delta,\overline{\Delta})\, \exp\left(\Delta^\dagger j + j^\dagger\Delta\right) = \exp\left(j^\dagger V j\right) \int \mathrm{d}\mu_V(\Delta',\overline{\Delta}') = \exp\left(j^\dagger V j\right),$$

where the last step is Lemma 17.4.

Proof 34.17 of Lemma 17.7 We use analyticity:

(a) G is entire on $\mathbb{C}^{2N}$. Let $\lambda_{\min} > 0$ be the smallest eigenvalue of V^{-1}, so $\Delta^\dagger V^{-1}\Delta \geq \lambda_{\min}|\Delta|^2$. By Cauchy–Schwarz, $\left|\Delta^\dagger j + K^\mathsf{T}\Delta\right| \leq |\Delta|\,(|j| + |K|)$. Therefore, for all $|j|, |K| \leq R$,

$$\left| e^{-\Delta^\dagger V^{-1}\Delta} e^{\Delta^\dagger j + K^\mathsf{T}\Delta} \right| \leq e^{-\lambda_{\min}|\Delta|^2 + 2R|\Delta|},$$

which is integrable over $\mathbb{R}^{2N}$ and independent of (j, K). The integrand is holomorphic in each j_a and K_a. By dominated convergence G is continuous, and by Fubini and Morera it is holomorphic in each variable separately; hence (Osgood) G is holomorphic on all of $\mathbb{C}^{2N}$. The same domination, with an extra polynomial factor in $|\Delta|$, justifies differentiating under the integral sign arbitrarily often. Clearly E is entire as well.

(b) $G = E$ on a real slice. Introduce new complex coordinates $(z, w) \in \mathbb{C}^{2N}$ through the invertible linear map

$$j = z + \mathrm{i}w, \qquad K = z - \mathrm{i}w, \qquad \Leftrightarrow \qquad z = \tfrac{1}{2}(j+K), \qquad w = \tfrac{1}{2\mathrm{i}}(j-K),$$

and set $H(z,w) \equiv G(z+\mathrm{i}w, z-\mathrm{i}w) - E(z+\mathrm{i}w, z-\mathrm{i}w)$, an entire function. If $z, w \in \mathbb{R}^N$, then $K = \overline{j}$, so $K^\mathsf{T} = j^\dagger$ and (17.2) gives $H(z,w) = 0$. Thus H vanishes on $\mathbb{R}^{2N} \subset \mathbb{C}^{2N}$.

(c) $H \equiv 0$. For a holomorphic function, the complex partial derivative $\partial/\partial z_a$ at a real point coincides with the real partial derivative in the direction $\operatorname{Re} z_a$, and similarly for w_a. Since H vanishes identically on $\mathbb{R}^{2N}$, all its real partial derivatives vanish there, in particular at the origin. Hence every Taylor coefficient of H at 0 vanishes. An entire function equals its Taylor series everywhere, so $H \equiv 0$, i.e. $G = E$ on all of $\mathbb{C}^{2N}$.

Proof 34.18 of Lemma 17.8 Since $\Delta^\dagger j + K^\mathsf{T}\Delta = \sum_a \left(\overline{\Delta}_a j_a + K_a \Delta_a\right)$, we have

$$\partial_j^\alpha \partial_K^\beta \exp\left(\Delta^\dagger j + K^\mathsf{T}\Delta\right) = \overline{\Delta}^\alpha \Delta^\beta \exp\left(\Delta^\dagger j + K^\mathsf{T}\Delta\right).$$

Differentiating G under the integral sign (allowed by part (a) of the proof of Lemma 17.7) and setting $j = K = 0$ gives $\partial_j^\alpha \partial_K^\beta G(0,0) = \int \mathrm{d}\mu_V\, \overline{\Delta}^\alpha \Delta^\beta$. On the other hand, the Taylor coefficients of a power series are $c_{\alpha\beta} = \partial_j^\alpha \partial_K^\beta E(0,0)/(\alpha!\beta!)$. Since $G = E$ by (17.4), the two derivatives coincide.

Proof 34.19 of Lemma 17.9 Even elements commute with each other and with complex numbers, so all manipulations of commuting variables are allowed. If the algebra has M generators, any product of more than $M/2$ bodiless even elements vanishes (each contains at least two generators). Hence every exponential series below terminates and is a finite sum.

Left side. The terms $\overline{\Delta}_a j_a$ and $K_a \Delta_a$ commute, so the exponential of their sum is the product of their exponentials. Expanding each factor,

$$\exp\left(\Delta^\dagger j + K^\mathsf{T}\Delta\right) = \prod_{a=1}^{N} \left(\sum_{k\geq 0} \frac{\overline{\Delta}_a^k j_a^k}{k!} \right) \left(\sum_{l\geq 0} \frac{K_a^l \Delta_a^l}{l!} \right) = \sum_{\alpha,\beta} \frac{\overline{\Delta}^\alpha \Delta^\beta}{\alpha!\,\beta!}\, j^\alpha K^\beta,$$

a finite sum. Each term is a complex polynomial in $(\Delta, \overline{\Delta})$ times a fixed Grassmann element, so the integral acts term by term, and by (17.5)

$$\int \mathrm{d}\mu_V(\Delta,\overline{\Delta}) \exp\left(\Delta^\dagger j + K^\mathsf{T}\Delta\right) = \sum_{\alpha,\beta} \frac{\alpha!\,\beta!\, c_{\alpha\beta}}{\alpha!\,\beta!}\, j^\alpha K^\beta = \sum_{\alpha,\beta} c_{\alpha\beta}\, j^\alpha K^\beta.$$

Right side. $\exp(K^\mathsf{T} V j) = \sum_n (K^\mathsf{T} V j)^n/n!$. Multiplying out the powers of $K^\mathsf{T} V j = \sum_{a,b} K_a V_{ab} j_b$ only uses commutativity and distributivity, i.e. exactly the operations that produce the complex power series of Lemma 17.8. By uniqueness of power-series coefficients the result is $\sum_{\alpha,\beta} c_{\alpha\beta} j^\alpha K^\beta$, which equals the left side.

Proof 34.20 of Theorem 17.10 Both lines are Lemma 17.9 with a particular choice of the even sources j, K.

First line. Choose $j = \mathrm{i}P$ and $K = \mathrm{i}\overline{Q}$, i.e. $K^\mathsf{T} = \mathrm{i}\overline{\mathrm{Q}}^\mathsf{T}$. Then

$$\Delta^\dagger j + K^\mathsf{T}\Delta = \mathrm{i}\,\Delta^\dagger P + \mathrm{i}\,\overline{\mathrm{Q}}^\mathsf{T}\Delta = \mathrm{i}\left(\Delta^\dagger P + \overline{\mathrm{Q}}^\mathsf{T}\Delta\right), \qquad K^\mathsf{T} V j = \mathrm{i}\cdot \mathrm{i}\,\overline{\mathrm{Q}}^\mathsf{T} V P = -\overline{\mathrm{Q}}^\mathsf{T} V P.$$

Second line. Choose $j = P$ and $K = \overline{Q}$, i.e. $K^\mathsf{T} = \overline{\mathrm{Q}}^\mathsf{T}$. Then $\Delta^\dagger j + K^\mathsf{T}\Delta = \Delta^\dagger P + \overline{\mathrm{Q}}^\mathsf{T}\Delta$ and $K^\mathsf{T} V j = +\overline{\mathrm{Q}}^\mathsf{T} V P$.

Inserting either choice into Lemma 17.9 gives the corresponding line of (17.6).

Proof 34.21 of Lemma 17.12 We simply complete the square:

$$-\frac{1}{2}\varphi^\mathsf{T} V^{-1}\varphi + j^\mathsf{T}\varphi = -\frac{1}{2}(\varphi - Vj)^\mathsf{T} V^{-1}(\varphi - Vj) + \frac{1}{2} j^\mathsf{T} V j. \tag{34.52}$$

Translation invariance of the Lebesgue integral removes the shift Vj, and the remaining normalized Gaussian integral equals one.

Proof 34.22 of Theorem 17.13 Both lines are the Gaussian identity (17.8) with matrix V and a particular choice of the source j.

First line. Choose $j = -\mathrm{i}\rho$. Since $(-\mathrm{i})^2 = -1$, one obtains

$$\int \mathrm{d}\mu_V(\varphi) \exp(-\mathrm{i}\rho^{\mathsf{T}}\varphi) = \exp\left(-\frac{1}{2}\rho^{\mathsf{T}} V \rho\right).$$

Second line. Choose $j = \rho$. Then (17.8) directly gives $\int \mathrm{d}\mu_V(\varphi) \exp(\rho^{\mathsf{T}}\varphi) = \exp\left(+\frac{1}{2}\rho^{\mathsf{T}} V \rho\right)$.

Rewriting the normalized measure $\mathrm{d}\mu_V$ in terms of $\mathrm{d}^N\varphi$ gives exactly (17.9).

Proof 34.23 of Lemma **??** By definition, $S_{\text{direct}} = \frac{1}{2}\sum_{a,b,c,d} \rho_{ab} V_{ab;cd} \rho_{cd}$. The first ρ carries the row labels (a, b) of V, and the second ρ carries the column labels (c, d) of V, in the same order. With $I = (a, b)$ and $J = (c, d)$, this is literally $\frac{1}{2}\sum_{I,J} \rho_I V_{IJ} \rho_J$. So, in the direct channel, the vector is ρ and the matrix is V.

Proof 34.24 of Lemma **??** Both sides are the sum of the same D^2 numbers, only listed in a different order. For $D = 2$:

$$\sum_{c,d} f(c, d) = f(1, 1) + f(1, 2) + f(2, 1) + f(2, 2),$$
$$\sum_{c,d} f(d, c) = f(1, 1) + f(2, 1) + f(1, 2) + f(2, 2).$$

The two lines contain the same four terms. Since the terms are even Grassmann elements in our application (see the proof of Lemma **??**), their order does not matter.

Proof 34.25 of Lemma **??** We go in three tiny steps.

1. Fix a and b, and apply (**??**) to the function $f(c, d) \equiv \rho_{ab} V_{ab;cd} \rho_{dc}$. Then $f(d, c) = \rho_{ab} V_{ab;dc} \rho_{cd}$, and hence

$$\sum_{c,d} \rho_{ab}\, V_{ab;cd}\, \rho_{dc} = \sum_{c,d} \rho_{ab}\, V_{ab;dc}\, \rho_{cd}.$$

2. Now the second ρ has its labels in the natural order (c, d). The price is that V now carries the swapped labels $V_{ab;dc}$. By definition (**??**), this is $K^{\mathrm{x}}_{ab;cd}$:

$$\sum_{c,d} \rho_{ab}\, V_{ab;dc}\, \rho_{cd} = \sum_{c,d} \rho_{ab}\, K^{\mathrm{x}}_{ab;cd}\, \rho_{cd}.$$

3. Sum over a, b, multiply by $\frac{1}{2}$, and write $I = (a, b)$, $J = (c, d)$. This gives $S_{\text{exchange}} = \frac{1}{2}\sum_{I,J} \rho_I K^{\mathrm{x}}_{IJ} \rho_J$, exactly as in Lemma **??**, but with K^{x} in place of V.

Proof 34.26 of Lemma **??**

1. The entries of ρ commute. Each $\rho_I = \overline{\psi}_a \psi_b$ contains two Grassmann generators. Moving $\rho_J = \overline{\psi}_c \psi_d$ past ρ_I means moving two generators past two generators, i.e. $2 \cdot 2 = 4$ swaps, each giving a factor -1. In total $(-1)^4 = +1$, so $\rho_I \rho_J = \rho_J \rho_I$.
2. Therefore
$$\rho^{\mathsf{T}} K^{\mathsf{T}} \rho = \sum_{I,J} \rho_I \, K_{JI} \, \rho_J = \sum_{I,J} \rho_J \, K_{JI} \, \rho_I = \sum_{I,J} \rho_I \, K_{IJ} \, \rho_J = \rho^{\mathsf{T}} K \rho,$$
where we used $\rho_I \rho_J = \rho_J \rho_I$ in the second step and renamed $I \leftrightarrow J$ in the third step.
3. Averaging $\rho^{\mathsf{T}} K \rho$ and $\rho^{\mathsf{T}} K^{\mathsf{T}} \rho$ gives $\rho^{\mathsf{T}} K_{\mathrm{s}} \rho$.

Proof 34.27 of Lemma **??** Combine Lemmas **??**, **??** and **??**. For the components, use $(K^{\mathsf{T}})_{ab;cd} = K_{cd;ab}$, so $(K^{\mathrm{x}})^{\mathsf{T}}_{ab;cd} = K^{\mathrm{x}}_{cd;ab} = V_{cd;ba}$.

Proof 34.28 of Theorem **??**

1. By (**??**), $S_X = \frac{1}{2} \rho^{\mathsf{T}} K^X_{\mathrm{s}} \rho$.
2. This is exactly the left-hand side of the first line of the master identity (17.9), with the matrix V there replaced by K^X_{s}. The master identity requires a real, symmetric, positive definite matrix: K^X_{s} is real and symmetric by construction and positive definite by assumption.
3. The master identity requires a vector of commuting entries. The entries ρ_I commute, as used in the proof of Lemma **??**. (The master identity was proven for $\rho \in \mathbb{C}^N$. Both sides are power series in ρ whose coefficients are Gaussian moments, so the identity holds coefficient by coefficient and therefore also for commuting even Grassmann elements ρ_I, where the series terminate.)
4. Reading off the right-hand side of the first line of (17.9) with $V \to K^X_{\mathrm{s}}$ gives (**??**).

Proof 34.29 of Corollary **??**

1. In (**??**), replace the names $c \to d$ and $d \to c$. This gives $\rho_{ab}\rho_{dc} = -\rho_{ac}\rho_{db}$, which is the middle equality.
2. In $-\frac{1}{2} \sum_{a,b,c,d} \rho_{ac} V_{ab;cd} \rho_{db}$, rename the summation labels $b \to d$, $c \to b$, $d \to c$ (and keep a). This gives $-\frac{1}{2} \sum_{a,b,c,d} \rho_{ab} V_{ad;bc} \rho_{cd} = \frac{1}{2} \rho^{\mathsf{T}} \widetilde{K}^{\mathrm{x}} \rho$.
3. Symmetrize as in Lemma **??**.

Proof 34.30 of Lemma **??** Choose the matrix-unit basis E_{ij} as a temporary basis. Its dual basis is E_{ji} and

$$\sum_{i,j} (E_{ij})_{mn} (E_{ji})_{pq} = \sum_{i,j} \delta_{mi} \delta_{nj} \delta_{pj} \delta_{qi} = \delta_{mq} \delta_{np}.$$

The relation is basis-independent because changing the matrix basis and changing the dual basis by the inverse transformation leaves the contraction unchanged.

Proof 34.31 of Theorem **??** Expand the four-index coefficient in the crossed basis using completeness:

$$M_{ab} N_{cd} = \sum_{A,B} C_{AB} (\Gamma^A)_{ad} (\Gamma^B)_{cb}. \tag{34.53}$$

Contract both sides with $(\Gamma_A)_{da}(\Gamma_B)_{bc}$ and sum all one-particle labels. The coefficient is

$$C_{AB} = (\Gamma_A)_{da} M_{ab} (\Gamma_B)_{bc} N_{cd} = \operatorname{tr}(\Gamma_A M \Gamma_B N).$$

Multiplying (34.53) by $\overline{\psi}_a \psi_b \overline{\psi}_c \psi_d$ and using the elementary reordering identity (**??**) produces one minus sign and yields (**??**).

Proof 34.32 of Corollary **??** Equation (**??**) is the coefficient formula in the proof of the Fierz identity (**??**). The permutation interchanges the two crossed labels twice when it is applied twice, so it returns $T_{ab;cd}$. This proves (**??**) without choosing a basis.

Proof 34.33 of Theorem **??** Use the orthonormal basis $\Gamma^0 = \sigma^0/\sqrt{2}$ and $\Gamma^i = \sigma^i/\sqrt{2}$, for which $\operatorname{tr}(\Gamma^A \Gamma^B) = \delta^{AB}$. The general completeness relation (**??**) gives the first identity. Multiplying that identity by two and solving for the Pauli term gives the second one.

Proof 34.34 of Corollary **??** Apply the Fierz identity (**??**) with $M = N = \sigma^0$ and the orthonormal Pauli basis. The trace coefficient is δ_{AB}, while $B_{\Gamma^0} = n/\sqrt{2}$ and $B_{\Gamma^i} = s^i/\sqrt{2}$. Thus

$$n^2 = -\left[\left(\frac{n}{\sqrt{2}}\right)^2 + \sum_i \left(\frac{s^i}{\sqrt{2}}\right)^2\right],$$

which is (**??**).

Proof 34.35 of Theorem **??** Put $q_\uparrow = \overline{\psi}_\uparrow \psi_\uparrow$ and $q_\downarrow = \overline{\psi}_\downarrow \psi_\downarrow$. Since $q_\uparrow^2 = q_\downarrow^2 = 0$ and the q's are even,

$$n^2 = (q_\uparrow + q_\downarrow)^2 = 2 q_\uparrow q_\downarrow = 2Q.$$

The spin-density identity gives $s^i s^i = -3n^2 = -6Q$. Finally,

$$\overline{P} P = \overline{\psi}_\uparrow \overline{\psi}_\downarrow \psi_\downarrow \psi_\uparrow = Q.$$

Equation (**??**) is an arbitrary linear combination of the first two equalities.

Proof 34.36 of Theorem **??** The Grassmann relations imply $\psi^2 = 0$ and $\overline{\psi}^2 = 0$. Hence the displayed monomial contains two identical generators of each type and vanishes. A nonzero local quartic interaction requires at least two distinguishable internal states, or a nonlocal label such as two different orbitals or sites.

Proof 34.37 of Theorem **??** Use the matrix basis $\Gamma^0 = \mathbf{1}/\sqrt{N}$ and $\Gamma^a = \sqrt{2} T^a$. It is orthonormal under the trace pairing, so its completeness relation is (**??**). The general Fierz identity with $M = N = \mathbf{1}$ gives

$$n^2 = -\left[\left(\frac{n}{\sqrt{N}}\right)^2 + 2 J^a J^a\right],$$

which is (**??**) after solving for $J^a J^a$.

Proof 34.38 of Theorem **??** Decompose an arbitrary matrix C into symmetric and antisymmetric parts. The symmetric part multiplies $\psi_a\psi_b = -\psi_b\psi_a$ and therefore vanishes. The second statement follows because every 2×2 antisymmetric matrix is proportional to ε.

Proof 34.39 of Theorem **??** Use $Q = n^2/2$ from (**??**) and apply the HST identity (17.9) with $N = 1$, $V = U$, and $\rho = n$.

Proof 34.40 of Theorem **??** Equation (**??**) gives $-UQ = +Us^i s^i/6$. The ordinary three-dimensional Gaussian identity

$$\left(\frac{a}{\pi}\right)^{3/2}\int \mathrm{d}^3\boldsymbol{\phi}\,\exp(-a\boldsymbol{\phi}^2+\boldsymbol{\phi}\cdot\boldsymbol{s}) = \exp\left(\frac{\boldsymbol{s}^2}{4a}\right)$$

with $a = 3/(2U)$ produces (**??**).

Proof 34.41 of Theorem **??** Apply the complex HST identity (17.6) with one complex composite. For the repulsive sign use $V = U$ and the first line (imaginary coupling). For the attractive sign use $V = g$ and the second line (real coupling). The normalization $\det(V^{-1})/\pi = 1/(\pi U)$, respectively $1/(\pi g)$, follows from $\int \mathrm{d}^2\Delta\, e^{-|\Delta|^2/U} = \pi U$.

Proof 34.42 of Theorem **??** The first equation is the direct substitution of the real HST identity. The finite-dimensional Berezin Gaussian identity is

$$\int \mathscr{D}(\overline{\psi},\psi)\,\exp(-\overline{\psi}M\psi) = \det M.$$

Apply it with $M = K + \mathrm{i}\varphi_A\Gamma^A$. The determinant is exact and contains all fermionic fluctuations around every auxiliary-field configuration.

Proof 34.43 of Corollary **??** Use $\delta \operatorname{Tr}\log M = \operatorname{Tr}(M^{-1}\delta M)$ and $\delta M = \mathrm{i}\,\delta\varphi_A\Gamma^A$. Differentiation of S_{eff} gives (**??**). The equation is an approximation only when one declares the integral over φ to be dominated by this saddle.

Proof 34.44 of Theorem **??** Integrate the total derivative

$$0 = \int \mathscr{D}\varphi\,\frac{\partial}{\partial\varphi_A}\exp\left[-\frac{1}{2}\varphi V^{-1}\varphi - \mathrm{i}\varphi\rho\right].$$

The derivative gives $-(V^{-1})_{AB}\varphi_B - \mathrm{i}\rho_A$. Taking the normalized expectation value and multiplying by $-V$ proves (**??**).

Proof 34.45 of Theorem **??** Substitute (**??**). Since $V'^{-1} = RVR^{\mathsf{T}}$, the three equalities follow by cancellation of $R^{-1}R$ and $R^{\mathsf{T}}R^{-\mathsf{T}}$. The Jacobian of a finite-dimensional linear field transformation is a constant and can be absorbed into the Gaussian normalization.

Proof 34.46 of Lemma **??** A quadratic form counts the pair (I,J) and (J,I) twice, hence the factor $1/2$. An unrestricted antisymmetric pair sum counts (a,b) and (b,a) twice on each side, hence $(2!)^{-2} = 1/4$. Passing from

one notation to the other changes the number of explicit permutations but not the polynomial. Omitting one of these factors doubles the interaction and changes the HST covariance by the same factor.

Proof 34.47 of Theorem **??** Items 1 and 3 are finite-dimensional tensor identities, proved by antisymmetrization and completeness. Item 4 is the identity (17.9) or (17.6). Item 5 is the Berezin Gaussian identity. Since each item is an equality, their composition is an equality. Replacing an integral by a saddle-point value or truncating its determinant expansion is not an identity and must therefore be stated as an additional approximation.

This entire section of proofs needs to be revised, cause we adjusted the prefactor convention for the functional derivati

Proof 34.48 of Lemma 18.2.

For the first equation we compute

$$\begin{aligned} W[j,\bar{j}] &= -\log \int \mathscr{D}(\psi,\overline{\psi}) \exp\left(-S[\psi,\overline{\psi}] + \sum(\bar{j}\psi + \overline{\psi} j)\right) \\ &= -\log \int \mathscr{D}(M\cdot\psi, \overline{M}\cdot\overline{\psi}) \exp\left(-S[M\cdot\psi, \overline{M}\cdot\overline{\psi}] + \sum_x \bar{j}(x)\,(M\cdot\psi)(x) + (\overline{M}\cdot\overline{\psi})(x)\, j(x)\right) \\ &= \dots \end{aligned}$$

using now

$$\oint_x \bar{j}(x)\,(M\cdot\psi)(x) = \sum_x \sum_y \bar{j}(x)\, M(x,y)\,\psi(y) = \sum_y \sum_x M^{\mathrm{T}}(y,x)\bar{j}(x)\,\psi(y) = \sum_y (M^{\mathrm{T}}\cdot\bar{j})(y)\,\psi(y)$$

and analogously one has

$$\sum_x (\overline{M}\cdot\overline{\psi})(x)\, j(x) = \sum_y \overline{\psi}(y)\,(\overline{M}^{\mathrm{T}}\cdot j)(y).$$

Then, it follows (together with Definition 18.1)

$$\begin{aligned} \dots &= -\log \int \mathscr{D}(\psi,\overline{\psi}) \exp\left(-S[\psi,\overline{\psi}] + \sum_y (M^{\mathrm{T}}\cdot\bar{j})(y)\,\psi(y) + \overline{\psi}(y)\,(\overline{M}^{\mathrm{T}}\cdot j)(y)\right) \\ &= W[\overline{M}^{\mathrm{T}}\cdot j, M^{\mathrm{T}}\cdot\bar{j}]. \end{aligned}$$

For the second equation one has

$$\begin{aligned} \phi[\bullet, \overline{M}^{\mathrm{T}}\cdot j, M^{\mathrm{T}}\cdot\bar{j}] &= -\frac{\vec{\partial}}{\partial(M^{\mathrm{T}}\cdot\bar{j})(\bullet)} W[\overline{M}^{\mathrm{T}}\cdot j, M^{\mathrm{T}}\cdot\bar{j}] \\ &= -\frac{\vec{\partial}}{\partial(M^{\mathrm{T}}\cdot\bar{j})(\bullet)} W[j,\bar{j}] \\ &= \dots \end{aligned}$$

Now one calculates

$$\bar{j}(x) = (M^{-\mathrm{T}}\cdot M^{\mathrm{T}}\cdot\bar{j})(x) = \sum_y M^{-\mathrm{T}}(x,y)\,(M^{\mathrm{T}}\cdot\bar{j})(y)$$

and therefore

$$\frac{\vec{\partial}}{\partial(M^{\mathrm{T}}\cdot\bar{j})(\bullet)} = \sum_x \left(\frac{\vec{\partial}}{\partial(M^{\mathrm{T}}\cdot\bar{j})(\bullet)}\bar{j}(x)\right)\frac{\vec{\partial}}{\partial\bar{j}(x)} = \sum_x M^{-\mathrm{T}}(x,\bullet)\frac{\vec{\partial}}{\partial\bar{j}(x)} = \sum_x M^{-1}(\bullet,x)\frac{\vec{\partial}}{\partial\bar{j}(x)}.$$

It then follows with Notation 16.31

$$\ldots = -\sum_x M^{-1}(\bullet, x)\left(\frac{\vec{\partial}}{\partial \bar{j}(x)} W[j,\bar{j}]\right) = \sum_x M^{-1}(\bullet, x)\,\phi[x, j, \bar{j}] = \left(M^{-1}\cdot\phi\right)[\bullet, j, \bar{j}],$$

Analogously, one obtains

$$\bar{\phi}[\bullet, \overline{M}^{\mathrm{T}}\cdot j, M^{\mathrm{T}}\cdot\bar{j}] = \frac{\vec{\partial}}{\partial(\overline{M}^{\mathrm{T}}\cdot j)(\bullet)} W[j,\bar{j}] = \sum_x \overline{M}^{-1}(\bullet, x)\left(\frac{\vec{\partial}}{\delta j(x)} W[j,\bar{j}]\right) = \left(\overline{M}^{-1}\cdot\bar{\phi}\right)[\bullet, j, \bar{j}].$$

Proof 34.49 of Theorem 18.3.

With Lemma 18.2 one can prove the theorem very easily:

$$\begin{aligned}\Gamma[M^{-1}\cdot\phi, \overline{M}^{-1}\cdot\bar{\phi}] &= W[\overline{M}^{\mathrm{T}}\cdot j, M^{\mathrm{T}}\cdot\bar{j}] + \sum_x (M^{\mathrm{T}}\cdot\bar{j})(x)\,(M^{-1}\cdot\phi)(x) + (\overline{M}^{-1}\cdot\bar{\phi})(x)\,(\overline{M}^{\mathrm{T}}\cdot j)(x)\\ &= W[j,\bar{j}] + \sum_x \bar{j}(x)\,\phi(x) + \bar{\phi}(x)\,j(x)\\ &= \Gamma[\phi,\bar{\phi}].\end{aligned}$$

Proof 34.50 of Theorem 20.4

TBDigitalized. (Negele, Orland p. 29, Altland p.163 for fermions, and Altland p. 159 for bosons.)

Proof 34.51 of Theorem 20.5

Proof 34.52 of Lemma 20.6

TBDigitalized, cf. Negele Orland page 30or Altland page 181 for fermions, Negele Orland page 21 or Altland p. 159 for bosons.

Proof 34.53 of Theorem 20.7

TBD.

Proof 34.54 of Theorem 20.8

- NO page 22, Altland page 160 (bosons)
- NO page 39, Altland page 181 f (fermions)

Proof 34.55 of Lemma 20.9

Follows by construction via the recipe of second quantization.

Proof 34.56 of Lemma 20.10

We obtain by direct computation ...

- Altland page 182.

Proof 34.57 of Lemma 20.11

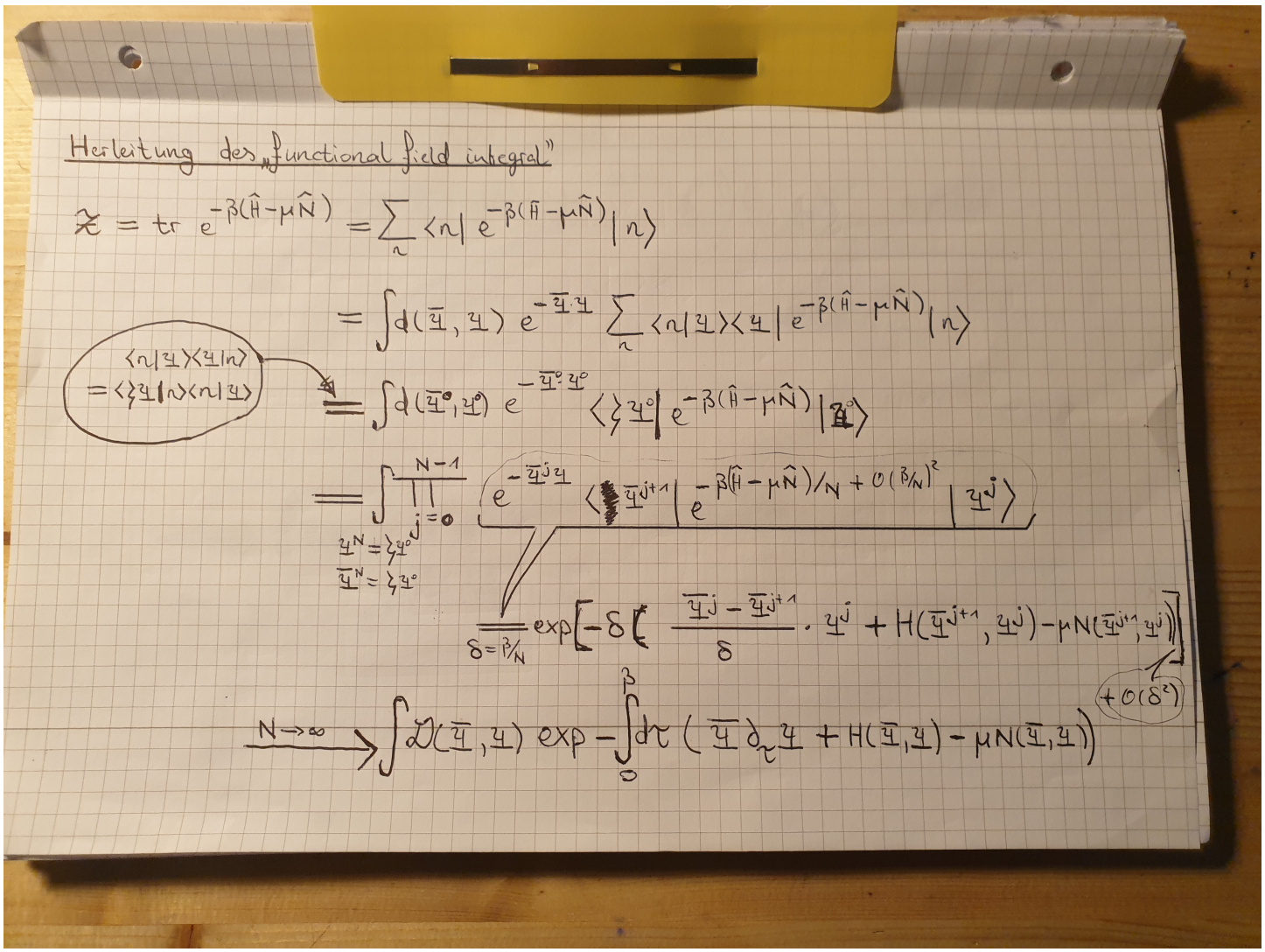
TBDIgitalized, cf. Negele Orland page 24 f.

Proof 34.58 of Lemma 20.12

By a direct computation we obtain

- TBDigitalized.

Proof 34.59 of Theorem 20.13



Proof 34.60 of Lemma 20.14

Shit... We need a finite set of Matsubara-frequencies...

We assume, without[4] loss of generality, that N (which is going to infinity) is even for bosons and it is odd for fermions. This allows us to introduce the *finite set of Matsubara-frequencies* $\Omega_{\zeta,N}$ as

$$\Omega_{\zeta,N} = \begin{cases} \left\{ 2n\pi/\hbar\beta \,\middle|\, n \in \{-N, -N+1, \dots, -1, 0, +1, \dots, N\} \right\} & \text{for bosons} \\ \left\{ (2n+1)\pi/\hbar\beta \,\middle|\, n \in \{-N, -N+1, \dots, -1, 0, +1, \dots, N\} \right\} & \text{for fermions} \end{cases} \tag{34.54}$$

Something in this direction...

We introduce (nostalgically) a discretization for the temporal component and denote the abbreviations

$$\psi(\tau) \equiv \psi(\tau^j) \equiv \psi^j = \frac{1}{\sqrt{\hbar\beta}} \sum_{\mathrm{i}\omega_n \in \mathrm{i}\Omega_\zeta} \psi(\mathrm{i}\omega_n) \mathrm{e}^{-\mathrm{i}\omega_n \hbar\beta j/N}, \qquad \overline{\psi}^j = \frac{1}{\sqrt{\hbar\beta}} \sum_{\mathrm{i}\omega_m \in \mathrm{i}\Omega_\zeta} \overline{\psi}(\mathrm{i}\omega_m) \mathrm{e}^{\mathrm{i}\omega_m \hbar\beta j/N} \tag{34.55}$$

[4] Note the entire proof remains perfectly valid for the respective other case; The notation becomes simply more tedious.

which we write equivalently, remembering that for each timestap there is an entire basis-index-set attached to the fields, as

$$\psi_\alpha^j = \frac{1}{\sqrt{\hbar\beta}} \sum_{\mathrm{i}\omega_n \in \mathrm{i}\Omega_\zeta} \psi_\alpha(\mathrm{i}\omega_n)\mathrm{e}^{-\mathrm{i}\omega_n\hbar\beta j/N}, \qquad \overline{\psi}_\alpha^j = \frac{1}{\sqrt{\hbar\beta}} \sum_{\mathrm{i}\omega_m \in \mathrm{i}\Omega_\zeta} \overline{\psi}_\alpha(\mathrm{i}\omega_m)\mathrm{e}^{\mathrm{i}\omega_m\hbar\beta j/N} \tag{34.56}$$

with $\alpha \in \mathcal{A}$. Before the substitution we have an integral measure as

$$\mathscr{D}(\overline{\psi}, \psi) = \lim_{N\to\infty} \prod_{n=1}^{N} \mathrm{d}(\overline{\psi}^n, \psi^n) = \lim_{N\to\infty} \prod_{n=1}^{N} \prod_{\alpha\in\mathcal{A}} \frac{\mathrm{d}\,\overline{\psi}_\alpha^n\, \mathrm{d}\,\psi_\alpha^n}{\pi^{(1+\zeta)/2}} \tag{34.57}$$

It obviously suffices to examine the transformation for a single $\alpha \in \mathcal{A}$.

We consider the bosonic case!

Recall the transformation-formula

$$\int_{g(\Omega)} f(x)\mathrm{d}x = \int_\Omega f(g(y))|\det J_g(y)|\mathrm{d}y \tag{34.58}$$

and now we introduce

$$x = \begin{pmatrix} \psi^1 \\ \vdots \\ \psi^N \\ \overline{\psi}^1 \\ \vdots \\ \overline{\psi}^N \end{pmatrix} \tag{34.59}$$

and

$$g(y) = \begin{pmatrix} \boldsymbol{M} & 0 \\ 0 & \overline{\boldsymbol{M}} \end{pmatrix} \begin{pmatrix} \psi_: \\ \overline{\psi}_: \end{pmatrix} = \begin{pmatrix} \psi^: \\ \overline{\psi}^: \end{pmatrix} \tag{34.60}$$

The equation $g(y) = x$ can now be rewritten as

$$\begin{pmatrix} \psi^: \\ \overline{\psi}^: \end{pmatrix} = \begin{pmatrix} f(1,1) & f(1,2) & \cdots & f(1,N) & 0 & 0 & \cdots & 0 \\ \vdots & & & \vdots & \vdots & 0 & & \vdots \\ f(N,1) & f(N,2) & \cdots & f(N,N) & 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 & f(1,1) & f(1,2) & \cdots & f(1,N) \\ \vdots & 0 & & \vdots & \vdots & & & \vdots \\ 0 & 0 & \cdots & 0 & f(N,1) & f(N,2) & \cdots & f(N,N) \end{pmatrix} \begin{pmatrix} \psi_: \\ \overline{\psi}_: \end{pmatrix} \tag{34.61}$$

with

$$f(j,n) = \frac{1}{\sqrt{\hbar\beta}}\mathrm{e}^{-\mathrm{i}\omega_n\hbar\beta j/N}. \tag{34.62}$$

Then we obtain for the transformation matrix $\boldsymbol{M}$ the identity

$$
\begin{aligned}
M_{k,:}\cdot\left(M^{\dagger}\right)_{:,l} &= \sum_{n=1}^{N} M_{k,n}\left(M^{\dagger}\right)_{n,l} \\
&= \sum_{n=1}^{N} M_{k,n}M^{*}_{l,n} \\
&= \sum_{n=1}^{N} f(k,n)f(l,n)^{*} \\
&= \frac{1}{\hbar\beta}\sum_{n=1}^{N} \mathrm{e}^{-\mathrm{i}\omega_n\hbar\beta k/N}\mathrm{e}^{+\mathrm{i}\omega_n\hbar\beta l/N} \\
&= \frac{1}{\hbar\beta}\sum_{n=1}^{N} \mathrm{e}^{-\mathrm{i}\omega_n\hbar\beta(l-k)/N} \\
&= \frac{1}{\hbar\beta}\sum_{n=1}^{N} \mathrm{e}^{-\mathrm{i}(2n+1-\theta(\zeta))(\pi/N)(l-k)} \\
&= \frac{1}{\hbar\beta}\mathrm{e}^{\mathrm{i}(1-\theta(\zeta))(\pi/N)(l-k)}\underbrace{\sum_{n=1}^{N}\mathrm{e}^{\mathrm{i}2n(\pi/N)(l-k)}}_{N\delta_{l,k}} \\
&= \frac{N}{\hbar\beta}\delta_{l,k}
\end{aligned}
\tag{34.63}
$$

Therefore, the matrix $\sqrt{\hbar\beta/N}\cdot\boldsymbol{M}$ is unitary! We therefore find

$$
|\det\begin{pmatrix}\boldsymbol{M} & 0\\ 0 & \boldsymbol{M}\end{pmatrix}| = \left(\sqrt{\frac{\hbar\beta}{N}}^{2N}\right)^{-1}\cdot|\det\text{"unitary matrix"}| = \left(\left(\frac{\hbar\beta}{N}\right)^{N}\right)^{-1} = \left(\frac{N}{\hbar\beta}\right)^{N} \tag{34.64}
$$

Further one finds for bosons

$$
\int \mathrm{d}(v^{\dagger},v)\mathrm{e}^{-v^{\dagger}Av} = \pi^{N}\left(\det A\right)^{-1} = \pi^{N}\left(\det A\right)^{-\zeta} \tag{34.65}
$$

therefore, the equation

$$
\int \mathrm{d}(\overline{\psi},\psi)\mathrm{e}^{-\overline{\psi}_n\epsilon\psi_n} = (\beta\epsilon)^{-\zeta} \tag{34.66}
$$

is being reproduced except for a diverging factor. Whereas ψ_n represents a single Grassmann-variable here, i.e.

$$
\psi_n \overset{here}{\neq} \psi_{j,n} \tag{34.67}
$$

We consider the fermionic case.

Recall the transformation-rule

$$\overline{\nu} = \left(\overline{M}\right)^{\text{inv}} \overline{\phi}, \quad \nu = M^{\text{inv}}\phi \quad \Rightarrow \quad \int \mathrm{d}(\overline{\phi},\phi) f(\overline{\phi},\phi) = \det\left(M^{\text{inv}}\overline{M}^{\text{inv}}\right) \int \mathrm{d}\left(\overline{\nu},\nu\right) f(\overline{\phi}(\overline{\nu}),\phi(\nu)) \tag{34.68}$$

Here we have

$$\overline{\psi}_{:} = \left(\overline{M}\right)^{\text{inv}} \overline{\psi}^{:}, \quad \psi_{:} = M^{\text{inv}}\psi^{:} \quad \Rightarrow \quad \int \mathrm{d}(\overline{\phi},\phi) f(\overline{\phi},\phi) = \det\left(\frac{\hbar\beta}{N}\right)^{N} \int \mathrm{d}\left(\overline{\nu},\nu\right) f(\overline{\phi}(\overline{\nu}),\phi(\nu)) \tag{34.69}$$

whereas we used

$$M^{inv} = M^{\dagger} \cdot \frac{\beta}{N} = \sqrt{\frac{\beta}{N}} \left(\sqrt{\frac{\beta}{N}}\right)^{\dagger} \quad \Rightarrow \quad \det M^{\text{inv}} = \left(\frac{\beta}{N}\right)^{N} \tag{34.70}$$

Proof 34.61 of Corollary 20.15

The discrete version of the partition-function reads

$$Z = \lim_{N\to\infty} \int_{\substack{\psi^N=\zeta\psi^0 \\ \overline{\psi}^N=\zeta\overline{\psi}^0}} \prod_{j=0}^{N} \mathrm{d}_{\zeta}(\overline{\psi}^j,\psi^j) \exp -\delta \sum_{j=0}^{N-1} -\frac{\overline{\psi}^{j+1}-\overline{\psi}^j}{\delta} \cdot \psi^j + H(\overline{\psi}^{j+1},\psi^j) - \mu N(\overline{\psi}^{j+1},\psi^j)$$

Now we examine each of the terms in the exponents individually, when we transform coordinates according to

$$\psi^j = \frac{1}{\hbar\beta} \sum_{\omega_n} \psi_{\omega_n} \mathrm{e}^{-\mathrm{i}\omega_n\tau_j}, \qquad \overline{\psi}^j = \frac{1}{\hbar\beta} \sum_{\omega_n} \overline{\psi}_{\omega_n} \mathrm{e}^{+\mathrm{i}\omega_n\tau_j} \tag{34.71}$$

for

$$n \in \left\{ -\frac{N-1}{2}, \ldots, -1, 0, +1, \ldots, \frac{N-1}{2} \right\} \tag{34.72}$$

We also notice that

$$\sum_{j=0}^{N-1} \mathrm{e}^{\mathrm{i}\tau_j(\omega_n-\omega_m)} = N\delta_{n,m} \tag{34.73}$$

The Derivative

Noticing that $1 \equiv \mathrm{e}^{\mathrm{i}\omega_n\tau_0}$ and remembering that $\delta = \hbar\beta/N$ we obtain

$$
\begin{aligned}
&\delta \sum_{j=0}^{N-1} -\frac{1}{\delta}\left(\frac{1}{\sqrt{\hbar\beta}}\sum_{\omega_n}\overline{\psi}_{\omega_n}\mathrm{e}^{\mathrm{i}\omega_n\tau_{j+1}} - \overline{\psi}_{\omega_n}\mathrm{e}^{\mathrm{i}\omega_n\tau_j}\right)\frac{1}{\sqrt{\hbar\beta}}\sum_{\omega_m}\psi_{\omega_m}\mathrm{e}^{-\mathrm{i}\omega_m\tau_j} \\
&= \delta \sum_{j=0}^{N-1} -\frac{1}{\delta\hbar\beta}\sum_{\omega_n}\overline{\psi}_{\omega_n}\left(\mathrm{e}^{\mathrm{i}\omega_n\tau_1}-1\right)\mathrm{e}^{\mathrm{i}\omega_n\tau_j}\sum_{\omega_m}\psi_{\omega_m}\mathrm{e}^{-\mathrm{i}\omega_m\tau_j} \\
&\approx \delta \sum_{j=0}^{N-1} -\frac{1}{\delta\hbar\beta}\sum_{\omega_n}\overline{\psi}_{\omega_n}\mathrm{i}\omega_n\delta\mathrm{e}^{\mathrm{i}\omega_n\tau_j}\sum_{\omega_m}\psi_{\omega_m}\mathrm{e}^{-\mathrm{i}\omega_m\tau_j} \\
&= \frac{\delta}{\hbar\beta}\sum_{\omega_n,\omega_m} -\mathrm{i}\omega_n\overline{\psi}_{\omega_n}\psi_{\omega_m}\sum_{j=0}^{N-1}\mathrm{e}^{\mathrm{i}\tau_j(\omega_n-\omega_m)} \\
&= \sum_{\omega_n} -\mathrm{i}\omega_n\overline{\psi}_{\omega_n}\psi_{\omega_n}
\end{aligned}
$$

The other Quadratic Terms

$$
\begin{aligned}
\delta\sum_{j=0}^{N-1}\overline{\psi}(\tau_{j+1})\psi(\tau_j) &= \frac{\delta}{\hbar\beta}\sum_{j=0}^{N-1}\sum_{\omega_n,\omega_m}\overline{\psi}_{\omega_n}\mathrm{e}^{\mathrm{i}\omega_n\tau_{j+1}}\psi_{\omega_m}\mathrm{e}^{-\mathrm{i}\omega_m\tau_j} \\
&= \sum_{\omega_n,\omega_m}\overline{\psi}_{\omega_n}\psi_{\omega_m}\frac{\delta}{\hbar\beta}\left(\sum_{j=0}^{N-1}\mathrm{e}^{\mathrm{i}(\omega_n-\omega_m)\tau_j}\right)\mathrm{e}^{\mathrm{i}\omega_n\tau_1} \\
&= \sum_{\omega_n}\overline{\psi}_{\omega_n}\psi_{\omega_n}\mathrm{e}^{\mathrm{i}\omega_n\delta}
\end{aligned}
$$

Proof 34.62 of Lemma 20.16 For the non-interacting case see, for example, [4] Chapter 4 or [38] Equation (2.137b), or [52] chapter 7.2 p. 139, 145, 149 or [13] p. 37, 38. For the interacting case, we refer to [38] again.

Proof 34.63 of Theorem 20.17

- Cf. Negele p. 70 following.
- Cf. Diehl QFT-1-Script 20, 21, page 98
- Cf. Coleman p. 428.

Proof 34.64 of Theorem 20.18

We compute straightforwardly

$$
\begin{aligned}
\mathscr{G}^{\ 0}_{\alpha,\alpha'}(\tau) &= -\frac{1}{\hbar}\langle\psi_\alpha(\tau)\overline{\psi}_{\alpha'}(0)\rangle \\
&= -\frac{1}{\hbar}\frac{1}{\hbar\beta}\sum_{\omega_n,\omega_m\in\Omega_\zeta}\langle\psi_\alpha(\omega_n)\overline{\psi}_{\alpha'}(\omega_m)\rangle\mathrm{e}^{-\mathrm{i}\omega_n\tau} \\
&= \dots
\end{aligned}
$$

now we use that the action is diagonal w.r.t. Matsubara-frequencies s.t. we obtain

$$\langle \psi_\alpha(\omega)\overline{\psi}_{\alpha'}(\omega_m)\rangle = \delta_{n,m}\langle \psi_\alpha(\omega_n)\overline{\psi}_{\alpha'}(\omega_n)\rangle \tag{34.74}$$

and therefore we obtain

$$\ldots = \frac{1}{\hbar\beta}\sum_{\omega_n \in \Omega_\zeta} \langle \psi_\alpha(\omega_n)\overline{\psi}_{\alpha'}(\omega_m)\rangle \mathrm{e}^{-\mathrm{i}\omega_n\tau} \equiv \frac{1}{\hbar\beta}\sum_{\omega_n \in \Omega_\zeta} \mathscr{G}_{0\,\alpha,\alpha'}(\mathrm{i}\omega_n)\mathrm{e}^{-\mathrm{i}\omega_n\tau} \tag{34.75}$$

Therefore we obtain for the non-interacting Green-function

$$\mathscr{G}_{0\,\alpha,\alpha'}(\mathrm{i}\omega_n) \equiv -\frac{1}{\hbar}\langle \psi_\alpha(\omega_n)\overline{\psi}_{\alpha'}(\omega_n)\rangle_0 = -\frac{1}{\hbar}\left(\left[-\mathrm{i}\omega_n + \frac{H-\mu}{\hbar}\right]^{\mathrm{inv}}\right)_{\alpha,\alpha'} = \frac{1}{\hbar}\left(\left[\mathrm{i}\omega_n - \frac{H-\mu}{\hbar}\right]^{\mathrm{inv}}\right)_{\alpha,\alpha'} \tag{34.76}$$

which completes the proof.

35. Appendix - Proofs for Part VI

Proof 35.1 of Lemma 23.15

The only non-trivial identity is the interaction-term. Using Lemma 20.14 and Corollary 1.12 we obtain

$$
\begin{aligned}
S_{\text{el-ph-int}}[\chi,\overline{\chi}] &= \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k},\mathbf{q}\in\mathrm{Q}\\ \tau\in(0,\hbar\beta)\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ m,n\in\{1,2,3,\dots\}\\ \sigma\in\{\downarrow,\uparrow\}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\hbar\sqrt{N_p}}\left(\phi_\nu(\tau,\mathbf{q})+\overline{\phi}_\nu(\tau,-\mathbf{q})\right)\overline{\psi}_{m\sigma}(\tau,\mathbf{k}+\mathbf{q})\psi_{n\sigma}(\tau,\mathbf{k}) \\
&= \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k},\mathbf{q}\in\mathrm{Q}\\ \tau\in(0,\hbar\beta)\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ m,n\in\{1,2,3,\dots\}\\ \sigma\in\{\downarrow,\uparrow\}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\hbar\sqrt{N_p}}\phi_\nu(\tau,\mathbf{q})\overline{\psi}_{m\sigma}(\tau,\mathbf{k}+\mathbf{q})\psi_{n\sigma}(\tau,\mathbf{k}) \\
&+ \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k},\mathbf{q}\in\mathrm{Q}\\ \tau\in(0,\hbar\beta)\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ m,n\in\{1,2,3,\dots\}\\ \sigma\in\{\downarrow,\uparrow\}}} \frac{g_{mn\nu}(\mathbf{k},-\mathbf{q})}{\hbar\sqrt{N_p}}\overline{\phi}_\nu(\tau,\mathbf{q})\overline{\psi}_{m\sigma}(\tau,\mathbf{k}-\mathbf{q})\psi_{n\sigma}(\tau,\mathbf{k}) \\
&= \frac{1}{(\hbar\beta)^{3/2}}\sum_{\substack{\omega_q\in\Omega_{+1}\\ \omega_n,\omega_k\in\mathrm{i}\Omega_{-1}}}\sum_{\substack{\mathbf{k},\mathbf{q}\in\mathrm{Q}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ m,n\in\{1,2,3,\dots\}\\ \sigma\in\{\downarrow,\uparrow\}}}\frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\hbar\sqrt{N_p}}\phi_\nu(\mathrm{i}\omega_q,\mathbf{q})\overline{\psi}_{m\sigma}(\mathrm{i}\omega_n,\mathbf{k}+\mathbf{q})\psi_{n\sigma}(\mathrm{i}\omega_k,\mathbf{k})\int_0^{\hbar\beta}\mathrm{d}\tau\,\mathrm{e}^{\mathrm{i}\tau(-\omega_q+\omega_n-\omega_k)} \\
&+ \frac{1}{(\hbar\beta)^{3/2}}\sum_{\substack{\omega_q\in\Omega_{+1}\\ \omega_n,\omega_k\in\mathrm{i}\Omega_{-1}}}\sum_{\substack{\mathbf{k},\mathbf{q}\in\mathrm{Q}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ m,n\in\{1,2,3,\dots\}\\ \sigma\in\{\downarrow,\uparrow\}}}\frac{g_{mn\nu}(\mathbf{k},-\mathbf{q})}{\hbar\sqrt{N_p}}\overline{\phi}_\nu(\mathrm{i}\omega_q,\mathbf{q})\overline{\psi}_{m\sigma}(\mathrm{i}\omega_n,\mathbf{k}-\mathbf{q})\psi_{n\sigma}(\mathrm{i}\omega_k,\mathbf{k})\int_0^{\hbar\beta}\mathrm{d}\tau\,\mathrm{e}^{\mathrm{i}\tau(+\omega_q+\omega_n-\omega_k)} \\
&= \frac{1}{\sqrt{\hbar\beta}}\sum_{\substack{\omega_q\in\Omega_{+1}\\ \omega_n,\omega_k\in\mathrm{i}\Omega_{-1}}}\sum_{\substack{\mathbf{k},\mathbf{q}\in\mathrm{Q}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ m,n\in\{1,2,3,\dots\}\\ \sigma\in\{\downarrow,\uparrow\}}}\frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\hbar\sqrt{N_p}}\phi_\nu(\mathrm{i}\omega_q,\mathbf{q})\overline{\psi}_{m\sigma}(\mathrm{i}\omega_n,\mathbf{k}+\mathbf{q})\psi_{n\sigma}(\mathrm{i}\omega_k,\mathbf{k})\,\delta_{\omega_n,\omega_k+\omega_q} \\
&+ \frac{1}{\sqrt{\hbar\beta}}\sum_{\substack{\omega_q\in\Omega_{+1}\\ \omega_n,\omega_k\in\mathrm{i}\Omega_{-1}}}\sum_{\substack{\mathbf{k},\mathbf{q}\in\mathrm{Q}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ m,n\in\{1,2,3,\dots\}\\ \sigma\in\{\downarrow,\uparrow\}}}\frac{g_{mn\nu}(\mathbf{k},-\mathbf{q})}{\hbar\sqrt{N_p}}\overline{\phi}_\nu(\mathrm{i}\omega_q,\mathbf{q})\overline{\psi}_{m\sigma}(\mathrm{i}\omega_n,\mathbf{k}-\mathbf{q})\psi_{n\sigma}(\mathrm{i}\omega_k,\mathbf{k})\,\delta_{\omega_n,\omega_k-\omega_q} \\
&= \frac{1}{\sqrt{\hbar\beta}}\sum_{\substack{k\in\mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ q\in\mathrm{i}\Omega_{+1}\times\mathrm{Q}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ m,n\in\{1,2,3,\dots\}\\ \sigma\in\{\downarrow,\uparrow\}}}\frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\hbar\sqrt{N_p}}\left(\phi_\nu(q)+\overline{\phi}_\nu(-q)\right)\overline{\psi}_{m\sigma}(q+k)\psi_{n\sigma}(k)
\end{aligned}
$$

Proof 35.2 of Lemma 23.16

By straightforward computation we obtain

$$\begin{aligned} S_{\text{el-ph-int}}[\chi,\overline{\chi}] &= \frac{1}{\sqrt{\hbar\beta}} \sum_{\substack{\omega_q \in \Omega_{+1} \\ \omega_k \in \mathrm{i}\Omega_{-1}}} \sum \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\hbar\sqrt{N_p}} \phi_\nu(\mathrm{i}\omega_q,\mathbf{q}) \overline{\psi}_{m\sigma}(\mathrm{i}\left(\omega_k+\omega_q\right),\mathbf{k}+\mathbf{q}) \psi_{n\sigma}(\mathrm{i}\omega_k,\mathbf{k}) \\ &+ \frac{1}{\sqrt{\hbar\beta}} \sum_{\substack{\omega_q \in \Omega_{+1} \\ \omega_k \in \mathrm{i}\Omega_{-1}}} \sum \frac{g_{mn\nu}(\mathbf{k},-\mathbf{q})}{\hbar\sqrt{N_p}} \overline{\phi}_\nu(\mathbf{q},\mathrm{i}\omega_q) \overline{\psi}_{m\sigma}(\mathbf{k}-\mathbf{q},\mathrm{i}\left(\omega_k-\omega_q\right)) \psi_{n\sigma}(\mathbf{k},\mathrm{i}\omega_k) \\ &= \sum_{\substack{\mathbf{q}\in\mathrm{Q} \\ \omega_q \in \Omega_{+1} \\ \nu \in \{1,\ldots,rd_{\mathbf{x}}\}}} \phi_\nu(\mathrm{i}\omega_q,\mathbf{q}) \rho_\nu(\mathrm{i}\omega_q,\mathbf{q}) \quad + \quad \overline{\phi}_\nu(\mathrm{i}\omega_q,\mathbf{q}) \rho_\nu(-\mathrm{i}\omega_q,-\mathbf{q}) \end{aligned}$$

with density-like-interaction

$$\rho_\nu(\mathrm{i}\omega_q,\mathbf{q}) = \frac{1}{\sqrt{\hbar\beta N_p}} \sum_{\substack{\mathbf{k}\in\mathrm{Q} \\ \sigma\in\{\downarrow,\uparrow\} \\ \omega_k \in \mathrm{i}\Omega_{-1} \\ n,m\in\{1,\ldots,\infty\}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\hbar} \overline{\psi}_{m\sigma}(\mathrm{i}\left(\omega_k+\omega_q\right),\mathbf{k}+\mathbf{q}) \psi_{n\sigma}(\mathrm{i}\omega_k,\mathbf{k}) \tag{35.1}$$

Proof 35.3 of Lemma 23.18

We keep in mind that

$$S_{\text{ph}}[\phi,\overline{\phi}] = \sum_{\substack{q\in\mathrm{i}\Omega_{+1}\times\mathrm{Q} \\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} \overline{\phi}_\nu(q) \left(-\frac{1}{\hbar}\mathscr{G}_{0,\nu}^{-\mathrm{B}}(q)\right) \phi_\nu(q) \tag{35.2}$$

and

$$S_{\substack{\text{el-ph-int} \\ [j_{\mathrm{B}},\bar{j}_{\mathrm{B}}]}}[\chi,\overline{\chi}] = \sum_{\substack{q\in\mathrm{i}\Omega_{+1}\times\mathrm{Q} \\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\}}} \phi_\nu(q) \left(\rho_\nu(q)-\bar{j}_\nu(q)\right) + \overline{\phi}_\nu(q) \left(\rho_\nu(-q)-j_\nu(q)\right)$$

Now we change the variables according to

$$\begin{aligned} \phi_\nu(q) &\mapsto \phi_\nu(q) + \hbar\mathscr{G}_{0,\nu}(q) \left(\rho_\nu(-q)-j_\nu(q)\right) ng \\ \overline{\phi}_\nu(q) &\mapsto \overline{\phi}_\nu(q) + \hbar\mathscr{G}_{0,\nu}(q) \left(\rho_\nu(q)-\bar{j}_\nu(q)\right) \end{aligned}$$

This yields

$$\begin{aligned}\left(S_{\text{ph}}+S_{\text{el-ph}}\right)[\overline{\chi},\chi] = &\sum_{\substack{q\in \mathrm{i}\Omega_{+1}\times \mathrm{Q}\\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\}}}\left[\overline{\phi}_{\nu}(q)+\hbar\mathscr{G}_{0\ \nu}^{\mathrm{B}}(q)\left(\rho_{\nu}(q)-\overline{j}_{\mathrm{B}\ \nu}(q)\right)\right]\left(-\frac{1}{\hbar}\mathscr{G}_{0\ \nu}^{-\mathrm{B}}(q)\right)\left[\phi_{\nu}(q)+\hbar\mathscr{G}_{0\ \nu}^{\mathrm{B}}(q)\left(\rho_{\nu}(-q)-j_{\mathrm{B}\ \nu}(q)\right)\right]\\ &+\sum_{\substack{q\in \mathrm{i}\Omega_{+1}\times \mathrm{Q}\\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\}}}\left[\phi_{\nu}(q)+\hbar\mathscr{G}_{0\ \nu}^{\mathrm{B}}(q)\left(\rho_{\nu}(-q)-j_{\mathrm{B}\ \nu}(q)\right)\right]\left(\rho_{\nu}(q)-\overline{j}_{\mathrm{B}\ \nu}(q)\right)\\ &+\sum_{\substack{q\in \mathrm{i}\Omega_{+1}\times \mathrm{Q}\\ nu\in\{1,\ldots,rd_{\mathbf{x}}\}}}\left[\overline{\phi}_{\nu}(q)+\hbar\mathscr{G}_{0\ \nu}^{\mathrm{B}}(q)\left(\rho_{\nu}(q)-\overline{j}_{\mathrm{B}\ \nu}(q)\right)\right]\left(\rho_{\nu}(-q)-j_{\mathrm{B}\ \nu}(q)\right)\end{aligned} \tag{35.3}$$

Now we obtain 8 terms in the total action, the first four from the first line, the next two (number 5 and 6) from the second line, and the last two (number 7 and 8) from the third line. We list them below:

$$S_1 \equiv \sum_{\substack{q\in \mathrm{i}\Omega_{+1}\times \mathrm{Q}\\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\}}}\overline{\phi}_{\nu}(q)\left(-\frac{1}{\hbar}\mathscr{G}_{0\ \nu}^{-\mathrm{B}}(q)\right)\phi_{\nu}(q) \tag{35.4}$$

$$S_2 \equiv -\hbar\sum_{\substack{q\in \mathrm{i}\Omega_{+1}\times \mathrm{Q}\\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\}}}\left(\rho_{\nu}(q)-\overline{j}_{\mathrm{B}\ \nu}(q)\right)\mathscr{G}_{0\ \nu}^{\mathrm{B}}(q)\left(\rho_{\nu}(-q)-j_{\mathrm{B}\ \nu}(q)\right) \tag{35.5}$$

$$S_3 \equiv -\sum_{\substack{q\in \mathrm{i}\Omega_{+1}\times \mathrm{Q}\\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\}}}\left(\rho_{\nu}(q)-\overline{j}_{\mathrm{B}\ \nu}(q)\right)\phi_{\nu}(q) \tag{35.6}$$

$$S_4 \equiv -\sum_{\substack{q\in \mathrm{i}\Omega_{+1}\times \mathrm{Q}\\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\}}}\overline{\phi}_{\nu}(q)\left(\rho_{\nu}(-q)-j_{\mathrm{B}\ \nu}(q)\right)$$

$$S_5 \equiv \sum_{\substack{q\in \mathrm{i}\Omega_{+1}\times \mathrm{Q}\\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\}}}\phi_{\nu}(q)\left(\rho_{\nu}(q)-\overline{j}_{\mathrm{B}\ \nu}(q)\right) \tag{35.7}$$

$$S_6 \equiv \hbar\sum_{\substack{q\in \mathrm{i}\Omega_{+1}\times \mathrm{Q}\\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\}}}\left(\rho_{\nu}(-q)-j_{\mathrm{B}\ \nu}(q)\right)\mathscr{G}_{0\ \nu}^{\mathrm{B}}(q)\left(\rho_{\nu}(q)-\overline{j}_{\mathrm{B}\ \nu}(q)\right) \tag{35.8}$$

$$S_7 \equiv \sum_{\substack{q\in \mathrm{i}\Omega_{+1}\times \mathrm{Q}\\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\}}}\overline{\phi}_{\nu}(q)\left(\rho_{\nu}(-q)-j_{\mathrm{B}\ \nu}(q)\right) \tag{35.9}$$

$$S_8 \equiv \hbar\sum_{\substack{q\in \mathrm{i}\Omega_{+1}\times \mathrm{Q}\\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\}}}\left(\rho_{\nu}(q)-\overline{j}_{\mathrm{B}\ \nu}(q)\right)\mathscr{G}_{0\ \nu}^{\mathrm{B}}(q)\left(\rho_{\nu}(-q)-j_{\mathrm{B}\ \nu}(q)\right) \tag{35.10}$$

Now we obtain

$$\text{"}2+6=0=3+5=4+7\text{"} \tag{35.11}$$

such that only 1 and 8 contribute. Then, when one integrates out the phonons (with Lemma 16.18) and we discard the divergent factor because it cancels out when we compute Green-functions, one obtains the effective electron-electron interaction, giving us

$$\begin{aligned} S_{\substack{\text{el-el-int}\\[j_{\mathrm{B}},\bar{j}_{\mathrm{B}}]}}[\psi,\overline{\psi}] &= +\hbar \sum_{\substack{q\in \mathrm{i}\Omega_{+1}\times \mathrm{Q}\\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} \left(\rho_\nu(q)-\bar{j}_{\underset{\nu}{\mathrm{B}}}(q)\right)\mathscr{G}^{\mathrm{B}}_{\underset{\nu}{0}}(q)\left(\rho_\nu(-q)-j_{\underset{\nu}{\mathrm{B}}}(q)\right)\\ &= +\hbar \sum_{\substack{q\in \mathrm{i}\Omega_{+1}\times \mathrm{Q}\\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} \overline{\left(\rho_\nu(-q)-j_{\underset{\nu}{\mathrm{B}}}(q)\right)}\mathscr{G}^{\mathrm{B}}_{\underset{\nu}{0}}(q)\left(\rho_\nu(-q)-j_{\underset{\nu}{\mathrm{B}}}(q)\right) \end{aligned}$$

For the latter identity: We compute straightforwardly for the source-independent term we obtain

$$\begin{aligned} S_{\text{el-el-int}}[\psi,\overline{\psi}] &= +\hbar \sum_{\substack{\mathbf{q}\in \mathrm{Q}\\ \omega_q\in\Omega_{+1}\\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} \rho_\nu(\mathrm{i}\omega_q,\mathbf{q})\mathscr{G}^{\mathrm{B}}_{\underset{\nu}{0}}(\mathbf{q},\mathrm{i}\omega_q)\rho_\nu(-\mathrm{i}\omega_q,-\mathbf{q})\\ &= + \sum_{\substack{\mathbf{q}\in \mathrm{Q}\\ \omega_q\in\Omega_{+1}\\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} \frac{\rho_\nu(\mathrm{i}\omega_q,+\mathbf{q})\rho_\nu(-\mathrm{i}\omega_q,-\mathbf{q})}{\mathrm{i}\omega_q-\omega_\nu(\mathbf{q})}\\ &= - \sum_{\substack{\mathbf{q}\in \mathrm{Q}\\ \omega_q\in\Omega_{+1}\\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} \frac{\rho_\nu(+\mathrm{i}\omega_q,+\mathbf{q})\rho_\nu(-\mathrm{i}\omega_q,-\mathbf{q})}{\omega_q^2+\omega_\nu^2(\mathbf{q})}\left(\mathrm{i}\omega_q+\omega_\nu(\mathbf{q})\right)\\ &= - \sum_{\substack{\mathbf{q}\in \mathrm{Q}\\ \omega_q\in\Omega_{+1}\\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} \frac{\omega_\nu(\mathbf{q})}{\omega_q^2+\omega_\nu^2(\mathbf{q})}\rho_\nu(+\mathrm{i}\omega_q,+\mathbf{q})\rho_\nu(-\mathrm{i}\omega_q,-\mathbf{q})\\ &\equiv - \sum_{\substack{q\in \mathrm{i}\Omega_{+1}\times \mathrm{Q}\\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} \frac{\omega_\nu(\mathbf{q})}{\omega_q^2+\omega_\nu^2(\mathbf{q})}\rho_\nu(+q)\rho_\nu(-q) \end{aligned}$$

whereas in the second last line we used $\omega_\nu(\mathbf{q})=\omega_\nu(-\mathbf{q})$.

Proof 35.4 of Lemma 23.19

Now we simplify the interaction-term

$$\begin{aligned} &\rho_\nu(+\mathrm{i}\omega_q,+\mathbf{q})\rho_\nu(-\mathrm{i}\omega_q,-\mathbf{q})\\ &= \frac{1}{\hbar\beta N_p} \sum_{\substack{\mathbf{k},\mathbf{k}'\in \mathrm{Q}\\ \omega_k,\omega_{k'}\in \mathrm{i}\Omega_{-1}\\ \sigma,\sigma'\in\{\downarrow,\uparrow\}\\ n,n',m,m'\in\{1,\dots,\infty\}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})g_{m'n'\nu}(\mathbf{k}',-\mathbf{q})}{\hbar^2}\overline{\psi}_{m\sigma}(\mathrm{i}\left(\omega_k+\omega_q\right),\mathbf{k}+\mathbf{q})\psi_{n\sigma}(\mathrm{i}\omega_k,\mathbf{k})\overline{\psi}_{m'\sigma'}(\mathrm{i}\left(\omega_{k'}-\omega_q\right),\mathbf{k}'-\mathbf{q})\psi_{n'\sigma'}(\mathrm{i}\omega_{k'},\mathbf{k}') \end{aligned} \tag{35.12}$$

introducing the four-momentum we can write this shorter as

$$\begin{aligned}\rho_\nu(q)\rho_\nu(-q) &= \frac{1}{\hbar\beta N_p}\sum_{\substack{k,k'\in \mathrm{Q}\times\Omega_{-1}\\ \sigma,\sigma'\in\{\downarrow,\uparrow\}\\ n,n',m,m'\in\{1,\dots,\infty\}}}\frac{g_{mn\nu}(\mathbf{k},\mathbf{q})g_{m'n'\nu}(\mathbf{k}',-\mathbf{q})}{\hbar^2}\overline{\psi}_{m\sigma}(k+q)\psi_{n\sigma}(k)\overline{\psi}_{m'\sigma'}(k'-q)\psi_{n'\sigma'}(k')\\ &= \frac{-1}{\hbar\beta N_p}\sum_{\substack{k,k'\in \mathrm{Q}\times\Omega_{-1}\\ \sigma,\sigma'\in\{\downarrow,\uparrow\}\\ n,n',m,m'\in\{1,\dots,\infty\}}}\frac{g_{mn\nu}(\mathbf{k},\mathbf{q})g_{m'n'\nu}(\mathbf{k}',-\mathbf{q})}{\hbar^2}\overline{\psi}_{m\sigma}(k+q)\overline{\psi}_{m'\sigma'}(k'-q)\psi_{n\sigma}(k)\psi_{n'\sigma'}(k')\end{aligned}$$

Therefore we obtain for the source-independent interaction-term

$$\begin{aligned}S_{\text{el-el-int}}[\psi,\overline{\psi}] &= \frac{+1}{\hbar\beta N_p}\sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ \mathrm{i}\omega_q\in\mathrm{i}\Omega_{+1}\\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}\\ k,k'\in\mathrm{Q}\times\Omega_{-1}\\ \sigma,\sigma'\in\{\downarrow,\uparrow\}\\ n,n',m,m'\in\{1,\dots,\infty\}}}\frac{\omega_\nu(\mathbf{q})}{\omega_q^2+\omega_\nu^2(\mathbf{q})}\frac{g_{mn\nu}(\mathbf{k},\mathbf{q})g_{m'n'\nu}(\mathbf{k}',-\mathbf{q})}{\hbar^2}\overline{\psi}_{m\sigma}(k+q)\overline{\psi}_{m'\sigma'}(k'-q)\psi_{n\sigma}(k)\psi_{n'\sigma'}(k')\\ &= \sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ \omega_q\in\Omega_{+1}\\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}\\ k,k'\in\mathrm{Q}\times\Omega_{-1}\\ \sigma,\sigma'\in\{\downarrow,\uparrow\}\\ n,n',m,m'\in\{1,\dots,\infty\}}}\overline{\psi}_{m\sigma}(k+q)\overline{\psi}_{m'\sigma'}(k'-q)\frac{+1}{\hbar\beta N_p}\frac{\omega_\nu(\mathbf{q})}{\omega_q^2+\omega_\nu^2(\mathbf{q})}\frac{g_{mn\nu}(\mathbf{k},\mathbf{q})g_{m'n'\nu}(\mathbf{k}',-\mathbf{q})}{\hbar^2}\psi_{n\sigma}(k)\psi_{n'\sigma'}(k')\\ &\overset{\mathbf{k}'\mapsto\mathbf{k}'+\mathbf{q}}{=} \sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ \omega_q\in\Omega_{+1}\\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}\\ k,k'\in\mathrm{Q}\times\Omega_{-1}\\ \sigma,\sigma'\in\{\downarrow,\uparrow\}\\ n,n',m,m'\in\{1,\dots,\infty\}}}\overline{\psi}_{m\sigma}(k+q)\overline{\psi}_{m'\sigma'}(k')\frac{-1}{\hbar\beta N_p}\frac{\omega_\nu(\mathbf{q})}{\omega_q^2+\omega_\nu^2(\mathbf{q})}\frac{g_{mn\nu}(\mathbf{k},\mathbf{q})g_{m'n'\nu}(\mathbf{k}'+\mathbf{q},-\mathbf{q})}{\hbar^2}\psi_{n'\sigma'}(k'+q)\psi_{n\sigma}(k)\\ &\overset{\text{Lemma 8.37}}{=} \sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ \omega_q\in\Omega_{+1}\\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}\\ k,k'\in\mathrm{Q}\times\Omega_{-1}\\ \sigma,\sigma'\in\{\downarrow,\uparrow\}\\ n,n',m,m'\in\{1,\dots,\infty\}}}\overline{\psi}_{m\sigma}(k+q)\overline{\psi}_{m'\sigma'}(k')\frac{-1}{\hbar\beta N_p}\frac{\omega_\nu(\mathbf{q})}{\omega_q^2+\omega_\nu^2(\mathbf{q})}\frac{g_{mn\nu}(\mathbf{k},\mathbf{q})g^*_{n'm'\nu}(\mathbf{k}',\mathbf{q})}{\hbar^2}\psi_{n'\sigma'}(k'+q)\psi_{n\sigma}(k)\end{aligned}\tag{35.13}$$

Now we introduce[1] the new fermionic Matsubara summation-variable $\mathrm{i}\Omega_{-1}\times\mathrm{Q}\ni p\equiv k+q$ in order to replace the summation over $q\equiv p-k$. This yields

[1] More concretely: For each k we introduce a p such that the equation $p\equiv k+q$ is fulfilled.

$$
\begin{aligned}
&S_{\text{el-el-int}}[\psi,\overline{\psi}] \\
&= \sum_{\substack{\nu\in\{1,\dots,rd_{\mathbf{x}}\}\\ p,k,k'\in \mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ \sigma,\sigma'\in\{\downarrow,\uparrow\}\\ n,n',m,m'\in\{1,\dots,\infty\}}} \overline{\psi}_{m\sigma}(p)\overline{\psi}_{m'\sigma'}(k')\frac{-1}{\hbar\beta N_p}\frac{\omega_\nu(\mathbf{p}-\mathbf{k})}{\omega_{p-k}^2+\omega_\nu^2(\mathbf{p}-\mathbf{k})}\frac{g_{mn\nu}(\mathbf{k},\mathbf{p}-\mathbf{k})g^*_{n'm'\nu}(\mathbf{k}',\mathbf{p}-\mathbf{k})}{\hbar^2}\psi_{n'\sigma'}(k'+p-k)\psi_{n\sigma}(k) \\
&= \sum_{\substack{p,k,k'\in \mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ \sigma,\sigma'\in\{\downarrow,\uparrow\}\\ n,n',m,m'\in\{1,\dots,\infty\}}} \overline{\psi}_{m\sigma}(p)\overline{\psi}_{m'\sigma'}(k')\frac{-1}{\hbar\beta N_p}\sum_{\nu\in\{1,\dots,rd_{\mathbf{x}}\}}\frac{\omega_\nu(\mathbf{p}-\mathbf{k})}{\omega_{p-k}^2+\omega_\nu^2(\mathbf{p}-\mathbf{k})}\frac{g_{mn\nu}(\mathbf{k},\mathbf{p}-\mathbf{k})g^*_{n'm'\nu}(\mathbf{k}',\mathbf{p}-\mathbf{k})}{\hbar^2}\psi_{n'\sigma'}(k'+p-k)\psi_{n\sigma}(k) \\
&= \sum_{\substack{p,p',k,k'\in \mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ \sigma,\sigma'\in\{\downarrow,\uparrow\}\\ n,n',m,m'\in\{1,\dots,\infty\}}} \overline{\psi}_{m\sigma}(p)\overline{\psi}_{m'\sigma'}(k')V_{m,m';n',n}(p,k';p',k)\psi_{n'\sigma'}(p')\psi_{n\sigma}(k)
\end{aligned}
\tag{35.14}
$$

with a quartic vertex over which we sum without any restrictions

$$
V_{m,m';n',n}(p,k';p',k)\equiv\frac{-1}{\hbar\beta N_p}\sum_{\nu\in\{1,\dots,rd_{\mathbf{x}}\}}\frac{\omega_\nu(\mathbf{p}-\mathbf{k})}{\omega_{p-k}^2+\omega_\nu^2(\mathbf{p}-\mathbf{k})}\frac{g_{mn\nu}(\mathbf{k},\mathbf{p}-\mathbf{k})g^*_{n'm'\nu}(\mathbf{k}',\mathbf{p}-\mathbf{k})}{\hbar^2}\delta_{p',k'+p-k} \tag{35.15}
$$

Now we will simplify this expression, by relabelling the indices. This yields, after replacing $k' \longleftrightarrow p'$, the following expression

$$
S_{\text{el-el-int}}[\psi,\overline{\psi}] = \sum_{\substack{p,k,k'\in \mathrm{Q}\times\Omega_{-1}\\ \sigma,\sigma'\in\{\downarrow,\uparrow\}\\ n,n',m,m'\in\{1,\dots,\infty\}}} \overline{\psi}_{m\sigma}(p)\overline{\psi}_{m'\sigma'}(p')V_{m,m';n',n}(p,p';k',k)\psi_{n'\sigma'}(k')\psi_{n\sigma}(k)
$$

with

$$
V_{m,m';n',n}(p,p';k',k) = \frac{-1}{\hbar\beta N_p}\sum_{\nu\in\{1,\dots,rd_{\mathbf{x}}\}}\frac{\omega_\nu(\mathbf{p}-\mathbf{k})}{\omega_{p_0-k_0}^2+\omega_\nu^2(\mathbf{p}-\mathbf{k})}\frac{g_{mn\nu}(\mathbf{k},\mathbf{p}-\mathbf{k})g^*_{n'm'\nu}(\mathbf{p}',\mathbf{p}-\mathbf{k})}{\hbar^2}\delta_{k',p'+p-k} \tag{35.16}
$$

Now we rewrite this even further to find a bilinearform

$$
\begin{aligned}
&S_{\text{el-el-int}}[\psi,\overline{\psi}] \\
&= \sum_{\substack{p,k,k'\in \mathrm{Q}\times\Omega_{-1}\\ \sigma,\sigma',\pi,\pi'\in\{\downarrow,\uparrow\}\\ n,n',m,m'\in\{1,\dots,\infty\}}} \overline{\psi}_{m\sigma}(p)\overline{\psi}_{m'\sigma'}(p')V^{\sigma,\sigma',\pi',\pi}_{m,m';n',n}(p,p';k',k)\psi_{n'\pi'}(k')\psi_{n\pi}(k)
\end{aligned}
$$

with

$$V^{\sigma,\sigma',\pi',\pi}_{m,m';n',n}(p,p';k',k) = \frac{-1}{\hbar\beta N_p}\sum_{\nu\in\{1,\dots,rd_{\mathbf{x}}\}}\frac{\omega_\nu(\mathbf{p}-\mathbf{k})}{\omega^2_{p_0-k_0}+\omega^2_\nu(\mathbf{p}-\mathbf{k})}\frac{g_{mn\nu}(\mathbf{k},\mathbf{p}-\mathbf{k})g^*_{n'm'\nu}(\mathbf{p}',\mathbf{p}-\mathbf{k})}{\hbar^2}\delta_{k'+k,p'+p}\delta_{\sigma,\pi}\delta_{\sigma',\pi'} \tag{35.17}$$

Now we condense the notation even further, by introducing the multi-index

$$\alpha \equiv (m_\alpha,\sigma_\alpha,\omega_\alpha,\mathbf{k}_\alpha) \in \{1,2,\dots\}\times\{\downarrow,\uparrow\}\times\Omega_{-1}\times\mathrm{Q} \equiv \Xi, \tag{35.18}$$

which then yields (notice the exchanged order of the Grassmann-fields)

$$S_{\text{el-el-int}}[\psi,\overline{\psi}] = \sum_{\alpha_1,\dots,\alpha_4\in\Xi}\overline{\psi}_{\alpha_1}\overline{\psi}_{\alpha_2}V_{\alpha_1,\alpha_2;\alpha_3,\alpha_4}\psi_{\alpha_4}\psi_{\alpha_3}$$

with Lemma 8.37

$$\begin{aligned}
&V_{\alpha_1,\alpha_2;\alpha_3,\alpha_4}\\
&= \frac{1}{\hbar\beta N_p}\sum_{\nu\in\{1,\dots,rd_{\mathbf{x}}\}}\frac{\omega_\nu(\mathbf{k}_{\alpha_1}-\mathbf{k}_{\alpha_4})}{\omega^2_{\alpha_1-\alpha_4}+\omega^2_\nu(\mathbf{k}_{\alpha_1}-\mathbf{k}_{\alpha_4})}\frac{g_{m_{\alpha_1}m_{\alpha_4}\nu}(\mathbf{k}_{\alpha_4},\mathbf{k}_{\alpha_1}-\mathbf{k}_{\alpha_4})g^*_{m_{\alpha_3}m_{\alpha_2}\nu}(\mathbf{k}_{\alpha_2},\mathbf{k}_{\alpha_1}-\mathbf{k}_{\alpha_4})}{\hbar^2}\delta_{k_{\alpha_3}+k_{\alpha_4},k_{\alpha_2}+k_{\alpha_1}}\delta_{\sigma_{\alpha_1},\sigma_{\alpha_4}}\delta_{\sigma_{\alpha_2},\sigma_{\alpha_3}}\\
&= \frac{1}{\hbar\beta N_p}\sum_{\nu\in\{1,\dots,rd_{\mathbf{x}}\}}\frac{\omega_\nu(\mathbf{k}_{\alpha_1}-\mathbf{k}_{\alpha_4})}{\omega^2_{\alpha_1-\alpha_4}+\omega^2_\nu(\mathbf{k}_{\alpha_1}-\mathbf{k}_{\alpha_4})}\frac{g_{m_{\alpha_1}m_{\alpha_4}\nu}(\mathbf{k}_{\alpha_4},\mathbf{k}_{\alpha_1}-\mathbf{k}_{\alpha_4})g_{m_{\alpha_2}m_{\alpha_3}\nu}(\mathbf{k}_{\alpha_2}+\mathbf{k}_{\alpha_1}-\mathbf{k}_{\alpha_4},-\mathbf{k}_{\alpha_1}+\mathbf{k}_{\alpha_4})}{\hbar^2}\delta_{k_{\alpha_3}+k_{\alpha_4},k_{\alpha_2}+k_{\alpha_1}}\delta_{\sigma_{\alpha_1},\sigma_{\alpha_4}}\delta_{\sigma_{\alpha_2},\sigma_{\alpha_3}}
\end{aligned} \tag{35.19}$$

Proof 35.5 of Corollary 23.20 We compute

$$\left(\sum_{\alpha_i}\psi^\dagger_{\alpha_1}\psi^\dagger_{\alpha_2}V_{\alpha_1,\alpha_2;\alpha_3,\alpha_4}\psi_{\alpha_4}\psi_{\alpha_3}\right)^\dagger = \sum_{\alpha_i}\psi^\dagger_{\alpha_3}\psi^\dagger_{\alpha_4}V^*_{\alpha_1,\alpha_2;\alpha_3,\alpha_4}\psi_{\alpha_2}\psi_{\alpha_1} = \sum_{\alpha_i}\psi^\dagger_{\alpha_1}\psi^\dagger_{\alpha_2}V_{\alpha_4,\alpha_3;\alpha_2,\alpha_1}\psi_{\alpha_4}\psi_{\alpha_3}$$

Therefore this is hermitian, if the following equation is fulfilled[2]

$$\begin{aligned}
&\sum_{\nu\in\{1,\dots,rd_{\mathbf{x}}\}}\frac{\omega_\nu(\mathbf{k}_{\alpha_1}-\mathbf{k}_{\alpha_4})}{\omega^2_{\alpha_1-\alpha_4}+\omega^2_\nu(\mathbf{k}_{\alpha_1}-\mathbf{k}_{\alpha_4})}\frac{g_{m_{\alpha_1}m_{\alpha_4}\nu}(\mathbf{k}_{\alpha_4},\mathbf{k}_{\alpha_1}-\mathbf{k}_{\alpha_4})g^*_{m_{\alpha_3}m_{\alpha_2}\nu}(\mathbf{k}_{\alpha_2},\mathbf{k}_{\alpha_1}-\mathbf{k}_{\alpha_4})}{\hbar^3\beta N_p}\\
&\overset{!}{=}\sum_{\nu\in\{1,\dots,rd_{\mathbf{x}}\}}\frac{\omega_\nu(\mathbf{k}_{\alpha_4}-\mathbf{k}_{\alpha_1})}{\omega^2_{\alpha_4-\alpha_1}+\omega^2_\nu(\mathbf{k}_{\alpha_4}-\mathbf{k}_{\alpha_1})}\frac{g^*_{m_{\alpha_4}m_{\alpha_1}\nu}(\mathbf{k}_{\alpha_1},\mathbf{k}_{\alpha_4}-\mathbf{k}_{\alpha_1})g_{m_{\alpha_2}m_{\alpha_3}\nu}(\mathbf{k}_{\alpha_3},\mathbf{k}_{\alpha_4}-\mathbf{k}_{\alpha_1})}{\hbar^3\beta N_p}
\end{aligned}$$

Now since

[2] Maybe we need to go through this proof again, since we symmetrized the expression.

$$g_{m_{\alpha_2} m_{\alpha_3} \nu}(\mathbf{k}_{\alpha_3}, \mathbf{k}_{\alpha_4} - \mathbf{k}_{\alpha_1}) = g^*_{m_{\alpha_3} m_{\alpha_2} \nu}(\mathbf{k}_{\alpha_3} + \mathbf{k}_{\alpha_4} - \mathbf{k}_{\alpha_1}, \mathbf{k}_{\alpha_1} - \mathbf{k}_{\alpha_4}) = g^*_{m_{\alpha_3} m_{\alpha_2} \nu}(\mathbf{k}_{\alpha_2}, \mathbf{k}_{\alpha_1} - \mathbf{k}_{\alpha_4})$$

etc, which proves the corollary.

Proof 35.6 of Corollary 23.22

Electrons:

One obtains through direct computation using Equation (20.37) and using further the identity relating Green-functions to functional derivatives

$$\begin{aligned}
\langle n_{n\sigma}(\mathbf{k}) \rangle &= \langle c^\dagger_{n\sigma}(\mathbf{k}) c_{n\sigma}(\mathbf{k}) \rangle \\
&= \frac{\delta^2}{\delta \bar{j}_{n,\sigma}(\tau = 0-, \mathbf{k}) \delta j_{n,\sigma}(\tau' = 0, \mathbf{k})} \frac{Z[j_{\mathrm{F}}, \bar{j}_{\mathrm{F}}, j_{\mathrm{B}}, \bar{j}_{\mathrm{B}}]}{Z} \Big|_{\bar{j}=j=0} \\
&= \frac{1}{\hbar \beta} \lim_{\delta \downarrow 0} \sum_{\omega_m \in \Omega_{-1}} \mathrm{e}^{+\mathrm{i}\omega_m \delta} \frac{\partial^2}{\partial \bar{j}_{n,\sigma}(\mathrm{i}\omega_m, \mathbf{k}) \partial j_{n,\sigma}(\mathrm{i}\omega_m, \mathbf{k})} \frac{Z[j_{\mathrm{F}}, \bar{j}_{\mathrm{F}}, j_{\mathrm{B}}, \bar{j}_{\mathrm{B}}]}{Z} \Big|_{\bar{j}=j=0}
\end{aligned}$$

whereas we used that the partition-function is diagonal w.r.t. the Matsubara-frequencies. After recalling the definition of the total electronic number operator as

$$\langle N \rangle = \sum_{\substack{\mathbf{k} \in \mathrm{Q} \\ \sigma \in \{\downarrow, \uparrow\} \\ n \in \{1,2,\ldots,\infty\}}} \langle n_{n\sigma}(\mathbf{k}) \rangle.$$

Follows from using the Lemma **??** as

$$\begin{aligned}
\langle H_{\mathrm{el}} \rangle &= \sum_{\substack{\mathbf{k} \in \mathrm{Q} \\ \sigma \in \{\uparrow, \downarrow\} \\ n \in \{1,\ldots,\infty\}}} \epsilon_{n\sigma}(\mathbf{k}) \left\langle c^\dagger_{n\sigma}(\mathbf{k}) c_{n\sigma}(\mathbf{k}) \right\rangle \\
&= \frac{1}{\hbar \beta} \lim_{\delta \downarrow 0} \sum_{\substack{\sigma \in \{\downarrow, \uparrow\} \\ k \in \mathrm{i}\Omega_{-1} \times \mathrm{Q} \\ n \in \{1,2,\ldots,\infty\}}} \epsilon_{n\sigma}(\mathbf{k}) \mathrm{e}^{+\mathrm{i}\omega_k \delta} \frac{\partial^2}{\partial \bar{j}_{n,\sigma}(k) \partial j_{n,\sigma}(k)} \frac{Z[j_{\mathrm{F}}, \bar{j}_{\mathrm{F}}, j_{\mathrm{B}}, \bar{j}_{\mathrm{B}}]}{Z} \Big|_{\bar{j}=j=0}
\end{aligned}$$

Phonons:

The equations for the phonons are derived analogously.

Interactions:

We first rewrite the interaction term as

$$\left\langle c^\dagger_{\mathbf{k}+\mathbf{q}m\sigma} c_{\mathbf{k}n\sigma} \left(b_{\mathbf{q}\nu} + b^\dagger_{-\mathbf{q}\nu} \right) \right\rangle = \left\langle \overline{\psi}_{\mathbf{k}+\mathbf{q}m\sigma}(0) \psi_{\mathbf{k}n\sigma}(0) \left(\phi_{\mathbf{q}\nu}(0) + \overline{\phi}_{-\mathbf{q}\nu}(0) \right) \right\rangle$$
$$= \frac{\delta^2}{\delta \bar{j}(\tau = 0-, \mathbf{k}n\sigma) \delta j(\tau = 0, \mathbf{k}+\mathbf{q}m\sigma)} \left(\frac{\delta}{\delta \bar{j}(\tau = 0-, \mathbf{q}\nu) + \delta j(\tau = 0, -\mathbf{q}\nu)} \right) \frac{Z[j, \bar{j}]}{Z} |_{j=\bar{j}=0} \tag{35.20}$$

Now we compute functional derivatives again. First we note that the functional derivatives can be expanded as

$$\frac{\delta}{\delta \bar{j}(\tau = 0, \mathbf{q}\nu)} = \frac{1}{\sqrt{\hbar\beta}} \sum_{\omega_m \in \Omega_{+1}} \frac{\partial}{\partial \bar{j}(\mathrm{i}\omega_m, \mathbf{q}\nu)}, \tag{35.21}$$

and

$$\frac{\delta}{\delta j(\tau = 0, -\mathbf{q}\nu)} = \frac{1}{\sqrt{\hbar\beta}} \sum_{\omega_m \in \Omega_{+1}} \frac{\partial}{\partial j(-\mathrm{i}\omega_m, -\mathbf{q}\nu)}. \tag{35.22}$$

We also expand the other functional derivatives as

$$\frac{\delta^2}{\delta \bar{j}(\tau = 0-, \mathbf{k}n\sigma) \delta j(\tau = 0, \mathbf{k}+\mathbf{q}m\sigma)} = \frac{1}{\hbar\beta} \lim_{\delta \downarrow 0} \sum_{\omega_{n,n'} \in \Omega_{-1}} \mathrm{e}^{\mathrm{i}\omega_n \delta} \frac{\partial^2}{\partial \bar{j}_{n,\sigma}(\mathrm{i}\omega_n, \mathbf{k}) \partial j_{m,\sigma}(\mathrm{i}\omega_{n'}, \mathbf{k}+\mathbf{q})} \tag{35.23}$$

which gives the desired result.

Proof 35.7 of Lemma 24.3 We use Lemma 20.16 and obtain the first equality. For the second equation, we notice that the expression can be rewritten with respect to the density of states as

$$\begin{aligned}
\Omega_{0,\mathrm{el}}(\mu, T, V) &= \frac{-1}{\beta} \sum_{\substack{\mathbf{k} \in \mathrm{Q} \\ \sigma \in \{\uparrow,\downarrow\} \\ m \in \{1,\ldots,\infty\}}} \mathrm{Log}\left(1 + \mathrm{e}^{-\beta(\epsilon_{m\mathbf{k}\sigma} - \mu)}\right) \\
&= \frac{-1}{\beta} \int \mathrm{d}E \sum_{\substack{\mathbf{k} \in \mathrm{Q} \\ \sigma \in \{\uparrow,\downarrow\} \\ m \in \{1,\ldots,\infty\}}} \mathrm{Log}\left(1 + \mathrm{e}^{-\beta(E-\mu)}\right) \delta(E - \epsilon_{m\mathbf{k}\sigma}) \\
&= \frac{-1}{\beta} \int \mathrm{d}E \, \mathrm{Log}\left(1 + \mathrm{e}^{-\beta(E-\mu)}\right) \rho_0(E - \mu) \\
&= \frac{-1}{\beta} \int \mathrm{d}E \, \mathrm{Log}\left(1 + \mathrm{e}^{-\beta E}\right) \rho_0(E)
\end{aligned}$$

Proof 35.8 of Lemma 25.3

We recall

$$\left\langle H_{0,\mathrm{el}} \right\rangle_0 (\mu, T, V) = \sum_{\substack{\mathbf{k} \in \mathrm{Q} \\ \sigma \in \{\uparrow,\downarrow\} \\ m \in \{1,2,\ldots,\infty\}}} \epsilon_{m\mathbf{k}\sigma} \, \mathrm{F}_\beta(\epsilon_{m,\sigma,\mathbf{k}} - \mu) \tag{35.24}$$

and then compute the temperature-derivative as

$$\partial_T \left\langle H_{0,\mathrm{el}} \right\rangle_0 (\mu, T, V) = \sum_{\substack{\mathbf{k}\in \mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,2,\ldots,\infty\}}} \epsilon_{m\mathbf{k}\sigma} \partial_T \, \mathrm{F}_1 \left(\beta(\epsilon_{m,\sigma,\mathbf{k}} - \mu)\right) = \ldots \tag{35.25}$$

Now we use chain and product rule to obtain

$$\begin{aligned} \partial_T \, \mathrm{F}_1 \left(\beta(\epsilon_{m,\sigma,\mathbf{k}} - \mu)\right) &= \left(\partial_T \, \mathrm{F}_1\right) \left(\beta(\epsilon_{m,\sigma,\mathbf{k}} - \mu)\right) && \cdot \partial_T \beta \left(\epsilon_{m,\sigma,\mathbf{k}} - \mu\right) \\ &\overset{\text{Lemma 9.63}}{=} -\frac{1}{4} \operatorname{sech}^2 \left(\frac{\epsilon_{m,\sigma,\mathbf{k}} - \mu}{2k_B T}\right) && \cdot \left(\partial_T \beta\right) (\epsilon_{m,\sigma,\mathbf{k}} - \mu) \\ &= -\frac{1}{4} \operatorname{sech}^2 \left(\frac{\epsilon_{m,\sigma,\mathbf{k}} - \mu}{2k_B T}\right) && \cdot \left(\frac{-1}{k_B T^2}\right) (\epsilon_{m,\sigma,\mathbf{k}} - \mu) \end{aligned} \tag{35.26}$$

which allows us to write the semi-final result as

$$\partial_T \langle H_{0,\mathrm{el}} \rangle_0 (\mu, T, V) = \ldots = \sum_{\substack{\mathbf{k}\in \mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\}}} \frac{\epsilon_{m\mathbf{k}\sigma}}{4} \operatorname{sech}^2 \left(\frac{\epsilon_{m\mathbf{k}\sigma} - \mu}{2k_B T}\right) \left[\frac{\epsilon_{m\mathbf{k}\sigma} - \mu}{k_B T^2}\right] = \star\star\star \tag{35.27}$$

Now we introduce

$$\rho(E) = \sum_{\substack{\mathbf{k}\in \mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,2,\ldots,\infty\}}} \delta(E - \xi_{m\mathbf{k}\sigma}) = \sum_{\substack{\mathbf{k}\in \mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,2,\ldots,\infty\}}} \delta(E + \mu - \epsilon_{m\mathbf{k}\sigma}) \tag{35.28}$$

and

$$\rho_{\mathrm{aux}}(E) = \sum_{\substack{\mathbf{k}\in \mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,2,\ldots,\infty\}}} \delta(E - \epsilon_{m\mathbf{k}\sigma}) \tag{35.29}$$

which implies $\rho_{\mathrm{aux}}(E + \mu) = \rho(E)$. This allows us to rewrite the expression as

$$\begin{aligned} \partial_T \langle H_{0,\mathrm{el}} \rangle_0 = \star &= \int \mathrm{d}E \, \rho(E) \frac{E + \mu}{4} \operatorname{sech}^2 \left(\frac{E}{2k_B T}\right) \quad \left[\frac{E}{k_B T^2}\right] \\ &= \int \mathrm{d}E \, \rho_{\mathrm{aux}}(E) \frac{E}{4} \operatorname{sech}^2 \left(\frac{E - \mu}{2k_B T}\right) \quad \left[\frac{E - \mu}{k_B T^2}\right] \\ &= \star\star \end{aligned} \tag{35.30}$$

We also recall the definition of the density of states from quantum espresso as

$$\rho_{\mathrm{QE}}(E) = \frac{1}{N_p} \sum_{\substack{\mathbf{k}\in \mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,2,\ldots,\infty\}}} \delta(E - \epsilon_{m\mathbf{k}\sigma}) = \frac{1}{N_p} \rho_{\mathrm{aux}}(E) \tag{35.31}$$

such that we obtain the final result

$$\frac{1}{N_x N_y N_z}\partial_T \langle H_{0,\mathrm{el}}\rangle_0(\mu,T,V) = \int \mathrm{d}E\, \rho_{\mathrm{QE}}(E)\frac{E}{4}\,\mathrm{sech}^2\left(\frac{E-\mu}{2k_B T}\right)\left[\frac{E-\mu(T)}{k_B T^2}\right] \tag{35.32}$$

which can also be (equivalently) rewritten as

$$\begin{aligned}\partial_T \frac{\langle H_{\mathrm{el}}\rangle_0}{N_x N_y N_z} &= \int \mathrm{d}E \quad \frac{E}{4} \quad \mathrm{sech}^2\left(\frac{E-\mu(T)}{2k_B T}\right) \quad \left[\frac{E-\mu(T)}{k_B T^2}\right] \quad \rho_{\mathrm{QE}}(E) \\ &= \frac{1}{N_x N_y N_z} \sum_{\substack{\mathbf{k}\in\mathrm{Q}\\ \sigma\in\{\uparrow,\downarrow\}\\ m\in\{1,\ldots,\infty\}}} \frac{\epsilon_{m\mathbf{k}\sigma}}{4} \quad \mathrm{sech}^2\left(\frac{\epsilon_{m\mathbf{k}\sigma}-\mu(T)}{2k_B T}\right) \quad \left[\frac{\epsilon_{m\mathbf{k}\sigma}-\mu(T)}{k_B T^2}\right]\end{aligned} \tag{35.33}$$

Proof 35.9 of Lemma 25.4 We compute the derivative w.r.t. the chemical potential and obtain the desired result with Lemma 9.63 and the chain-rule. This gives basically immediately the desired result

$$\partial_\mu \frac{\langle H_{\mathrm{el}}\rangle_0}{N_x N_y N_z} = \frac{\beta}{4} \int \mathrm{d}E \quad E \quad \mathrm{sech}^2\left(\frac{E-\mu}{2k_B T}\right) \quad \rho_{\mathrm{QE}}(E) \tag{35.34}$$

Proof 35.10 of Theorem 25.10

We use Equation (23.20) and compute

$$\frac{\partial}{\partial j_{n\sigma}(k)} Z[j,\bar{j}] = -\int \mathscr{D}(\overline{\psi},\psi)\,\overline{\psi}_{n\sigma}(k)\exp\left(\bar{j}_{\mathrm{el}}\psi + \overline{\psi} j_{\mathrm{el}}\right)\exp -\left(S_{\mathrm{el}} + S_{\substack{\text{el-el-int}\\ [j_{\mathrm{ph}},\bar{j}_{\mathrm{ph}}]}}\right)[\psi,\overline{\psi}] \tag{35.35}$$

and this yields for the double-derivative

$$\frac{\partial^2}{\partial \bar{j}_{n\sigma}(k)\partial j_{n\sigma}(k)} Z[j,\bar{j}] = -\int \mathscr{D}(\overline{\psi},\psi)\,\psi_{n\sigma}(k)\overline{\psi}_{n\sigma}(k)\exp\left(\bar{j}_{\mathrm{el}}\psi + \overline{\psi} j_{\mathrm{el}}\right)\exp -\left(S_{\mathrm{el}} + S_{\substack{\text{el-el-int}\\ [j_{\mathrm{ph}},\bar{j}_{\mathrm{ph}}]}}\right)[\psi,\overline{\psi}] \tag{35.36}$$

hence we obtain

$$\frac{\partial^2}{\partial \bar{j}_{n\sigma}(k)\partial j_{n\sigma}(k)} \frac{Z[j,\bar{j}]}{Z}\Big|_{j=\bar{j}=0} = -\langle \psi_{n\sigma}(k)\overline{\psi}_{n\sigma}(k)\rangle = +\mathscr{G}^{n,n}_{\sigma,\sigma}(k,k) \tag{35.37}$$

whereas in the last step we used Equation TBReferenced.

I think the other identity is proven in Waste-Folder 1

Proof 35.11 of Theorem 25.9

We perform a calculation analogously to Equation (33.162)

$$\begin{aligned}
\langle H_{\text{el}} \rangle &= \sum_{\substack{\mathbf{k}\in \text{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\}}} \epsilon_{m\mathbf{k}\sigma} \langle n_{m\mathbf{k}\sigma} \rangle \\
&= \frac{\hbar}{\mathrm{i}} \sum_{\substack{\mathbf{k}\in \text{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\}}} \epsilon_{m\mathbf{k}\sigma} G^{<}_{\substack{m,m \\ \mathbf{k},\mathbf{k} \\ \sigma,\sigma}}(t=0) \\
&= \frac{1}{2\pi\mathrm{i}} \oint \sum_{\substack{\mathbf{k}\in \text{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\} \\ E\in(-\infty,+\infty)}} \epsilon_{m\mathbf{k}\sigma} G^{<}_{\substack{m,m \\ \mathbf{k},\mathbf{k} \\ \sigma,\sigma}}(E) \\
&= \frac{-1}{\pi} \lim_{\eta\to 0} \oint \sum_{\substack{\mathbf{k}\in \text{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\} \\ E\in(-\infty,+\infty)}} \epsilon_{m\mathbf{k}\sigma} \, \mathrm{F}_\beta(E) \, \mathrm{Im} \; G^{\text{ret}}_{\substack{m,m \\ \mathbf{k},\mathbf{k} \\ \sigma,\sigma}}(E+\mathrm{i}\eta).
\end{aligned} \tag{35.38}$$

Proof 35.12 of Theorem 25.11

We divide the proof in consecutive steps.

1. We first compute the first derivative as

$$\frac{\partial}{\partial j_\nu(q)} Z[j,\bar{j}] = \int \mathscr{D}(\overline{\psi},\psi) \, \left(\frac{-\partial}{\partial j_\nu(q)} S_{\substack{\text{el-el-int} \\ [j,\bar{j}]}}[\psi,\overline{\psi}] \right) \exp -S_{[j,\bar{j}]}[\psi,\overline{\psi}] \tag{35.39}$$

2. We then compute the second derivative with Equation (23.20) as

$$\frac{\partial^2}{\partial \bar{j}_\nu(q) \partial j_\nu(q)} Z[j,\bar{j}] = \int \mathscr{D}(\overline{\psi},\psi) \left[\frac{-\partial^2}{\partial \bar{j}_\nu(q) \partial j_\nu(q)} S_{\substack{\text{el-el-int} \\ [j,\bar{j}]}}[\psi,\overline{\psi}] + \left(\frac{-\partial}{\partial j_\nu(q)} S_{\substack{\text{el-el-int} \\ [j,\bar{j}]}}[\psi,\overline{\psi}] \right) \left(\frac{-\partial}{\partial \bar{j}_\nu(q)} S_{\substack{\text{el-el-int} \\ [j,\bar{j}]}}[\psi,\overline{\psi}] \right) \right] \exp -S_{[j,\bar{j}]}[\psi,\overline{\psi}] \tag{35.40}$$

3. We then compute the individual terms with Equation (23.16)

$$\frac{\partial}{\partial j_\nu(q)} S_{\substack{\text{el-el-int} \\ [j,\bar{j}]}}[\psi,\overline{\psi}] = \hbar \bar{j}_\nu(q) \mathscr{G}_{0,\nu}(q) - \hbar \rho_\nu(q) \mathscr{G}_{0,\nu}(q) \tag{35.41}$$

4. and for the other derivative we have with Equation (23.16)

$$\frac{\partial}{\partial \bar{j}_\nu(q)} S_{\substack{\text{el-el-int} \\ [j,\bar{j}]}}[\psi,\overline{\psi}] = \hbar \mathscr{G}_{0,\nu}(q) j_\nu(q) - \hbar \mathscr{G}_{0,\nu}(q) \rho_\nu(-q) \tag{35.42}$$

5. and for the double-derivative we have

$$\frac{\partial^2}{\partial \bar{j}_\nu(q) \partial j_\nu(q)} S_{\substack{\text{el-el-int} \\ [j,\bar{j}]}}[\psi,\overline{\psi}] = \hbar \mathscr{G}_{0,\nu}(q) \tag{35.43}$$

Combining these results, we obtain

$$\begin{aligned}
\frac{\partial^2}{\partial \bar{j}_\nu(q) \partial j_\nu(q)} \frac{Z[j,\bar{j}]}{Z}\Big|_{j=\bar{j}=0} &= -\hbar \mathscr{G}_{0,\nu}(q) + \mathscr{G}^2_{0,\nu}(q) \frac{1}{Z} \int \mathscr{D}(\overline{\psi},\psi) \, \left(\hbar^2 \rho_\nu(q) \rho_\nu(-q) \right) \exp -S_{[j,\bar{j}]}[\psi,\overline{\psi}] \\
&= -\hbar \mathscr{G}_{0,\nu}(q) + \mathscr{G}^2_{0,\nu}(q) \hbar^2 \left\langle \rho_\nu(q) \rho_\nu(-q) \right\rangle \\
&= \star \star \star
\end{aligned} \tag{35.44}$$

Now we focus on the second term, which can be expanded using

$$\rho_\nu(q) = \frac{1}{\sqrt{\hbar\beta N_p}} \sum_{\substack{\sigma\in\{\downarrow,\uparrow\}\\ k\in \mathrm{i}\Omega_{-1}\times\mathbb{Q}\\ n,m\in\{1,\dots,\infty\}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\hbar}\overline{\psi}_{m\sigma}(k+q)\psi_{n\sigma}(k) \tag{35.45}$$

which implies for the product

$$\begin{aligned}\mathcal{G}^2_{0,\nu}(q)\hbar^2\left\langle\rho_\nu(q)\rho_\nu(-q)\right\rangle &= \frac{\mathcal{G}^2_{0,\nu}(q)}{\hbar\beta N_p} \sum_{\substack{\sigma,\sigma'\in\{\downarrow,\uparrow\}\\ k,k'\in \mathrm{i}\Omega_{-1}\times\mathbb{Q}\\ n,n',m,m'\in\{1,\dots,\infty\}}} g_{mn\nu}(\mathbf{k},\mathbf{q})g_{m'n'\nu}(\mathbf{k}',-\mathbf{q})\left\langle\overline{\psi}_{m\sigma}(k+q)\psi_{n\sigma}(k)\overline{\psi}_{m'\sigma'}(k'-q)\psi_{n'\sigma'}(k')\right\rangle\\ &= \frac{\mathcal{G}^2_{0,\nu}(q)}{\hbar\beta N_p} \sum_{\substack{\sigma,\sigma'\in\{\downarrow,\uparrow\}\\ k,k'\in \mathrm{i}\Omega_{-1}\times\mathbb{Q}\\ n,n',m,m'\in\{1,\dots,\infty\}}} g_{mn\nu}(\mathbf{k},\mathbf{q})g_{m'n'\nu}(\mathbf{k}',-\mathbf{q})\left\langle\psi_{n\sigma}(k)\psi_{n'\sigma'}(k')\overline{\psi}_{m'\sigma'}(k'-q)\overline{\psi}_{m\sigma}(k+q)\right\rangle\end{aligned} \tag{35.46}$$

Now we use the Bethe-Salpeter-equation TBReferenced and Equation Exp. Value as GF to approximate[3] the expectation-value as

$$\begin{aligned}&\left\langle\psi_{n\sigma}(k)\psi_{n'\sigma'}(k')\overline{\psi}_{m'\sigma'}(k'-q)\overline{\psi}_{m\sigma}(k+q)\right\rangle\\ &\approx \hbar^2\left(\underset{\sigma,\sigma}{\mathcal{G}_{n,m}}(k,k+q)\underset{\sigma',\sigma'}{\mathcal{G}_{n',m'}}(k',k'-q) - \underset{\sigma,\sigma'}{\mathcal{G}_{n,m'}}(k,k'-q)\underset{\sigma',\sigma}{\mathcal{G}_{n',m}}(k',k+q)\right) + \mathcal{O}(g^2)\\ &= \hbar^2\left(\delta_{q,0}\delta_{n,m}\delta_{n',m'}\mathcal{G}_{n,\sigma}(k)\mathcal{G}_{n',\sigma'}(k') - \delta_{k+q,k'}\delta_{n,m'}\delta_{n',m}\delta_{\sigma,\sigma'}\mathcal{G}_{n,\sigma}(k)\mathcal{G}_{n',\sigma'}(k')\right) + \mathcal{O}(g^2)\end{aligned} \tag{35.47}$$

Plugging this into the equation above yields the final results

$$\begin{aligned}\star\star\star &= -\hbar\mathcal{G}_{0,\nu}(q) \quad + \quad \frac{\hbar}{\beta N_p}\mathcal{G}^2_{0,\nu}(q)\delta_{q,0}\sum_{\substack{k,k'\in \mathrm{i}\Omega_{-1}\times\mathbb{Q}\\ n,n'\in\{1,\dots,\infty\}\\ \sigma,\sigma'\in\{\downarrow,\uparrow\}}} g_{nn\nu}(\mathbf{k},0)g_{n'n'\nu}(\mathbf{k}',0)\mathcal{G}_{n,\sigma}(k)\mathcal{G}_{n',\sigma'}(k')\\ &\quad - \frac{\hbar}{\beta N_p}\mathcal{G}^2_{0,\nu}(q)\sum_{\substack{k\in \mathrm{i}\Omega_{-1}\times\mathbb{Q}\\ n,n'\in\{1,\dots,\infty\}\\ \sigma\in\{\downarrow,\uparrow\}}} g_{n'n\nu}(\mathbf{k},\mathbf{q})g_{nn'\nu}(\mathbf{k}+\mathbf{q},-\mathbf{q})\mathcal{G}_{n,\sigma}(k)\mathcal{G}_{n',\sigma}(k+q) \quad + \quad \mathcal{O}(g^4)\\ &= -\hbar\mathcal{G}_{0,\nu}(q) \quad + \quad \frac{\hbar}{\beta N_p}\mathcal{G}^2_{0,\nu}(q)\delta_{q,0}\sum_{\substack{k,k'\in \mathrm{i}\Omega_{-1}\times\mathbb{Q}\\ n,n'\in\{1,\dots,\infty\}\\ \sigma,\sigma'\in\{\downarrow,\uparrow\}}} g_{nn\nu}(\mathbf{k},0)g_{n'n'\nu}(\mathbf{k}',0)\mathcal{G}_{n,\sigma}(k)\mathcal{G}_{n',\sigma'}(k')\\ &\quad - \frac{\hbar}{\beta N_p}\mathcal{G}^2_{0,\nu}(q)\sum_{\substack{k\in \mathrm{i}\Omega_{-1}\times\mathbb{Q}\\ n,n'\in\{1,\dots,\infty\}\\ \sigma\in\{\downarrow,\uparrow\}}} |g_{n'n\nu}(\mathbf{k},\mathbf{q})|^2\mathcal{G}_{n,\sigma}(k)\mathcal{G}_{n',\sigma}(k+q) \quad + \quad \mathcal{O}(g^4)\end{aligned} \tag{35.48}$$

since we can now replace $\mathcal{G}$ with $\mathcal{G}_0$ since the corrections will only contribute to higher orders in g, which proves the theorem.

[3] In order to go beyond this approximation: See TBDigitalized, TBD6.

Proof 35.13 of Lemma 25.12

We combine Theorem 25.11 with Equation (23.24) to obtain

$$\begin{aligned}\langle H_{\text{ph}}\rangle \approx &-\frac{1}{\hbar\beta}\sum_{\substack{q\in \mathrm{i}\Omega_{+1}\times\mathbb{Q}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}}} \mathrm{e}^{+\mathrm{i}\omega_q 0^+}\Omega_\nu(\mathbf{q})\hbar\mathscr{G}_{0,\nu}(q)\\ &+\frac{1}{\hbar\beta}\sum_{\substack{q\in \mathrm{i}\Omega_{+1}\times\mathbb{Q}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}}} \mathrm{e}^{+\mathrm{i}\omega_q 0^+}\Omega_\nu(\mathbf{q})\frac{\hbar}{\beta N_p}\mathscr{G}^2_{0,\nu}(q)\delta_{q,0}\sum_{\substack{k,k'\in \mathrm{i}\Omega_{-1}\times\mathbb{Q}\\ n,n'\in\{1,\dots,\infty\}\\ \sigma,\sigma'\in\{\downarrow,\uparrow\}}} g_{nn\nu}(\mathbf{k},0)g_{n'n'\nu}(\mathbf{k}',0)\mathscr{G}_{n,\sigma}(k)\mathscr{G}_{n',\sigma'}(k')\\ &-\frac{1}{\hbar\beta}\sum_{\substack{q\in \mathrm{i}\Omega_{+1}\times\mathbb{Q}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}}} \mathrm{e}^{+\mathrm{i}\omega_q 0^+}\Omega_\nu(\mathbf{q})\frac{\hbar}{\beta N_p}\mathscr{G}^2_{0,\nu}(q)\sum_{\substack{k\in \mathrm{i}\Omega_{-1}\times\mathbb{Q}\\ n,n'\in\{1,\dots,\infty\}\\ \sigma\in\{\downarrow,\uparrow\}}} |g_{n'n\nu}(\mathbf{k},\mathbf{q})|^2\mathscr{G}_{n,\sigma}(k)\mathscr{G}_{n',\sigma}(k+q)\end{aligned} \tag{35.49}$$

Now simplifying the appearing terms and neglecting terms of the order $\mathcal{O}(g^4)$ and rearranging the terms yields the desired result.

Proof 35.14 of Corollary 25.13

First Term We compute the phononic, non-interacting contribution and introduce $q \equiv (\mathrm{i}\omega_n, \mathbf{q})$

$$\begin{aligned}\frac{1}{\hbar\beta}\sum_{\mathrm{i}\omega_n\in\mathrm{i}\Omega_{+1}}\left(-\hbar\mathscr{G}_{0,\nu}(q)\right) &= \frac{-1}{\hbar\beta}\sum_{\mathrm{i}\omega_n\in\mathrm{i}\Omega_{+1}}\frac{1}{\mathrm{i}\omega_n-\omega_\nu(\mathbf{q})}\\ &\overset{\text{Corollary 15.22}}{=} \mathrm{B}_{\hbar\beta}(\omega_\nu(\mathbf{q}))\end{aligned} \tag{35.50}$$

Second Term For the mix-terms we compute

$$\begin{aligned}\frac{1}{\beta^2}\sum_{\substack{\omega_k\in\Omega_{-1}\\ \omega_q\in\Omega_{+1}}}\mathscr{G}^2_{0,\nu}(q)\mathscr{G}_{0,n,\sigma}(k)\mathscr{G}_{0,n',\sigma}(k+q) &= \frac{1}{\beta^2\hbar^4}\sum_{\substack{\omega_k\in\Omega_{-1}\\ \omega_q\in\Omega_{+1}}}\frac{1}{\left(\mathrm{i}\omega_q-\omega_\nu(\mathbf{q})\right)^2}\cdot\frac{1}{\mathrm{i}\omega_k-\xi_{n,\sigma,\mathbf{k}}/\hbar}\cdot\frac{1}{\mathrm{i}\omega_{k+q}-\xi_{n',\sigma,\mathbf{k}+\mathbf{q}}/\hbar}\\ &= \dots\end{aligned} \tag{35.51}$$

We now decompose $\Omega_{-1}\ni\omega_{q+k}\equiv\omega_q+\omega_k$, then we can evaluate the sum over ω_k first as

$$\begin{aligned}\dots &= \frac{1}{\hbar^3\beta}\sum_{\omega_q\in\Omega_{+1}}\frac{1}{\left(\mathrm{i}\omega_q-\omega_\nu(\mathbf{q})\right)^2}\cdot\underbrace{\frac{1}{\hbar\beta}\sum_{\omega_k\in\Omega_{-1}}\frac{1}{\mathrm{i}\omega_k-\xi_{n,\sigma,\mathbf{k}}/\hbar}\cdot\frac{1}{\mathrm{i}\omega_k+\mathrm{i}\omega_q-\xi_{n',\sigma,\mathbf{k}+\mathbf{q}}/\hbar}}_{=S_{-1}\equiv\sum_{\omega_k\in\Omega_{-1}}h(\omega_k)}\\ &= \dots\end{aligned} \tag{35.52}$$

We now consider the function

$$\begin{aligned}\mathbb{C}-Z\ni z\mapsto h(-\mathrm{i}z) &= \frac{1}{\hbar\beta}\cdot\frac{1}{z-\xi_{n,\sigma,\mathbf{k}}/\hbar}\cdot\frac{1}{z+\mathrm{i}\omega_q-\xi_{n',\sigma,\mathbf{k}+\mathbf{q}}/\hbar}\\ &= \frac{1}{\hbar\beta}\cdot\frac{1}{z-z_1}\cdot\frac{1}{z-z_2}\end{aligned} \tag{35.53}$$

with first order poles

$$z_1 = \xi_{n,\sigma,\mathbf{k}}/\hbar, \qquad z_2 = \xi_{n',\sigma,\mathbf{k}+\mathbf{q}}/\hbar - \mathrm{i}\omega_q \tag{35.54}$$

This gives with Theorem 15.20 (a version of the Residue-theorem)

$$S_{-1} = \sum_{\omega_k \in \Omega_{-1}} h(\omega_k) = -\zeta \sum_{l=1}^{2} \mathrm{Res}(f_\zeta(z), z = z_l)|_{\zeta=-1} \tag{35.55}$$

with auxiliary function

$$f_\zeta(z)|_{\zeta=-1} = g_\zeta(z) h(-\mathrm{i}z)|_{\zeta=-1} = \hbar\beta n^\zeta_{\hbar\beta}(z) h(-\mathrm{i}z)|_{\zeta=-1} \tag{35.56}$$

This gives for the first residue

$$\begin{aligned} \mathrm{Res}(f_\zeta(z), z = z_1)|_{\zeta=-1} &= \lim_{z \to z_1} (z - z_1) f_\zeta(z)|_{\zeta=-1} \\ &= \lim_{z \to z_1} (z - z_2)^{-1} \, \mathrm{F}_{\hbar\beta}(z) \\ &= \frac{\mathrm{F}_\beta(\xi_{n,\sigma,\mathbf{k}})}{\xi_{n,\sigma,\mathbf{k}}/\hbar - \xi_{n',\sigma,\mathbf{k}+\mathbf{q}}/\hbar + \mathrm{i}\omega_q} \end{aligned} \tag{35.57}$$

For the second residue we obtain likewise

$$\begin{aligned} \mathrm{Res}(f_\zeta(z), z = z_2)|_{\zeta=-1} &= \lim_{z \to z_2} (z - z_2) f_\zeta(z)|_{\zeta=-1} \\ &= \lim_{z \to z_2} (z - z_1)^{-1} \, \mathrm{F}_{\hbar\beta}(z) \\ &= \frac{\mathrm{F}_\beta(\xi_{n',\sigma,\mathbf{k}+\mathbf{q}} - \mathrm{i}\hbar\omega_q)}{\xi_{n',\sigma,\mathbf{k}+\mathbf{q}}/\hbar - \xi_{n,\sigma,\mathbf{k}}/\hbar - \mathrm{i}\omega_q} \\ &\overset{\star}{=} \frac{\mathrm{F}_\beta(\xi_{n',\sigma,\mathbf{k}+\mathbf{q}})}{\xi_{n',\sigma,\mathbf{k}+\mathbf{q}}/\hbar - \xi_{n,\sigma,\mathbf{k}}/\hbar - \mathrm{i}\omega_q} \end{aligned} \tag{35.58}$$

whereas in $\star$ we used Remark 9.65.1. Summing up the residues yields then

$$\begin{aligned} \ldots &= \frac{\mathrm{F}_\beta(\xi_{n,\sigma,\mathbf{k}}) - \mathrm{F}_\beta(\xi_{n',\sigma,\mathbf{k}+\mathbf{q}})}{\hbar^2} \underbrace{\frac{1}{\hbar\beta} \sum_{\omega_q \in \Omega_{+1}} \frac{1}{\left(\mathrm{i}\omega_q - \omega_\nu(\mathbf{q})\right)^2} \cdot \frac{1}{\mathrm{i}\omega_q + \xi_{n,\sigma,\mathbf{k}}/\hbar - \xi_{n',\sigma,\mathbf{k}+\mathbf{q}}/\hbar}}_{= S_{+1} \equiv \sum_{\omega_q \in \Omega_{+1}} h(\omega_q)} \\ &= \ldots \end{aligned} \tag{35.59}$$

We now, again, consider the function

$$\begin{aligned} \mathbb{C} - Z \ni z \mapsto h(-\mathrm{i}z) &= \frac{1}{\hbar\beta} \cdot \frac{1}{(z - \omega_\nu(\mathbf{q}))^2} \cdot \frac{1}{z + \xi_{n,\sigma,\mathbf{k}}/\hbar - \xi_{n',\sigma,\mathbf{k}+\mathbf{q}}/\hbar} \\ &= \frac{1}{\hbar\beta} \cdot \frac{1}{(z - z_2)^2} \cdot \frac{1}{z - z_1} \end{aligned} \tag{35.60}$$

with poles of different order

- $z_1 = \xi_{n',\sigma,\mathbf{k}+\mathbf{q}}/\hbar - \xi_{n,\sigma,\mathbf{k}}/\hbar$ (first order pole)
- $z_2 = \omega_\nu(\mathbf{q})$ (second order pole)

This gives with Theorem 15.20

$$S_{+1} = \sum_{\omega_q \in \Omega_{+1}} h(\omega_q) = -\sum_{l=1}^{2} \mathrm{Res}(f_{+1}(z), z = z_l) = \star\star\star \tag{35.61}$$

with auxiliary function

$$f_{+1}(z) = \hbar\beta\, \mathrm{B}_{\hbar\beta}(z) h(-\mathrm{i}z) = \hbar\beta\, \mathrm{B}_{\hbar\beta}(z) \cdot \frac{1}{\hbar\beta} \cdot \frac{1}{(z-z_2)^2} \cdot \frac{1}{z-z_1} = \mathrm{B}_{\hbar\beta}(z) \cdot \frac{1}{(z-z_2)^2} \cdot \frac{1}{z-z_1} \tag{35.62}$$

This gives for the first residue

$$-\mathrm{Res}(f_{+1}(z), z = z_1) = -\lim_{z \to z_1} (z-z_2)^{-2}\, \mathrm{B}_{\hbar\beta}(z) = \frac{-\,\mathrm{B}_\beta(\xi_{n',\sigma,\mathbf{k}+\mathbf{q}} - \xi_{n,\sigma,\mathbf{k}})}{\left(\xi_{n',\sigma,\mathbf{k}+\mathbf{q}}/\hbar - \xi_{n,\sigma,\mathbf{k}}/\hbar - \omega_\nu(\mathbf{q})\right)^2} \tag{35.63}$$

Now we compute the second residue

$$-\mathrm{Res}(f_{+1}(z), z = z_2) = -\lim_{z \to z_2} \frac{\mathrm{d}}{\mathrm{d}z} \left[(z-z_1)^{-1}\, \mathrm{B}_{\hbar\beta}(z)\right] = \square\square\square \tag{35.64}$$

which gives with Lemma 9.64 the result

$$\begin{aligned} \square\square\square &= \lim_{z \to z_2} -\Big[-(z-z_1)^{-2}\, \mathrm{B}_{\hbar\beta}(z) + (z-z_1)^{-1} \cdot (-\hbar\beta)\, \mathrm{B}_{\hbar\beta}(z) \left(1 + \mathrm{B}_{\hbar\beta}(z)\right) \Big] \\ &= \frac{\mathrm{B}_\beta(\Omega_\nu(\mathbf{q}))}{\left(\omega_\nu(\mathbf{q}) + \xi_{n,\sigma,\mathbf{k}}/\hbar - \xi_{n',\sigma,\mathbf{k}+\mathbf{q}}/\hbar\right)^2} + \frac{\hbar\beta\, \mathrm{B}_\beta(\Omega_\nu(\mathbf{q})) \left(1 + \mathrm{B}_\beta(\Omega_\nu(\mathbf{q}))\right)}{\omega_\nu(\mathbf{q}) + \xi_{n,\sigma,\mathbf{k}}/\hbar - \xi_{n',\sigma,\mathbf{k}+\mathbf{q}}/\hbar} \end{aligned} \tag{35.65}$$

This gives the result

$$\star\star\star = \boxed{\text{TBD}}. \tag{35.66}$$

Using now Equation (TBReferenced) we obtain the final expression as

$$\begin{aligned} &\frac{1}{\beta^2} \sum_{\substack{\omega_k \in \Omega_{-1} \\ \omega_q \in \Omega_{+1}}} \mathscr{G}^2_{0,\nu}(q) \mathscr{G}_{0,n,\sigma}(k) \mathscr{G}_{0,n',\sigma}(k+q) \\ &= \dots \\ &= \frac{\mathrm{F}_\beta(\xi_{n,\sigma,\mathbf{k}}) - \mathrm{F}_\beta(\xi_{n',\sigma,\mathbf{k}+\mathbf{q}})}{\hbar^2} \Big[\frac{\mathrm{B}_\beta(\Omega_\nu(\mathbf{q})) - \mathrm{B}_\beta(\xi_{n',\sigma,\mathbf{k}+\mathbf{q}} - \xi_{n,\sigma,\mathbf{k}})}{\left(\omega_\nu(\mathbf{q}) + \xi_{n,\sigma,\mathbf{k}}/\hbar - \xi_{n',\sigma,\mathbf{k}+\mathbf{q}}/\hbar\right)^2} + \frac{\hbar\beta\, \mathrm{B}_\beta(\Omega_\nu(\mathbf{q})) \left(1 + \mathrm{B}_\beta(\Omega_\nu(\mathbf{q}))\right)}{\omega_\nu(\mathbf{q}) + \xi_{n,\sigma,\mathbf{k}}/\hbar - \xi_{n',\sigma,\mathbf{k}+\mathbf{q}}/\hbar} \Big] \end{aligned} \tag{35.67}$$

now we use Lemma 9.66 to obtain

$$\mathrm{B}_\beta(\Omega_\nu(\mathbf{q}))\left(1+\mathrm{B}_\beta(\Omega_\nu(\mathbf{q}))\right) = 4^{-1}\,\mathrm{csch}^2\left(\frac{\beta\Omega_\nu(\mathbf{q})}{2}\right) \tag{35.68}$$

which proves the corollary. Notice that Equation (35.67) has the right unit, namely Energy^{-2}.

Proof 35.15 of Lemma 25.14

We first simplify Equation (23.25): We use Equation (23.20) to integrate out the phonons, such that we can obtain

$$\frac{\partial}{\partial\bar{j}(\mathrm{i}\omega_m,\mathbf{q}\nu)}Z[j,\bar{j}] = \int\mathscr{D}(\overline{\psi},\psi)\left(\frac{-\partial}{\partial\bar{j}(\mathrm{i}\omega_m,\mathbf{q}\nu)}S_{\substack{\text{el-el-int}\\[j_{\text{ph}},\bar{j}_{\text{ph}}]}}[\psi,\overline{\psi}]\right)\exp - S_{j,\bar{j}}[\psi,\overline{\psi}] \tag{35.69}$$

and

$$\frac{\partial}{\partial j(-\mathrm{i}\omega_m,-\mathbf{q}\nu)}Z[j,\bar{j}] = \int\mathscr{D}(\overline{\psi},\psi)\left(\frac{-\partial}{\partial j(-\mathrm{i}\omega_m,-\mathbf{q}\nu)}S_{\substack{\text{el-el-int}\\[j_{\text{ph}},\bar{j}_{\text{ph}}]}}[\psi,\overline{\psi}]\right)\exp - S_{j,\bar{j}}[\psi,\overline{\psi}] \tag{35.70}$$

Now we use Equation (23.16) to obtain the explicit form of these derivatives as

$$\frac{-\partial}{\partial j(\mathrm{i}\omega_m,\mathbf{q}\nu)}S_{\substack{\text{el-el-int}\\[j_{\text{ph}},\bar{j}_{\text{ph}}]}}[\psi,\overline{\psi}] = -\hbar\bar{j}_\nu(q)\mathscr{G}_{0,\nu}(q)+\hbar\rho_\nu(q)\mathscr{G}_{0,\nu}(q) \tag{35.71}$$

and

$$\frac{-\partial}{\partial\bar{j}(\mathrm{i}\omega_m,\mathbf{q}\nu)}S_{\substack{\text{el-el-int}\\[j_{\text{ph}},\bar{j}_{\text{ph}}]}}[\psi,\overline{\psi}] = -\hbar\mathscr{G}_{0,\nu}(-q)j_\nu(-q)+\hbar\mathscr{G}_{0,\nu}(-q)\rho_\nu(q) \tag{35.72}$$

Now we can use Equation (23.20) again to obtain

$$\frac{\partial}{\partial j_{m,\sigma}(\mathrm{i}\omega_{n'},\mathbf{k}+\mathbf{q})}Z[j,\bar{j}] = \int\mathscr{D}(\overline{\psi},\psi)\underbrace{\left(\frac{\partial}{\partial j_{m,\sigma}(\mathrm{i}\omega_{n'},\mathbf{k}+\mathbf{q})}\sum\overline{\psi}j_{\text{el}}\right)}_{=-\psi_{m\sigma}(\mathrm{i}\omega_{n'},\mathbf{k}+\mathbf{q})}\exp - S_{[j,\bar{j}]}[\psi,\overline{\psi}] \tag{35.73}$$

This implies that

$$\frac{\partial^2}{\partial\bar{j}_{n,\sigma}(\mathrm{i}\omega_n,\mathbf{k})\partial j_{m,\sigma}(\mathrm{i}\omega_{n'},\mathbf{k}+\mathbf{q})}\frac{Z[j,\bar{j}]}{Z}|_{j=\bar{j}=0} = \left\langle\overline{\psi}_{m\sigma}(\mathrm{i}\omega_{n'},\mathbf{k}+\mathbf{q})\psi_{n\sigma}(\mathrm{i}\omega_n,\mathbf{k})\right\rangle \tag{35.74}$$

Now we combine this with Equation (22.24) to obtain the desired result:

$$\begin{aligned}\langle H_{\text{int}}\rangle &= \sum_{\substack{\mathbf{k},\mathbf{q}\in\mathrm{Q}\\ \sigma\in\{\downarrow,\uparrow\}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ n,m\in\{1,\dots,\infty\}\\ \omega_m\in\Omega_{+1}\\ \omega_n,\omega_{n'}\in\Omega_{-1}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})\hbar}{\sqrt{N_p}\sqrt{\hbar\beta}^3}\quad \left\langle \overline{\psi}_{m\sigma}(\mathrm{i}\omega_{n'},\mathbf{k}+\mathbf{q})\psi_{n\sigma}(\mathrm{i}\omega_n,\mathbf{k})\Big[\rho_\nu(\mathrm{i}\omega_m,\mathbf{q})\mathscr{G}_{0,\nu}(\mathrm{i}\omega_m,\mathbf{q})+\mathscr{G}_{0,\nu}(-\mathrm{i}\omega_m,-\mathbf{q})\rho_\nu(\mathrm{i}\omega_m,\mathbf{q})\Big]\right\rangle \\ &= \sum_{\substack{k\in\mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ q\in\mathrm{i}\Omega_{+1}\times\mathrm{Q}\\ \sigma\in\{\downarrow,\uparrow\}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ n,m\in\{1,\dots,\infty\}\\ \omega_{n'}\in\Omega_{-1}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})\hbar}{\sqrt{N_p}\sqrt{\hbar\beta}^3}\quad \left\langle \overline{\psi}_{m\sigma}(\mathrm{i}\omega_{n'},\mathbf{k}+\mathbf{q})\psi_{n\sigma}(\mathrm{i}\omega_n,\mathbf{k})\Big[\rho_\nu(q)\mathscr{G}_{0,\nu}(q)+\mathscr{G}_{0,\nu}(-q)\rho_\nu(q)\Big]\right\rangle\end{aligned} \tag{35.75}$$

Proof 35.16 of Corollary 25.15

We decompose Equation (25.16) as

$$\begin{aligned}\langle H_{\text{int}}\rangle &= \sum_{\substack{k\in\mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ q\in\mathrm{i}\Omega_{+1}\times\mathrm{Q}\\ \sigma\in\{\downarrow,\uparrow\}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ n,m\in\{1,\dots,\infty\}\\ \omega_{n'}\in\Omega_{-1}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})\hbar}{\sqrt{N_p}\sqrt{\hbar\beta}^3}\quad \left\langle \overline{\psi}_{m\sigma}(\mathrm{i}\omega_{n'},\mathbf{k}+\mathbf{q})\psi_{n\sigma}(\mathrm{i}\omega_n,\mathbf{k})\Big[\rho_\nu(q)\mathscr{G}_{0,\nu}(q)+\mathscr{G}_{0,\nu}(-q)\rho_\nu(q)\Big]\right\rangle \\ &\equiv \qquad\qquad \mathrm{I} \qquad + \qquad \mathrm{II}\end{aligned} \tag{35.76}$$

We focus on the first term I and compute

$$\begin{aligned}\mathrm{I} &= \sum_{\substack{k,\widetilde{k}\in\mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ q\in\mathrm{i}\Omega_{+1}\times\mathrm{Q}\\ \sigma,\widetilde{\sigma}\in\{\downarrow,\uparrow\}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ n,\widetilde{n},m,\widetilde{m}\in\{1,\dots,\infty\}\\ \omega_{n'}\in\Omega_{-1}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})g_{\widetilde{m}\widetilde{n}\nu}(\widetilde{\mathbf{k}},\mathbf{q})}{N_p(\hbar\beta)^2}\left\langle \overline{\psi}_{m\sigma}(\mathrm{i}\omega_{n'},\mathbf{k}+\mathbf{q})\psi_{n\sigma}(k)\overline{\psi}_{\widetilde{m}\widetilde{\sigma}}(\widetilde{k}+q)\psi_{\widetilde{n}\widetilde{\sigma}}(\widetilde{k})\right\rangle\mathscr{G}_{0,\nu}(q) \\ &= \dots\end{aligned} \tag{35.77}$$

Now we simplify the correlator as

$$\begin{aligned}&\left\langle \overline{\psi}_{m\sigma}(\mathrm{i}\omega_{n'},\mathbf{k}+\mathbf{q})\psi_{n\sigma}(k)\overline{\psi}_{\widetilde{m}\widetilde{\sigma}}(\widetilde{k}+q)\psi_{\widetilde{n}\widetilde{\sigma}}(\widetilde{k})\right\rangle \\ &= -\left\langle \psi_{n\sigma}(k)\psi_{\widetilde{n}\widetilde{\sigma}}(\widetilde{k})\overline{\psi}_{m\sigma}(\mathrm{i}\omega_{n'},\mathbf{k}+\mathbf{q})\overline{\psi}_{\widetilde{m}\widetilde{\sigma}}(\widetilde{k}+q)\right\rangle \\ &= -\Big[\left\langle \psi_{n\sigma}(k)\overline{\psi}_{\widetilde{m}\widetilde{\sigma}}(\widetilde{k}+q)\right\rangle_0\left\langle \psi_{\widetilde{n}\widetilde{\sigma}}(\widetilde{k})\overline{\psi}_{m\sigma}(\mathrm{i}\omega_{n'},\mathbf{k}+\mathbf{q})\right\rangle_0 \quad - \left\langle \psi_{n\sigma}(k)\overline{\psi}_{m\sigma}(\mathrm{i}\omega_{n'},\mathbf{k}+\mathbf{q})\right\rangle_0\left\langle \psi_{\widetilde{n}\widetilde{\sigma}}(\widetilde{k})\overline{\psi}_{\widetilde{m}\widetilde{\sigma}}(\widetilde{k}+q)\right\rangle_0 + \mathcal{O}(g^2)\Big] \\ &= -\hbar^2\Big[\mathscr{G}_{\substack{0\\ n,\widetilde{m}\\ \sigma,\widetilde{\sigma}}}(k,\widetilde{k}+q)\mathscr{G}_{\substack{0\\ \widetilde{n},m\\ \widetilde{\sigma},\sigma}}\begin{pmatrix}\mathrm{i}\omega_{\widetilde{k}},\mathrm{i}\omega_{n'}\\ \widetilde{\mathbf{k}},\mathbf{k}+\mathbf{q}\end{pmatrix} \quad - \mathscr{G}_{\substack{0\\ n,m\\ \sigma,\sigma}}\begin{pmatrix}\mathrm{i}\omega_k,\mathrm{i}\omega_{n'}\\ \mathbf{k},\mathbf{k}+\mathbf{q}\end{pmatrix}\mathscr{G}_{\substack{0\\ \widetilde{n},\widetilde{m}\\ \widetilde{\sigma},\widetilde{\sigma}}}(\widetilde{k},\widetilde{k}+q)\Big]\end{aligned} \tag{35.78}$$

This gives a natural decomposition for

$$\mathrm{I} = \dots = \mathrm{I1} + \mathrm{I2} \tag{35.79}$$

Now we simplify

$$I1 = \sum_{\substack{k,\tilde{k}\in \mathrm{i}\Omega_{-1}\times\mathbb{Q} \\ (\mathrm{i}\omega_q,\mathbf{q})\equiv q\in \mathrm{i}\Omega_{+1}\times\mathbb{Q} \\ \sigma,\tilde{\sigma}\in\{\downarrow,\uparrow\} \\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\} \\ n,\tilde{n},m,\tilde{m}\in\{1,\ldots,\infty\} \\ \omega_{n'}\in\Omega_{-1}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})g_{\tilde{m}\tilde{n}\nu}(\widetilde{\mathbf{k}},\mathbf{q})}{N_p\beta^2}\cdot(-1)\cdot\left[\delta_{n,\tilde{m}}\delta_{\sigma,\tilde{\sigma}}\delta_{k-q,\tilde{k}}\mathscr{G}_{0,n,\sigma}(k)\delta_{\tilde{n},m}\delta_{\omega_{\tilde{k}},\omega_{n'}}\delta_{\widetilde{\mathbf{k}},\mathbf{k}+\mathbf{q}}\mathscr{G}_{0,m,\sigma}(\mathrm{i}\omega_k,\mathbf{k})\right] \tag{35.80}$$
$$= \star\star\star$$

Now we use the individual delta-functions to ...

1. kill $\tilde{m}$,
2. kill $\tilde{\sigma}$,
3. kill $\tilde{k}$,
4. kill $\tilde{n}$,
5. kill $\omega_{n'}$ as $\tilde{k}$ is already killed,
6. kill $\mathbf{q}$ as $\tilde{k}$ is already killed.

This allows us to simplify

$$\begin{aligned}
\star\star\star &= \sum_{\substack{k\in \mathrm{i}\Omega_{-1}\times\mathbb{Q} \\ \mathrm{i}\omega_q\in\Omega_{+1} \\ \sigma\in\{\downarrow,\uparrow\} \\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\} \\ n,m\in\{1,\ldots,\infty\}}} \frac{g_{mn\nu}(\mathbf{k},0)g_{nm\nu}(\mathbf{k},0)}{N_p\beta^2}\cdot(-1)\cdot\mathscr{G}_{0,n,\sigma}(k)\mathscr{G}_{0,m,\sigma}(\mathrm{i}\omega_{k-q},\mathbf{k}) \\
&= \sum_{\substack{\mathbf{k}\in\mathbb{Q} \\ \sigma\in\{\downarrow,\uparrow\} \\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\} \\ n,m\in\{1,\ldots,\infty\}}} \frac{-|g_{mn\nu}(\mathbf{k},0)|^2}{N_p\beta^2\hbar^2}\sum_{\substack{\mathrm{i}\omega_k\in\Omega_{-1} \\ \mathrm{i}\omega_q\in\Omega_{+1}}}\frac{1}{\mathrm{i}\omega_k-\xi_{n,\sigma}/\hbar}\cdot\frac{1}{\mathrm{i}\omega_k-\mathrm{i}\omega_q-\xi_{m,\sigma}/\hbar} \\
&= \sum_{\substack{\mathbf{k}\in\mathbb{Q} \\ \sigma\in\{\downarrow,\uparrow\} \\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\} \\ n,m\in\{1,\ldots,\infty\}}} \frac{-|g_{mn\nu}(\mathbf{k},0)|^2}{N_p}\frac{1}{\hbar\beta}\sum_{\omega_k\in\Omega_{-1}}\frac{1}{\mathrm{i}\omega_k-\xi_{n,\sigma}/\hbar}\cdot\underbrace{\frac{1}{\hbar\beta}\sum_{\omega_q\in\Omega_{+1}}\frac{1}{\mathrm{i}\omega_q-\mathrm{i}\omega_k+\xi_{m,\sigma}/\hbar}}_{=-\mathrm{B}_\beta(\xi_{m,\sigma}-\mathrm{i}\hbar\omega_k)}
\end{aligned} \tag{35.81}$$

whereas we used corollary 16.15 (or something).

Intermezzo: We now simplify $\mathrm{B}_\beta(\bullet-\mathrm{i}\hbar\omega_k)$ ... TBContinued.

Proof 35.17 of Theorem 25.16

For **the electronic contribution** of the expectation-value we simply refer to Theorem 25.9.

For **the phononic contribution**, we simplify refer to Corollary 25.13.

For **the interaction contribution**, we refer to Theorem TBCreated after PP3 has been digitalized.

Proof 35.18 of Lemma 25.19 We compute the derivative of Equation (24.26) as

$$\begin{aligned}\left(\partial_T F\right)(\mu,T) &= \langle N\rangle(\mu,T)\\ &= \partial_T \frac{-1}{\pi}\lim_{\delta\to 0}\sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}\in \mathrm{Q}\\ \sigma\in\{\uparrow,\downarrow\}\\ m\in\{1,\dots,\infty\}\\ E\in(-\infty,+\infty)}} \mathrm{F}_\beta(E)\,\mathrm{Im}\,G^{\mathrm{ret}}_{\substack{m,m\\ \sigma,\sigma}}(E+\mathrm{i}\delta,\mathbf{k})\\ &= \frac{-1}{\pi}\lim_{\delta\to 0}\sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}\in \mathrm{Q}\\ \sigma\in\{\uparrow,\downarrow\}\\ m\in\{1,\dots,\infty\}\\ E\in(-\infty,+\infty)}} \left[\left(\partial_T\,\mathrm{F}_\beta(E)\right)\mathrm{Im}\,G^{\mathrm{ret}}_{\substack{m,m\\ \sigma,\sigma}}(E+\mathrm{i}\delta,\mathbf{k}) + \mathrm{F}_\beta(E)\,\mathrm{Im}\,\partial_T G^{\mathrm{ret}}_{\substack{m,m\\ \sigma,\sigma}}(E+\mathrm{i}\delta,\mathbf{k})\right]\\ &= \dots\end{aligned} \tag{35.82}$$

Now we use Lemma 9.66, i.e. we use the Equation

$$\partial_T\,\mathrm{F}_\beta(E) = \frac{E}{k_B T^2}\,\mathrm{F}_\beta(E)\left(1-\mathrm{F}_\beta(E)\right) \tag{35.83}$$

and for the other derivative we have

$$\partial_T G^{\mathrm{ret}}_{m,\sigma,\mathbf{k}}(E+\mathrm{i}\delta) = \partial_T \frac{1}{E+\mathrm{i}\delta-\left(\epsilon_{m\mathbf{k}\sigma}+\Sigma^{\mathrm{ret}}_{m,\sigma,\mathbf{k}}(E+\mathrm{i}\delta)-\mu\right)} = \frac{\partial_T\Sigma^{\mathrm{ret}}_{m,\sigma,\mathbf{k}}(E+\mathrm{i}\delta)}{E+\mathrm{i}\delta-\left(\epsilon_{m\mathbf{k}\sigma}+\Sigma^{\mathrm{ret}}_{m,\sigma,\mathbf{k}}(E+\mathrm{i}\delta)-\mu\right)^2} \tag{35.84}$$

Now we compute the derivative and use the diagonal bands approximation for the self-energy and use Lemma 9.66

$$\begin{aligned}\partial_T\Sigma^{\mathrm{ret}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta) &= \sum_{\substack{\mathbf{q}\in \mathrm{Q}\\ n\in\{1,\dots,\infty\}\\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} \frac{|g_{nm\nu}(\mathbf{k},\mathbf{q})|^2}{N_p}\left[\partial_T\frac{\mathrm{B}_\beta(\Omega_\nu(\mathbf{q}))+\mathrm{F}_\beta(\xi_{n\sigma\mathbf{k}+\mathbf{q}})}{E+\mathrm{i}\delta-\xi_{n\sigma\mathbf{k}+\mathbf{q}}+\Omega_\nu(\mathbf{q})}+\partial_T\frac{\mathrm{B}_\beta(\Omega_\nu(\mathbf{q}))+1-\mathrm{F}_\beta(\xi_{n\sigma\mathbf{k}+\mathbf{q}})}{E+\mathrm{i}\delta-\xi_{n\sigma\mathbf{k}+\mathbf{q}}-\Omega_\nu(\mathbf{q})}\right]\\ &= \sum_{\substack{\mathbf{q}\in \mathrm{Q}\\ n\in\{1,\dots,\infty\}\\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} \frac{|g_{nm\nu}(\mathbf{k},\mathbf{q})|^2}{4k_BT^2N_p}\left[\frac{\Omega_\nu(\mathbf{q})\,\mathrm{csch}^2(\beta\Omega_\nu(\mathbf{q})/2)+\xi_{n\sigma\mathbf{k}+\mathbf{q}}\,\mathrm{sech}^2(\beta\xi_{n\sigma\mathbf{k}+\mathbf{q}}/2)}{E+\mathrm{i}\delta-\xi_{n\sigma\mathbf{k}+\mathbf{q}}+\Omega_\nu(\mathbf{q})}+\frac{\Omega_\nu(\mathbf{q})\,\mathrm{csch}^2(\beta\Omega_\nu(\mathbf{q})/2)-\xi_{n\sigma\mathbf{k}+\mathbf{q}}\,\mathrm{sech}^2(\beta\xi_{n\sigma\mathbf{k}+\mathbf{q}}/2)}{E+\mathrm{i}\delta-\xi_{n\sigma\mathbf{k}+\mathbf{q}}-\Omega_\nu(\mathbf{q})}\right]\end{aligned} \tag{35.85}$$

now we multiply both sides of this equation with k_BT^2. For the Hartree-contribution we obtain with Equation (21.10) the equation

$$\begin{aligned}\partial_T\Sigma^{\mathrm{Hartree}}_{m\sigma\mathbf{k}}(\bullet) &= -\sum_{\substack{\mathbf{q}\in \mathrm{Q}\\ \sigma'\in\{\downarrow,\uparrow\}\\ n\in\{1,2,\dots\}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}}} \frac{g_{mm\nu}(\mathbf{k},0)g_{nn\nu}(\mathbf{q},0)}{N_p}\frac{1}{\Omega_\nu(\mathbf{q}'\equiv 0)}\partial_T\left(\mathrm{F}_\beta(\xi_{n\sigma'\mathbf{q}})\right)\\ &= \dots\end{aligned} \tag{35.86}$$

now we use Lemma 9.66 and obtain finally

$$\ldots = - \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ \sigma'\in\{\downarrow,\uparrow\} \\ n\in\{1,2,\ldots\} \\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} \frac{g_{mm\nu}(\mathbf{k},0)g_{nn\nu}(\mathbf{q},0)}{N_p} \frac{1}{\Omega_\nu(\mathbf{q}'\equiv 0)} \frac{\xi_{n\sigma'\mathbf{q}}}{4k_{\mathrm{B}}T^2} \partial_T \left(\operatorname{sech}^2 \frac{\xi_{n\sigma'\mathbf{q}}}{2k_{\mathrm{B}}T}\right)^2 \tag{35.87}$$

Proof 35.19 of Lemma 25.20 We rewrite the particle-number equation as

$$\langle N\rangle(\mu,T) = \frac{-1}{\pi} \lim_{\delta\to 0} \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}\in \mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\} \\ E\in(-\infty,+\infty)}} \mathrm{F}_\beta(E)\,\mathrm{Im}\,\frac{1}{E+\mu+\mathrm{i}\delta - \left(\epsilon_{m\sigma\mathbf{k}} + \widetilde{\Sigma}^{\mathrm{ret}}_{m\sigma\mathbf{k}}(E+\mu+\mathrm{i}\delta)\right)} = \ldots \tag{35.88}$$

whereas we introduced

$$\widetilde{\Sigma}^{\mathrm{ret}}_{m\sigma\mathbf{k}}(E+\mu+\mathrm{i}\delta) = \widetilde{\Sigma}^{\mathrm{Hartree}}_{m\sigma\mathbf{k}}(E+\mu+\mathrm{i}\delta) + \widetilde{\Sigma}^{\mathrm{Fock}}_{m\sigma\mathbf{k}}(E+\mu+\mathrm{i}\delta) \tag{35.89}$$

with Hartree-contribution

$$\widetilde{\Sigma}^{\mathrm{Hartree}}_{m\sigma\mathbf{k}}(\bullet) = - \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ \sigma'\in\{\downarrow,\uparrow\} \\ n\in\{1,2,\ldots\} \\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} \frac{g_{mm\nu}(\mathbf{k},0)g_{nn\nu}(\mathbf{q},0)}{N_p} \frac{\mathrm{F}_\beta(\epsilon_{n\sigma'\mathbf{q}}-\mu)}{\Omega_\nu(\mathbf{q}'=0)} \tag{35.90}$$

and Fock-contribution

$$\widetilde{\Sigma}^{\mathrm{Fock}}_{m\sigma\mathbf{k}}(E+\mu+\mathrm{i}\delta) = \sum_{\substack{\mathbf{q}\in \mathrm{Q} \\ n\in\{1,2,\ldots\} \\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} \frac{|g_{nm\nu}(\mathbf{k},\mathbf{q})|^2}{N_p} \left[\frac{\mathrm{B}_\beta(\Omega_\nu(\mathbf{q})) + \mathrm{F}_\beta(\xi_{\mathbf{q}+\mathbf{k}n\sigma})}{E+\mu+\mathrm{i}\delta-\epsilon_{\mathbf{q}+\mathbf{k}n\sigma}+\Omega_\nu(\mathbf{q})} + \frac{\mathrm{B}_\beta(\Omega_\nu(\mathbf{q})) + 1 - \mathrm{F}_\beta(\xi_{\mathbf{q}+\mathbf{k}n\sigma})}{E+\mu+\mathrm{i}\delta-\epsilon_{\mathbf{q}+\mathbf{k}n\sigma}-\Omega_\nu(\mathbf{q})}\right] \tag{35.91}$$

now, using the substitution-rule allows us to rewrite the above Equation as

$$\langle N\rangle(\mu,T) = \ldots = \frac{-1}{\pi} \lim_{\delta\to 0} \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}\in \mathrm{Q} \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\} \\ E\in(-\infty,+\infty)}} \mathrm{F}_\beta(E-\mu)\,\mathrm{Im}\,\frac{1}{E+\mathrm{i}\delta - \left(\epsilon_{m\sigma\mathbf{k}} + \widetilde{\Sigma}^{\mathrm{ret}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta)\right)} \tag{35.92}$$

Now we use Equation (TBReferenced) together with Lemma TBReferenced, and introduce the function

$$g(\mu) = \beta(E-\mu) \quad \text{which implies} \quad \left(\frac{\mathrm{d}g}{\mathrm{d}\mu}\right)(\mu) = -\beta \tag{35.93}$$

such that we obtain

$$\mathrm{F}_\beta(E-\mu) = \mathrm{F}(g(\mu)) \tag{35.94}$$

which implies with the chain-rule

$$\partial_\mu \left(\mathrm{F}\circ g\right)(\mu) = \left(\partial_\mu \mathrm{F}\right)(g(\mu)) \cdot \left(\frac{\mathrm{d}g}{\mathrm{d}\mu}\right)(\mu) = \frac{1}{4}\,\mathrm{sech}^2\left(\beta\frac{E-\mu}{2}\right)\cdot\beta \tag{35.95}$$

Analogously we obtain

$$\partial_\mu \widetilde{\Sigma}^{\mathrm{ret}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta) = \partial_\mu \widetilde{\Sigma}^{\mathrm{Hartree}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta) + \partial_\mu \widetilde{\Sigma}^{\mathrm{Fock}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta) \tag{35.96}$$

with Hartree-contribution

$$\partial_\mu \widetilde{\Sigma}^{\mathrm{Hartree}}_{m\sigma\mathbf{k}}(\bullet) = -\sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ \sigma'\in\{\downarrow,\uparrow\}\\ n\in\{1,2,\ldots\}\\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} \frac{g_{mm\nu}(\mathbf{k},0)g_{nn\nu}(\mathbf{q},0)}{4N_p}\frac{\beta}{\Omega_\nu(\mathbf{q}'=0)}\,\mathrm{sech}^2\left(\beta\xi_{n\sigma'\mathbf{q}}/2\right) \tag{35.97}$$

and Fock-contribution

$$\partial_\mu \widetilde{\Sigma}^{\mathrm{Fock}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta) = \sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ n\in\{1,2,\ldots\}\\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} \frac{|g_{nm\nu}(\mathbf{k},\mathbf{q})|^2}{4N_p k_B T}\mathrm{sech}^2(\beta\xi_{\mathbf{q}+\mathbf{k}n\sigma}/2)\left[\frac{1}{E+\mathrm{i}\delta-\epsilon_{\mathbf{q}+\mathbf{k}n\sigma}+\Omega_\nu(\mathbf{q})}-\frac{1}{E+\mathrm{i}\delta-\epsilon_{\mathbf{q}+\mathbf{k}n\sigma}-\Omega_\nu(\mathbf{q})}\right] \tag{35.98}$$

Now we can compute the derivative as

$$\langle N\rangle(\mu,T) = \frac{-1}{\pi}\lim_{\delta\to 0}\sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}\in\mathrm{Q}\\ \sigma\in\{\uparrow,\downarrow\}\\ m\in\{1,\ldots,\infty\}\\ E\in(-\infty,+\infty)}} \mathrm{F}_\beta(E-\mu)\,\mathrm{Im}\left[E+\mathrm{i}\delta-\left(\epsilon_{m\sigma\mathbf{k}}+\widetilde{\Sigma}^{\mathrm{ret}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta)\right)\right]^{-1} \tag{35.99}$$

which implies

$$\begin{aligned}
\partial_\mu\langle N\rangle(\mu,T) &= \frac{-1}{\pi}\lim_{\delta\to 0}\sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}\in\mathrm{Q}\\ \sigma\in\{\uparrow,\downarrow\}\\ m\in\{1,\ldots,\infty\}\\ E\in(-\infty,+\infty)}} \frac{\beta}{4}\,\mathrm{sech}^2\left(\beta\frac{E-\mu}{2}\right)\mathrm{Im}\left[E+\mathrm{i}\delta-\left(\epsilon_{m\sigma\mathbf{k}}+\widetilde{\Sigma}^{\mathrm{ret}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta)\right)\right]^{-1}\\
&\quad+\frac{-1}{\pi}\lim_{\delta\to 0}\sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}\in\mathrm{Q}\\ \sigma\in\{\uparrow,\downarrow\}\\ m\in\{1,\ldots,\infty\}\\ E\in(-\infty,+\infty)}} \mathrm{F}_\beta(E-\mu)\cdot(-1)^2\cdot\mathrm{Im}\,\frac{\partial_\mu\widetilde{\Sigma}^{\mathrm{ret}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta)}{\left(E+\mathrm{i}\delta-\left(\epsilon_{m\sigma\mathbf{k}}+\widetilde{\Sigma}^{\mathrm{ret}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta)\right)\right)^2}\\
&= \frac{-1}{\pi}\lim_{\delta\to 0}\sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}\in\mathrm{Q}\\ \sigma\in\{\uparrow,\downarrow\}\\ m\in\{1,\ldots,\infty\}\\ E\in(-\infty,+\infty)}} \frac{\beta}{4}\Bigg[\mathrm{sech}^2(\beta E/2)\,\mathrm{Im}\,\frac{1}{E+\mathrm{i}\delta-\left(\xi_{m\sigma\mathbf{k}}+\Sigma^{\mathrm{ret}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta)\right)}\\
&\qquad+\mathrm{F}_\beta(E)\,\mathrm{Im}\,\frac{\sigma_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta)}{\left[E+\mathrm{i}\delta-\left(\xi_{m\sigma\mathbf{k}}+\Sigma^{\mathrm{ret}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta)\right)\right]^2}\Bigg]
\end{aligned} \tag{35.100}$$

whereas we introduced the notation

$$\sigma_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta) = \sigma^{\mathrm{Hartree}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta) + \sigma^{\mathrm{Fock}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta), \tag{35.101}$$

with the Hartree-contribution

$$\sigma^{\text{Hartree}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta) = -\sum_{\substack{\mathbf{q}\in \mathrm{Q}\\ \sigma'\in\{\downarrow,\uparrow\}\\ n\in\{1,2,\dots\}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}}} \frac{g_{mm\nu}(\mathbf{k},0)g_{nn\nu}(\mathbf{q},0)}{N_p}\frac{1}{\Omega_\nu(\mathbf{q}'=0)}\operatorname{sech}^2\left(\beta\xi_{n\sigma'\mathbf{q}}/2\right) \tag{35.102}$$

and the Fock-contribution

$$\sigma^{\text{Fock}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta) = \sum_{\substack{\mathbf{q}\in \mathrm{Q}\\ n\in\{1,2,\dots\}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}}} \frac{|g_{nm\nu}(\mathbf{k},\mathbf{q})|^2}{N_p}\operatorname{sech}^2(\beta\xi_{\mathbf{q}+\mathbf{k}n\sigma}/2)\left[\frac{1}{E+\mathrm{i}\delta-\xi_{\mathbf{q}+\mathbf{k}n\sigma}+\Omega_\nu(\mathbf{q})}-\frac{1}{E+\mathrm{i}\delta-\xi_{\mathbf{q}+\mathbf{k}n\sigma}-\Omega_\nu(\mathbf{q})}\right] \tag{35.103}$$

Proof 35.20 of Lemma 25.21

We compute the derivative of Equation (25.18) as

$$\begin{aligned}
\partial_T\langle H_{\text{el}}\rangle &= \partial_T\frac{-1}{\pi}\lim_{\delta\to 0}\iint_{\substack{\mathbf{k}\in\mathrm{Q}\\ \sigma\in\{\uparrow,\downarrow\}\\ m\in\{1,\dots,\infty\}\\ E\in(-\infty,+\infty)}} \epsilon_{m\mathbf{k}\sigma}\,\mathrm{F}_\beta(E)\operatorname{Im}G^{\text{ret}}_{\substack{m,m\\ \sigma,\sigma}}(E+\mathrm{i}\delta,\mathbf{k})\\
&= \frac{-1}{\pi}\lim_{\delta\to 0}\iint_{\substack{\mathbf{k}\in\mathrm{Q}\\ \sigma\in\{\uparrow,\downarrow\}\\ m\in\{1,\dots,\infty\}\\ E\in(-\infty,+\infty)}} \epsilon_{m\mathbf{k}\sigma}\left[\left(\partial_T\,\mathrm{F}_\beta(E)\right)\operatorname{Im}G^{\text{ret}}_{\substack{m,m\\ \sigma,\sigma}}(E+\mathrm{i}\delta,\mathbf{k})+\mathrm{F}_\beta(E)\operatorname{Im}\partial_T G^{\text{ret}}_{\substack{m,m\\ \sigma,\sigma}}(E+\mathrm{i}\delta,\mathbf{k})\right]\\
&= \dots
\end{aligned} \tag{35.104}$$

Now we use Lemma 9.66, i.e. we use the Equation

$$\mathrm{d}_T\,\mathrm{F}_\beta(E) = \frac{E}{k_B T^2}\,\mathrm{F}_\beta(E)\left(1-\mathrm{F}_\beta(E)\right) \tag{35.105}$$

and for the other derivative we have

$$\partial_T G^{\text{ret}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta) = \partial_T\frac{1}{E+\mathrm{i}\delta-\left(\epsilon_{m\mathbf{k}\sigma}+\Sigma^{\text{ret}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta)-\mu\right)} = \frac{\partial_T\Sigma^{\text{ret}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta)}{E+\mathrm{i}\delta-\left(\epsilon_{m\mathbf{k}\sigma}+\Sigma^{\text{ret}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta)-\mu\right)^2} \tag{35.106}$$

Now we compute the derivative and use the diagonal bands approximation for the self-energy and use Lemma 9.66

$$\begin{aligned}
\partial_T\Sigma^{\text{ret}}_{m\sigma\mathbf{k}}(E+\mathrm{i}\delta) &= \sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ n\in\{1,\dots,\infty\}\\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}}\frac{|g_{nm\nu}(\mathbf{k},\mathbf{q})|^2}{N_p}\left[\partial_T\frac{\mathrm{B}_\beta(\Omega_\nu(\mathbf{q}))+\mathrm{F}_\beta(\xi_{n\sigma\mathbf{k}+\mathbf{q}})}{E+\mathrm{i}\delta-\xi_{n\sigma\mathbf{k}+\mathbf{q}}+\Omega_\nu(\mathbf{q})}+\partial_T\frac{\mathrm{B}_\beta(\Omega_\nu(\mathbf{q}))+1-\mathrm{F}_\beta(\xi_{n\sigma\mathbf{k}+\mathbf{q}})}{E+\mathrm{i}\delta-\xi_{n\sigma\mathbf{k}+\mathbf{q}}-\Omega_\nu(\mathbf{q})}\right]\\
&= \sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ n\in\{1,\dots,\infty\}\\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}}\frac{|g_{nm\nu}(\mathbf{k},\mathbf{q})|^2}{4k_BT^2N_p}\left[\frac{\Omega_\nu(\mathbf{q})\operatorname{csch}^2(\beta\Omega_\nu(\mathbf{q})/2)+\xi_{n\sigma\mathbf{k}+\mathbf{q}}\operatorname{sech}^2(\beta\xi_{n\sigma\mathbf{k}+\mathbf{q}}/2)}{E+\mathrm{i}\delta-\xi_{n\sigma\mathbf{k}+\mathbf{q}}+\Omega_\nu(\mathbf{q})}+\frac{\Omega_\nu(\mathbf{q})\operatorname{csch}^2(\beta\Omega_\nu(\mathbf{q})/2)-\xi_{n\sigma\mathbf{k}+\mathbf{q}}\operatorname{sech}^2(\beta\xi_{n\sigma\mathbf{k}+\mathbf{q}}/2)}{E+\mathrm{i}\delta-\xi_{n\sigma\mathbf{k}+\mathbf{q}}-\Omega_\nu(\mathbf{q})}\right]
\end{aligned} \tag{35.107}$$

Proof 35.21 of Lemma 25.23

Taking the temperature-derivative of

$$\langle H_{\text{ph}} \rangle_0 = \sum_{\substack{\mathbf{q} \in \text{Q} \\ \nu \in \{1,2,\dots,rd_{\mathbf{x}}\}}} \Omega_\nu(\mathbf{q})\, \text{B}_\beta(\Omega_\nu(\mathbf{q})) \tag{35.108}$$

and using Lemma 9.66 we obtain the desired result.

Now we take care of the corrections. We compute the derivative

$$\begin{aligned}
\text{d}_T \langle \delta H_{\text{ph}} \rangle \approx & \sum_{\nu \in \{1,2,\dots,rd_{\mathbf{x}}\}} A_\nu \text{d}_T \left(B_\nu\right)^2 \\
& - \text{d}_T \sum_{\substack{\mathbf{k},\mathbf{q} \in \text{Q} \\ \nu \in \{1,2,\dots,rd_{\mathbf{x}}\} \\ n,n' \in \{1,\dots,\infty\} \\ \sigma \in \{\downarrow,\uparrow\}}} \frac{\Omega_\nu(\mathbf{q})}{N_p} |g_{n'n\nu}(\mathbf{k},\mathbf{q})|^2 \left(\text{F}_\beta(\xi_{n,\sigma,\mathbf{k}}) - \text{F}_\beta(\xi_{n',\sigma,\mathbf{k}+\mathbf{q}})\right) \left[\frac{\text{B}_\beta(\Omega_\nu(\mathbf{q})) - \text{B}_\beta(\xi_{n',\sigma,\mathbf{k}+\mathbf{q}} - \xi_{n,\sigma,\mathbf{k}})}{\left(\Omega_\nu(\mathbf{q}) + \xi_{n,\sigma,\mathbf{k}} - \xi_{n',\sigma,\mathbf{k}+\mathbf{q}}\right)^2} + \frac{1}{4} \frac{\beta\, \text{csch}(\beta\Omega_\nu(\mathbf{q})/2)^2}{\Omega_\nu(\mathbf{q}) + \xi_{n,\sigma,\mathbf{k}} - \xi_{n',\sigma,\mathbf{k}+\mathbf{q}}} \right]
\end{aligned}$$

we neglect the first term for the beginning, since it only contributes for crystals with more than one atom in the UC and focus on the second term, which can be computed as

$$\begin{aligned}
& - \text{d}_T \sum_{\substack{\mathbf{k},\mathbf{q} \in \text{Q} \\ \nu \in \{1,2,\dots,rd_{\mathbf{x}}\} \\ n,n' \in \{1,\dots,\infty\} \\ \sigma \in \{\downarrow,\uparrow\}}} \frac{\Omega_\nu(\mathbf{q})}{N_p} |g_{n'n\nu}(\mathbf{k},\mathbf{q})|^2 \left(\text{F}_\beta(\xi_{n,\sigma,\mathbf{k}}) - \text{F}_\beta(\xi_{n',\sigma,\mathbf{k}+\mathbf{q}})\right) \left[\frac{\text{B}_\beta(\Omega_\nu(\mathbf{q})) - \text{B}_\beta(\xi_{n',\sigma,\mathbf{k}+\mathbf{q}} - \xi_{n,\sigma,\mathbf{k}})}{\left(\Omega_\nu(\mathbf{q}) + \xi_{n,\sigma,\mathbf{k}} - \xi_{n',\sigma,\mathbf{k}+\mathbf{q}}\right)^2} + \frac{1}{4} \frac{\beta\, \text{csch}(\beta\Omega_\nu(\mathbf{q})/2)^2}{\Omega_\nu(\mathbf{q}) + \xi_{n,\sigma,\mathbf{k}} - \xi_{n',\sigma,\mathbf{k}+\mathbf{q}}} \right] \\
= & - \sum_{\substack{\mathbf{k},\mathbf{q} \in \text{Q} \\ \nu \in \{1,2,\dots,rd_{\mathbf{x}}\} \\ n,n' \in \{1,\dots,\infty\} \\ \sigma \in \{\downarrow,\uparrow\}}} \frac{\Omega_\nu(\mathbf{q})}{N_p} |g_{n'n\nu}(\mathbf{k},\mathbf{q})|^2 \left[\text{d}_T \left(\text{F}_\beta(\xi_{n,\sigma,\mathbf{k}}) - \text{F}_\beta(\xi_{n',\sigma,\mathbf{k}+\mathbf{q}})\right) \right] \left[\frac{\text{B}_\beta(\Omega_\nu(\mathbf{q})) - \text{B}_\beta(\xi_{n',\sigma,\mathbf{k}+\mathbf{q}} - \xi_{n,\sigma,\mathbf{k}})}{\left(\Omega_\nu(\mathbf{q}) + \xi_{n,\sigma,\mathbf{k}} - \xi_{n',\sigma,\mathbf{k}+\mathbf{q}}\right)^2} + \frac{1}{4} \frac{\beta\, \text{csch}(\beta\Omega_\nu(\mathbf{q})/2)^2}{\Omega_\nu(\mathbf{q}) + \xi_{n,\sigma,\mathbf{k}} - \xi_{n',\sigma,\mathbf{k}+\mathbf{q}}} \right] \\
& - \sum_{\substack{\mathbf{k},\mathbf{q} \in \text{Q} \\ \nu \in \{1,2,\dots,rd_{\mathbf{x}}\} \\ n,n' \in \{1,\dots,\infty\} \\ \sigma \in \{\downarrow,\uparrow\}}} \frac{\Omega_\nu(\mathbf{q})}{N_p} |g_{n'n\nu}(\mathbf{k},\mathbf{q})|^2 \left(\text{F}_\beta(\xi_{n,\sigma,\mathbf{k}}) - \text{F}_\beta(\xi_{n',\sigma,\mathbf{k}+\mathbf{q}})\right) \left[\text{d}_T \frac{\text{B}_\beta(\Omega_\nu(\mathbf{q})) - \text{B}_\beta(\xi_{n',\sigma,\mathbf{k}+\mathbf{q}} - \xi_{n,\sigma,\mathbf{k}})}{\left(\Omega_\nu(\mathbf{q}) + \xi_{n,\sigma,\mathbf{k}} - \xi_{n',\sigma,\mathbf{k}+\mathbf{q}}\right)^2} + \frac{1}{4} \text{d}_T \frac{\beta\, \text{csch}(\beta\Omega_\nu(\mathbf{q})/2)^2}{\Omega_\nu(\mathbf{q}) + \xi_{n,\sigma,\mathbf{k}} - \xi_{n',\sigma,\mathbf{k}+\mathbf{q}}} \right]
\end{aligned}$$

Using now again Lemma 9.66 we obtain the stated result for the first two terms. For the last term, we note the identity

$$\frac{\text{d}}{\text{d}x} \text{csch}(x) = -\coth(x)\, \text{csch}(x) \tag{35.109}$$

which gives

$$\begin{aligned}
& \text{d}_T \left(\frac{1}{k_B T} \cdot \text{csch}^2 \left(\frac{\Omega_\nu(\mathbf{q})}{2k_B T} \right) \right) \\
= & \frac{-1}{k_B T^2} \text{csch}^2 \left(\frac{\Omega_\nu(\mathbf{q})}{2k_B T} \right) + \frac{1}{k_B T} \cdot 2 \cdot \text{csch} \left(\frac{\Omega_\nu(\mathbf{q})}{2k_B T} \right) \cdot \left(-\coth \left(\frac{\Omega_\nu(\mathbf{q})}{2k_B T} \right) \cdot \text{csch} \left(\frac{\Omega_\nu(\mathbf{q})}{2k_B T} \right) \cdot \left(\frac{-\Omega_\nu(\mathbf{q})}{2k_B T^2} \right) \right) \\
= & \frac{-1}{k_B T^2} \text{csch}^2 \left(\frac{\Omega_\nu(\mathbf{q})}{2k_B T} \right) \cdot \left[1 - \frac{\Omega_\nu(\mathbf{q})}{k_B T} \coth \left(\frac{\Omega_\nu(\mathbf{q})}{2k_B T} \right) \right]
\end{aligned} \tag{35.110}$$

Proof 35.22 of Theorem 26.53

There are many couplings contributing. We will „divide and conquer“ the problem. The Kronecker-deltas for the spin yield the enumeration

- $\alpha_1 \equiv (m_{\alpha_1}, \sigma_{\alpha_1}, k_{\alpha_1}) = (m_{\alpha_1}, \sigma, k_{\alpha_1})$
- $\alpha_2 \equiv (m_{\alpha_2}, \sigma_{\alpha_2}, k_{\alpha_2}) = (m_{\alpha_2}, \pi, k_{\alpha_2})$
- $\alpha_3 \equiv (m_{\alpha_3}, \sigma_{\alpha_3}, k_{\alpha_3}) = (m_{\alpha_3}, \pi, k_{\alpha_3})$
- $\alpha_4 \equiv (m_{\alpha_4}, \sigma_{\alpha_4}, k_{\alpha_4}) = (m_{\alpha_4}, \sigma, k_{\alpha_4})$

Spin-Singlet Contributions

Case 1: $\sigma = \uparrow$ and $\pi = \downarrow$. Then we obtain

- $\alpha_1 \equiv (m_{\alpha_1}, \sigma_{\alpha_1}, k_{\alpha_1}) = (m_{\alpha_1}, \uparrow, k_{\alpha_1})$
- $\alpha_2 \equiv (m_{\alpha_2}, \sigma_{\alpha_2}, k_{\alpha_2}) = (m_{\alpha_2}, \downarrow, k_{\alpha_2})$
- $\alpha_3 \equiv (m_{\alpha_3}, \sigma_{\alpha_3}, k_{\alpha_3}) = (m_{\alpha_3}, \downarrow, k_{\alpha_3})$
- $\alpha_4 \equiv (m_{\alpha_4}, \sigma_{\alpha_4}, k_{\alpha_4}) = (m_{\alpha_4}, \uparrow, k_{\alpha_4})$

Then we can proceed by enumerating the momenta in the following way

- $\alpha_1 \equiv (m_{\alpha_1}, \sigma_{\alpha_1}, k_{\alpha_1}) = (m_{\alpha_1}, \uparrow, k_{\alpha_1})$
- $\alpha_2 \equiv (m_{\alpha_2}, \sigma_{\alpha_2}, k_{\alpha_2}) = (m_{\alpha_2}, \downarrow, -k)$
- $\alpha_3 \equiv (m_{\alpha_3}, \sigma_{\alpha_3}, k_{\alpha_3}) = (m_{\alpha_3}, \downarrow, k_{\alpha_3})$
- $\alpha_4 \equiv (m_{\alpha_4}, \sigma_{\alpha_4}, k_{\alpha_4}) = (m_{\alpha_4}, \uparrow, k')$

Momentum conservation yields then

- $\alpha_1 \equiv (m_{\alpha_1}, \sigma_{\alpha_1}, k_{\alpha_1}) = (m_{\alpha_1}, \uparrow, k_{\alpha_1})$
- $\alpha_2 \equiv (m_{\alpha_2}, \sigma_{\alpha_2}, k_{\alpha_2}) = (m_{\alpha_2}, \downarrow, -k)$
- $\alpha_3 \equiv (m_{\alpha_3}, \sigma_{\alpha_3}, k_{\alpha_3}) = (m_{\alpha_3}, \downarrow, k_{\alpha_1} - k - k')$
- $\alpha_4 \equiv (m_{\alpha_4}, \sigma_{\alpha_4}, k_{\alpha_4}) = (m_{\alpha_4}, \uparrow, k')$

Now we replace the summation over $k_{\alpha_1} \mapsto k_{\alpha_1} + k$.

- $\alpha_1 \equiv (m_{\alpha_1}, \sigma_{\alpha_1}, k_{\alpha_1}) = (m_{\alpha_1}, \uparrow, k_{\alpha_1} + k)$
- $\alpha_2 \equiv (m_{\alpha_2}, \sigma_{\alpha_2}, k_{\alpha_2}) = (m_{\alpha_2}, \downarrow, -k)$
- $\alpha_3 \equiv (m_{\alpha_3}, \sigma_{\alpha_3}, k_{\alpha_3}) = (m_{\alpha_3}, \downarrow, k_{\alpha_1} - k')$
- $\alpha_4 \equiv (m_{\alpha_4}, \sigma_{\alpha_4}, k_{\alpha_4}) = (m_{\alpha_4}, \uparrow, k')$

And now we write $k_{\alpha_1} \equiv q$ and obtain finally

- $\alpha_1 \equiv (m_{\alpha_1}, \sigma_{\alpha_1}, k_{\alpha_1}) = (m_{\alpha_1}, \uparrow, q + k)$
- $\alpha_2 \equiv (m_{\alpha_2}, \sigma_{\alpha_2}, k_{\alpha_2}) = (m_{\alpha_2}, \downarrow, -k)$
- $\alpha_3 \equiv (m_{\alpha_3}, \sigma_{\alpha_3}, k_{\alpha_3}) = (m_{\alpha_3}, \downarrow, q - k')$
- $\alpha_4 \equiv (m_{\alpha_4}, \sigma_{\alpha_4}, k_{\alpha_4}) = (m_{\alpha_4}, \uparrow, k')$

This gives for the matrix-element

$$
\begin{aligned}
&V_{\alpha_1,\alpha_2;\alpha_3,\alpha_4} \\
&= \frac{-1}{\hbar\beta N_p} \sum_{\nu\in\{1,\ldots,rd_{\mathbf{x}}\}} \frac{\omega_\nu(\mathbf{k}+\mathbf{q}-\mathbf{k}')}{\omega^2_{k+q-k'}+\omega^2_\nu(\mathbf{k}+\mathbf{q}-\mathbf{k}')} \frac{g_{m_{\alpha_1}m_{\alpha_4}\nu}(\mathbf{k}',\mathbf{k}+\mathbf{q}-\mathbf{k}')g^*_{m_{\alpha_3}m_{\alpha_2}\nu}(-\mathbf{k},\mathbf{k}+\mathbf{q}-\mathbf{k}')}{\hbar^2} \\
&= \frac{-1}{\hbar\beta N_p} \sum_{\nu\in\{1,\ldots,rd_{\mathbf{x}}\}} \frac{\omega_\nu(\mathbf{k}+\mathbf{q}-\mathbf{k}')}{\omega^2_{k+q-k'}+\omega^2_\nu(\mathbf{k}+\mathbf{q}-\mathbf{k}')} \frac{g_{m_{\alpha_1}m_{\alpha_4}\nu}(\mathbf{k}',\mathbf{k}+\mathbf{q}-\mathbf{k}')g_{m_{\alpha_2}m_{\alpha_3}\nu}(\mathbf{q}-\mathbf{k}',-(\mathbf{k}+\mathbf{q}-\mathbf{k}'))}{\hbar^2}
\end{aligned}
$$

Case 2: $\sigma = \downarrow$ and $\pi = \uparrow$. Then we obtain

- $\alpha_1 \equiv (m_{\alpha_1}, \sigma_{\alpha_1}, k_{\alpha_1}) = (m_{\alpha_1}, \downarrow, k_{\alpha_1})$
- $\alpha_2 \equiv (m_{\alpha_2}, \sigma_{\alpha_2}, k_{\alpha_2}) = (m_{\alpha_2}, \uparrow, k_{\alpha_2})$
- $\alpha_3 \equiv (m_{\alpha_3}, \sigma_{\alpha_3}, k_{\alpha_3}) = (m_{\alpha_3}, \uparrow, k_{\alpha_3})$
- $\alpha_4 \equiv (m_{\alpha_4}, \sigma_{\alpha_4}, k_{\alpha_4}) = (m_{\alpha_4}, \downarrow, k_{\alpha_4})$

Then we can proceed by enumerating the momenta in the following way

- $\alpha_1 \equiv (m_{\alpha_1}, \sigma_{\alpha_1}, k_{\alpha_1}) = (m_{\alpha_1}, \downarrow, -k)$
- $\alpha_2 \equiv (m_{\alpha_2}, \sigma_{\alpha_2}, k_{\alpha_2}) = (m_{\alpha_2}, \uparrow, k_{\alpha_2})$
- $\alpha_3 \equiv (m_{\alpha_3}, \sigma_{\alpha_3}, k_{\alpha_3}) = (m_{\alpha_3}, \uparrow, k')$
- $\alpha_4 \equiv (m_{\alpha_4}, \sigma_{\alpha_4}, k_{\alpha_4}) = (m_{\alpha_4}, \downarrow, k_{\alpha_4})$

Momentum conservation yields then

- $\alpha_1 \equiv (m_{\alpha_1}, \sigma_{\alpha_1}, k_{\alpha_1}) = (m_{\alpha_1}, \downarrow, -k)$
- $\alpha_2 \equiv (m_{\alpha_2}, \sigma_{\alpha_2}, k_{\alpha_2}) = (m_{\alpha_2}, \uparrow, k_{\alpha_2})$
- $\alpha_3 \equiv (m_{\alpha_3}, \sigma_{\alpha_3}, k_{\alpha_3}) = (m_{\alpha_3}, \uparrow, k')$
- $\alpha_4 \equiv (m_{\alpha_4}, \sigma_{\alpha_4}, k_{\alpha_4}) = (m_{\alpha_4}, \downarrow, k_{\alpha_2} - k - k')$

Now we replace the summation over $k_{\alpha_2} \mapsto k_{\alpha_2} + k$.

- $\alpha_1 \equiv (m_{\alpha_1}, \sigma_{\alpha_1}, k_{\alpha_1}) = (m_{\alpha_1}, \downarrow, -k)$
- $\alpha_2 \equiv (m_{\alpha_2}, \sigma_{\alpha_2}, k_{\alpha_2}) = (m_{\alpha_2}, \uparrow, k_{\alpha_2} + k)$
- $\alpha_3 \equiv (m_{\alpha_3}, \sigma_{\alpha_3}, k_{\alpha_3}) = (m_{\alpha_3}, \uparrow, k')$
- $\alpha_4 \equiv (m_{\alpha_4}, \sigma_{\alpha_4}, k_{\alpha_4}) = (m_{\alpha_4}, \downarrow, k_{\alpha_2} - k')$

And now we write $k_{\alpha_2} \equiv q$ and obtain

- $\alpha_1 \equiv (m_{\alpha_1}, \sigma_{\alpha_1}, k_{\alpha_1}) = (m_{\alpha_1}, \downarrow, -k)$
- $\alpha_2 \equiv (m_{\alpha_2}, \sigma_{\alpha_2}, k_{\alpha_2}) = (m_{\alpha_2}, \uparrow, q + k)$
- $\alpha_3 \equiv (m_{\alpha_3}, \sigma_{\alpha_3}, k_{\alpha_3}) = (m_{\alpha_3}, \uparrow, k')$
- $\alpha_4 \equiv (m_{\alpha_4}, \sigma_{\alpha_4}, k_{\alpha_4}) = (m_{\alpha_4}, \downarrow, q - k')$

finally we exchange $m_{\alpha_1} \leftrightarrow m_{\alpha_2}$ and (simultaneously) $m_{\alpha_3} \leftrightarrow m_{\alpha_4}$ which leads to

- $\alpha_1 \equiv (m_{\alpha_2}, \sigma_{\alpha_1}, k_{\alpha_1}) = (m_{\alpha_2}, \downarrow, -k)$
- $\alpha_2 \equiv (m_{\alpha_1}, \sigma_{\alpha_2}, k_{\alpha_2}) = (m_{\alpha_1}, \uparrow, q+k)$
- $\alpha_3 \equiv (m_{\alpha_4}, \sigma_{\alpha_3}, k_{\alpha_3}) = (m_{\alpha_4}, \uparrow, k')$
- $\alpha_4 \equiv (m_{\alpha_3}, \sigma_{\alpha_4}, k_{\alpha_4}) = (m_{\alpha_3}, \downarrow, q-k')$

This gives for the matrix-element

$$
\begin{aligned}
&V_{\alpha_1,\alpha_2;\alpha_3,\alpha_4} \\
&= \frac{-1}{\hbar\beta N_p} \sum_{\nu \in \{1,\ldots,rd_{\mathrm{x}}\}} \frac{\omega_\nu(-\mathbf{k}-\mathbf{q}+\mathbf{k}')}{\omega^2_{-k-q+k'} + \omega^2_\nu(-\mathbf{k}-\mathbf{q}+\mathbf{k}')} \frac{g_{m_{\alpha_2} m_{\alpha_3} \nu}(\mathbf{q}-\mathbf{k}', -\mathbf{k}-\mathbf{q}+\mathbf{k}') g^*_{m_{\alpha_4} m_{\alpha_1} \nu}(\mathbf{q}+\mathbf{k}, -\mathbf{k}-\mathbf{q}+\mathbf{k}')}{\hbar^2} \\
&= \frac{-1}{\hbar\beta N_p} \sum_{\nu \in \{1,\ldots,rd_{\mathrm{x}}\}} \frac{\omega_\nu(-\mathbf{k}-\mathbf{q}+\mathbf{k}')}{\omega^2_{-k-q+k'} + \omega^2_\nu(-\mathbf{k}-\mathbf{q}+\mathbf{k}')} \frac{g_{m_{\alpha_2} m_{\alpha_3} \nu}(\mathbf{q}-\mathbf{k}', -\mathbf{k}-\mathbf{q}+\mathbf{k}') g_{m_{\alpha_1} m_{\alpha_4} \nu}(\mathbf{k}', +\mathbf{k}+\mathbf{q}-\mathbf{k}')}{\hbar^2}
\end{aligned}
$$

Spin-Triplet-Contributions

Case 1: $\sigma = \uparrow$ and $\pi = \uparrow$. Then we obtain by the exact same calculations as above

- $\alpha_1 \equiv (m_{\alpha_1}, \sigma_{\alpha_1}, k_{\alpha_1}) = (m_{\alpha_1}, \uparrow, q+k)$
- $\alpha_2 \equiv (m_{\alpha_2}, \sigma_{\alpha_2}, k_{\alpha_2}) = (m_{\alpha_2}, \uparrow, -k)$
- $\alpha_3 \equiv (m_{\alpha_3}, \sigma_{\alpha_3}, k_{\alpha_3}) = (m_{\alpha_3}, \uparrow, q-k')$
- $\alpha_4 \equiv (m_{\alpha_4}, \sigma_{\alpha_4}, k_{\alpha_4}) = (m_{\alpha_4}, \uparrow, k')$

This gives for the matrix-element

$$\begin{aligned}
&V^{\uparrow\uparrow}_{\alpha_1,\alpha_2;\alpha_3,\alpha_4} \\
&= \frac{-1}{\hbar\beta N_p} \sum_{\nu \in \{1,\ldots,rd_{\mathbf{x}}\}} \frac{\omega_\nu(\mathbf{k}+\mathbf{q}-\mathbf{k}')}{\omega^2_{k+q-k'} + \omega^2_\nu(\mathbf{k}+\mathbf{q}-\mathbf{k}')} \frac{g_{m_{\alpha_1} m_{\alpha_4} \nu}(\mathbf{k}', \mathbf{k}+\mathbf{q}-\mathbf{k}') g^*_{m_{\alpha_3} m_{\alpha_2} \nu}(-\mathbf{k}, \mathbf{k}+\mathbf{q}-\mathbf{k}')}{\hbar^2} \\
&= \frac{-1}{\hbar\beta N_p} \sum_{\nu \in \{1,\ldots,rd_{\mathbf{x}}\}} \frac{\omega_\nu(\mathbf{k}+\mathbf{q}-\mathbf{k}')}{\omega^2_{k+q-k'} + \omega^2_\nu(\mathbf{k}+\mathbf{q}-\mathbf{k}')} \frac{g_{m_{\alpha_1} m_{\alpha_4} \nu}(\mathbf{k}', \mathbf{k}+\mathbf{q}-\mathbf{k}') g_{m_{\alpha_2} m_{\alpha_3} \nu}(\mathbf{q}-\mathbf{k}', -(\mathbf{k}+\mathbf{q}-\mathbf{k}'))}{\hbar^2}
\end{aligned}$$

Case 2: $\sigma = \downarrow$ and $\pi = \downarrow$. Then we obtain by the exact same calculations as above

- $\alpha_1 \equiv (m_{\alpha_1}, \sigma_{\alpha_1}, k_{\alpha_1}) = (m_{\alpha_1}, \downarrow, q+k)$
- $\alpha_2 \equiv (m_{\alpha_2}, \sigma_{\alpha_2}, k_{\alpha_2}) = (m_{\alpha_2}, \downarrow, -k)$
- $\alpha_3 \equiv (m_{\alpha_3}, \sigma_{\alpha_3}, k_{\alpha_3}) = (m_{\alpha_3}, \downarrow, q-k')$
- $\alpha_4 \equiv (m_{\alpha_4}, \sigma_{\alpha_4}, k_{\alpha_4}) = (m_{\alpha_4}, \downarrow, k')$

This gives for the matrix-element

$$\begin{aligned}
&V^{\downarrow\downarrow}_{\alpha_1,\alpha_2;\alpha_3,\alpha_4} \\
&= \frac{-1}{\hbar\beta N_p} \sum_{\nu \in \{1,\ldots,rd_{\mathbf{x}}\}} \frac{\omega_\nu(\mathbf{k}+\mathbf{q}-\mathbf{k}')}{\omega^2_{k+q-k'} + \omega^2_\nu(\mathbf{k}+\mathbf{q}-\mathbf{k}')} \frac{g_{m_{\alpha_1} m_{\alpha_4} \nu}(\mathbf{k}', \mathbf{k}+\mathbf{q}-\mathbf{k}') g^*_{m_{\alpha_3} m_{\alpha_2} \nu}(-\mathbf{k}, \mathbf{k}+\mathbf{q}-\mathbf{k}')}{\hbar^2} \\
&= \frac{-1}{\hbar\beta N_p} \sum_{\nu \in \{1,\ldots,rd_{\mathbf{x}}\}} \frac{\omega_\nu(\mathbf{k}+\mathbf{q}-\mathbf{k}')}{\omega^2_{k+q-k'} + \omega^2_\nu(\mathbf{k}+\mathbf{q}-\mathbf{k}')} \frac{g_{m_{\alpha_1} m_{\alpha_4} \nu}(\mathbf{k}', \mathbf{k}+\mathbf{q}-\mathbf{k}') g_{m_{\alpha_2} m_{\alpha_3} \nu}(\mathbf{q}-\mathbf{k}', -(\mathbf{k}+\mathbf{q}-\mathbf{k}'))}{\hbar^2}
\end{aligned}$$

Proof 35.23 of Theorem 26.55 We decompose the spin-singlet contributions as

$$S[\psi, \overline{\psi}] \equiv S^{\mathrm{ET}}[\psi, \overline{\psi}] + S^{\mathrm{NET}}[\psi, \overline{\psi}] + S^{\mathrm{RPC}}[\psi, \overline{\psi}] \tag{35.111}$$

whereas for the ([N]on-)[E]liashberg-[T]heory contribution

$$S^{\mathrm{ET}}[\psi,\overline{\psi}] = \sum_{\substack{k,k'\in \mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ m,n\in\{1,2,3\ldots\}}} \overline{\psi}_{m\uparrow}(k)\overline{\psi}_{m\downarrow}(-k)V^{\mathrm{ET}}_{\substack{\downarrow\uparrow\\ m,n}}(k,k')\psi_{n\downarrow}(-k')\psi_{n\uparrow}(k') + \sum_{\substack{\sigma\in\{\downarrow,\uparrow\}\\ k,k'\in \mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ m,n\in\{1,2,3\ldots\}}} \overline{\psi}_{m\sigma}(k)\overline{\psi}_{m\sigma}(-k)V^{\mathrm{ET}}_{\substack{\sigma\sigma\\ m,n}}(k,k')\psi_{n\sigma}(-k')\psi_{n\sigma}(k')$$

$$S^{\mathrm{NET}}_{\downarrow\uparrow}[\psi,\overline{\psi}] = \sum_{\substack{q,k\in \mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ m,n\in\{1,2,3\ldots\}}} \overline{\psi}_{m\uparrow}(q+k)\overline{\psi}_{n\downarrow}(-k)V^{\mathrm{NET}}_{\substack{\downarrow\uparrow\\ m,n}}(q,k)\psi_{m\downarrow}(q+k)\psi_{n\uparrow}(-k) + \sum_{\substack{\sigma\in\{\downarrow,\uparrow\}\\ q,k\in \mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ m,n\in\{1,2,3\ldots\}}} \overline{\psi}_{m\sigma}(q+k)\overline{\psi}_{n\sigma}(-k)V^{\mathrm{NET}}_{\substack{\sigma\sigma\\ m,n}}(q,k)\psi_{m\sigma}(q+k)\psi_{n\sigma}(-k)$$

we have, when we take the double contributions into account, the vertices

$$2V^{\mathrm{ET}}_{\substack{\sigma\sigma\\ m,n}}(k,k') = V^{\mathrm{ET}}_{\substack{\downarrow\uparrow\\ m,n}}(k,k') = \frac{-2}{\hbar\beta N_p}\sum_{\nu\in\{1,\ldots,rd_{\mathbf{x}}\}}\frac{\omega_\nu(\mathbf{k}-\mathbf{k}')}{\omega^2_{k-k'}+\omega^2_\nu(\mathbf{k}-\mathbf{k}')}\frac{|g_{mn\nu}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{\hbar^2} \tag{35.112}$$

$$2V^{\mathrm{NET}}_{\substack{\sigma\sigma\\ m,n}}(q,k) = V^{\mathrm{NET}}_{\substack{\downarrow\uparrow\\ m,n}}(q,k) = \frac{-2}{\hbar\beta N_p}\sum_{\nu\in\{1,\ldots,rd_{\mathbf{x}}\}}\frac{\omega_\nu(2\mathbf{k}+\mathbf{q})}{\omega^2_{2k+q}+\omega^2_\nu(2\mathbf{k}+\mathbf{q})}\frac{|g_{mn\nu}(-\mathbf{k},2\mathbf{k}+\mathbf{q})|^2}{\hbar^2} \tag{35.113}$$

and the [R]andom [P]hase [C]ancellations are all the remaining contributions (which have complex vertices).

Proof 35.24 of Lemma 26.63

We compute straightforwardly

$$\eta_m(\tau,\mathbf{k}) = \frac{1}{\sqrt{\hbar\beta}}\sum_{\omega_n\in\mathrm{i}\Omega_{-1}}\eta_m(\mathbf{k},\mathrm{i}\omega_n)\mathrm{e}^{-\mathrm{i}\omega_n\tau} = \frac{1}{\sqrt{\hbar\beta}}\sum_{\mathrm{i}\omega_n\in\mathrm{i}\Omega_{-1}}\begin{pmatrix}\psi_{m\uparrow}(\mathrm{i}\omega_n,\mathbf{k})\\ \overline{\psi}_{m\downarrow}(-\mathrm{i}\omega_n,-\mathbf{k})\end{pmatrix}\mathrm{e}^{-\mathrm{i}\omega_n\tau} = \begin{pmatrix}\psi_{m\uparrow}(\tau,\mathbf{k})\\ \overline{\psi}_{m\downarrow}(\tau,-\mathbf{k})\end{pmatrix}$$

whereas in the last step we replaced $\omega_n \mapsto -\omega_n$ in the second component. Likewise, one obtains also

$$\overline{\eta}^{\mathrm{T}}_m(\tau,\mathbf{k}) = \begin{pmatrix}\overline{\psi}_{m\uparrow}(\tau,\mathbf{k})\\ \psi_{m\downarrow}(\tau,-\mathbf{k})\end{pmatrix} \tag{35.114}$$

Proof 35.25 of Corollary 26.64 We note that the action can be rewritten in imaginary-time space as

$$
\begin{aligned}
S_{\text{int}}[\delta_{\downarrow\uparrow},\bar{\delta}_{\downarrow\uparrow},\psi,\overline{\psi}] &= \sum_{\substack{k\in \mathrm{i}\Omega_{-1}\times\mathbb{Q}\\ m\in\{1,2,3,\dots\}}} \overline{\eta}^{\mathrm{T}}_m(k)\left(-\frac{1}{\hbar}\mathscr{G}^{-1}{}_{\substack{m\\ [\delta_{\downarrow\uparrow},\bar{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}(k)\right)\eta_m(k)\\
&= \oint\!\!\!\!\!\!\sum_{\substack{\mathbf{k}\in\mathbb{Q}\\ m\in\{1,2,3,\dots\}\\ \tau,\tau'\in(0,\beta\hbar)}} \overline{\eta}^{\mathrm{T}}_m(\mathbf{k},\tau)\left(-\frac{1}{\hbar}\frac{1}{\hbar\beta}\sum_{\mathrm{i}\omega_n\in\mathrm{i}\Omega_{-1}}\mathscr{G}^{-1}{}_{\substack{m\\ [\delta_{\downarrow\uparrow},\bar{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}(\mathrm{i}\omega_n,\mathbf{k})\,\mathrm{e}^{-\mathrm{i}\omega_n(\tau'-\tau)}\right)\eta_m(\tau',\mathbf{k})\\
&\equiv \oint\!\!\!\!\!\!\sum_{\substack{\mathbf{k}\in\mathbb{Q}\\ m\in\{1,2,3,\dots\}\\ \tau,\tau'\in(0,\beta\hbar)}} \overline{\eta}^{\mathrm{T}}_m(\tau,\mathbf{k})\left(-\frac{1}{\hbar}\mathscr{G}^{-1}{}_{\substack{m\\ [\delta_{\downarrow\uparrow},\bar{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}(\tau-\tau',\mathbf{k})\right)\eta_m(\tau',\mathbf{k})
\end{aligned}
$$

Now the identities follow by simply using the usual relations from [Draft Summary].

Proof 35.26 of Corollary 26.67

Searching for stationary points yields the equation

$$
\begin{aligned}
0 &= \left(\frac{\partial}{\partial\delta(\Gamma)}S_{\text{tot}}\right)[\delta_{\downarrow\uparrow},\bar{\delta}_{\downarrow\uparrow}]\\
&= -\sum_{A\in\Pi}\bar{\delta}(A)\Lambda^{\text{ET}}_{\downarrow\uparrow}(A,\Gamma) - \operatorname{Tr}\mathscr{G}_{\substack{[\delta_{\downarrow\uparrow},\bar{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}\frac{\partial}{\partial\delta(\Gamma)}\mathscr{G}^{-1}_{\substack{[\delta_{\downarrow\uparrow},\bar{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}
\end{aligned}
\tag{35.115}
$$

Multiplying now from both sides with the inverse of $\Lambda^{\text{ET}}_{\downarrow\uparrow}$ from the right yields the gap-equation

$$
\bar{\delta}(B) = -\sum_{A\in\Pi}\operatorname{Tr}\left(\mathscr{G}_{\substack{[\delta_{\downarrow\uparrow},\bar{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}\frac{\partial}{\partial\delta(A)}\mathscr{G}^{-1}_{\substack{[\delta_{\downarrow\uparrow},\bar{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}\right)V^{\text{ET}}_{\downarrow\uparrow}(A,B)
\tag{35.116}
$$

[CP7] Summation index corrected from B to A.

Referring now to the multi-indices in Equation (44.23) and the matrix-elements in Equation (26.182), and partially performing the trace over the non-vanishing contributions, we obtain for each band and each four-momentum the desired equations.

Proof 35.27 of Lemma 26.68

Recalling that the Gorkov-Green-function block-diagonal w.r.t. bands and wave-vectors with individual blocks

$$
-\frac{1}{\hbar}\mathscr{G}^{-1}{}_{\substack{m\\ [\delta_{\downarrow\uparrow},\bar{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}(k) = \begin{pmatrix} -\frac{1}{\hbar}\mathscr{G}^{-\mathrm{F}}_{0\,m\uparrow}(k) & \delta_{m\downarrow\uparrow}(k)\\ \bar{\delta}_{m\downarrow\uparrow}(k) & +\frac{1}{\hbar}\mathscr{G}^{-\mathrm{F}}_{0\,m\downarrow}(-k)\end{pmatrix}
\tag{35.117}
$$

which allows us on the one hand to compute the derivative

$$
\frac{\partial}{\partial\delta_{m\downarrow\uparrow}(k)}\mathscr{G}^{-1}{}_{\substack{m\\ [\delta_{\downarrow\uparrow},\bar{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}} = \begin{pmatrix}0 & -\hbar\\ 0 & 0\end{pmatrix}
\tag{35.118}
$$

and by inversion of the equation

$$-\hbar\mathscr{G}\underset{\substack{[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}{\phantom{\mathscr{G}}}^{m}(k)=\begin{pmatrix}-\frac{1}{\hbar}\mathscr{G}\underset{m\uparrow}{\phantom{\mathscr{G}}}_{0}^{-\mathrm{F}}(k) & \delta_{m\downarrow\uparrow}(k)\\ \overline{\delta}_{m\downarrow\uparrow}(k) & +\frac{1}{\hbar}\mathscr{G}\underset{m\downarrow}{\phantom{\mathscr{G}}}_{0}^{-\mathrm{F}}(-k)\end{pmatrix}^{-1}\quad\Longleftrightarrow\quad\mathscr{G}\underset{\substack{[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}{\phantom{\mathscr{G}}}^{m}(k)=-\frac{1}{\hbar}\begin{pmatrix}-\frac{1}{\hbar}\mathscr{G}\underset{m\uparrow}{\phantom{\mathscr{G}}}_{0}^{-\mathrm{F}}(k) & \delta_{m\downarrow\uparrow}(k)\\ \overline{\delta}_{m\downarrow\uparrow}(k) & +\frac{1}{\hbar}\mathscr{G}\underset{m\downarrow}{\phantom{\mathscr{G}}}_{0}^{-\mathrm{F}}(-k)\end{pmatrix}^{-1}\tag{35.119}$$

Recalling that one has for the non-interacting Green-functions the relations (we are considering a spin-degenerate system)

$$\begin{aligned}-\frac{1}{\hbar}\mathscr{G}\underset{m\uparrow}{\phantom{\mathscr{G}}}_{0}^{-\mathrm{F}}(k)&=-\mathrm{i}\omega_n+(\epsilon_m(\mathbf{k})-\mu)/\hbar\\ +\frac{1}{\hbar}\mathscr{G}\underset{m\downarrow}{\phantom{\mathscr{G}}}_{0}^{-\mathrm{F}}(-k)&=-\mathrm{i}\omega_n-(\epsilon_m(-\mathbf{k})-\mu)/\hbar\end{aligned}$$

we obtain for the inverse with the rule for 2×2 matrices

$$\mathscr{G}\underset{\substack{[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}{\phantom{\mathscr{G}}}^{m}(k)=-\frac{1}{\hbar}\frac{\begin{pmatrix}-\mathrm{i}\omega_k-(\epsilon_m(-\mathbf{k})-\mu)/\hbar & -\delta_{m\downarrow\uparrow}(k)\\ -\overline{\delta}_{m\downarrow\uparrow}(k) & -\mathrm{i}\omega_k+(\epsilon_m(\mathbf{k})-\mu)/\hbar\end{pmatrix}}{\mathrm{Det}\begin{pmatrix}-\frac{1}{\hbar}\mathscr{G}\underset{m\uparrow}{\phantom{\mathscr{G}}}_{0}^{-\mathrm{F}}(k) & \delta_{m\downarrow\uparrow}(k)\\ \overline{\delta}_{m\downarrow\uparrow}(k) & +\frac{1}{\hbar}\mathscr{G}\underset{m\downarrow}{\phantom{\mathscr{G}}}_{0}^{-\mathrm{F}}(-k)\end{pmatrix}}\tag{35.120}$$

we therefore obtain ONLY IN THE CASE OF INVERSION SYMMETRIC CRYSTALS[4]

$$\mathrm{Det}\begin{pmatrix}-\frac{1}{\hbar}\mathscr{G}\underset{m\uparrow}{\phantom{\mathscr{G}}}_{0}^{-\mathrm{F}}(k) & \delta_{m\downarrow\uparrow}(k)\\ \overline{\delta}_{m\downarrow\uparrow}(k) & +\frac{1}{\hbar}\mathscr{G}\underset{m\downarrow}{\phantom{\mathscr{G}}}_{0}^{-\mathrm{F}}(-k)\end{pmatrix}=-\omega_k^2-\frac{\left(\epsilon_m(\mathbf{k})-\mu\right)^2}{\hbar^2}-|\delta_{m\downarrow\uparrow}(k)|^2\tag{35.121}$$

which simplifies the expression above to

$$\mathscr{G}\underset{\substack{[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}{\phantom{\mathscr{G}}}^{m}(k)=-\frac{1}{\hbar}\frac{\begin{pmatrix}+\mathrm{i}\omega_k+(\epsilon_m(-\mathbf{k})-\mu)/\hbar & +\delta_{m\downarrow\uparrow}(k)\\ +\overline{\delta}_{m\downarrow\uparrow}(k) & +\mathrm{i}\omega_k-(\epsilon_m(\mathbf{k})-\mu)/\hbar\end{pmatrix}}{+\omega_k^2+\frac{\left(\epsilon_m(\mathbf{k})-\mu\right)^2}{\hbar^2}+|\delta_{m\downarrow\uparrow}(k)|^2}\tag{35.122}$$

Proof 35.28 of Lemma 26.69 We first notice that

$$\mathscr{G}\underset{\substack{[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}{\phantom{\mathscr{G}}}_{m,12}(k)=\mathscr{G}\underset{\substack{[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}{\phantom{\mathscr{G}}}_{m,21}(k)^*\tag{35.123}$$

[4] In this case one finds $\epsilon_m(-\mathbf{k})=\epsilon_m(+\mathbf{k})$

and obtain therefore

$$\begin{aligned}\underset{\text{Gorkov}}{\mathscr{G}_{\substack{m,12\\[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]}}}(\tau-\tau') &= \frac{1}{\hbar\beta}\sum_{\mathrm{i}\omega_n\in\mathrm{i}\Omega_{-1}}\underset{\text{Gorkov}}{\mathscr{G}_{\substack{m,12\\[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]}}}(\mathrm{i}\omega_n,\mathbf{k})\mathrm{e}^{-\mathrm{i}\omega_n(\tau-\tau')}\\ &= \frac{1}{\hbar\beta}\sum_{\mathrm{i}\omega_n\in\mathrm{i}\Omega_{-1}}\frac{\delta_{m\downarrow\uparrow}(k)}{\omega_n^2+\left(\epsilon_m(\mathbf{k})-\mu\right)^2/\hbar^2+|\delta_{m\downarrow\uparrow}(k)|^2}\mathrm{e}^{-\mathrm{i}\omega_n(\tau-\tau')}\end{aligned}$$

And on the other hand we obtain

$$\begin{aligned}\underset{\text{Gorkov}}{\mathscr{G}_{\substack{m,21\\[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]}}}(\tau'-\tau) &= \frac{1}{\hbar\beta}\sum_{\mathrm{i}\omega_n\in\mathrm{i}\Omega_{-1}}\underset{\text{Gorkov}}{\mathscr{G}_{\substack{m,21\\[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]}}}(\mathrm{i}\omega_n,\mathbf{k})\mathrm{e}^{-\mathrm{i}\omega_n(\tau'-\tau)}\\ &= \frac{1}{\hbar\beta}\sum_{\mathrm{i}\omega_n\in\mathrm{i}\Omega_{-1}}\frac{\overline{\delta}_{m\downarrow\uparrow}(k)}{\omega_n^2+\left(\epsilon_m(\mathbf{k})-\mu\right)^2/\hbar^2+|\delta_{m\downarrow\uparrow}(k)|^2}\mathrm{e}^{+\mathrm{i}\omega_n(\tau-\tau')}\\ &= \underset{\text{Gorkov}}{\mathscr{G}_{\substack{m,12\\[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]}}}(\tau-\tau')^*\end{aligned}$$

Thus, we obtain in the sense of generalized matrices the desired identity.

Proof 35.29 of Theorem 26.70

Combining the results TBReferenced and TBReferenced gives us

$$\begin{aligned}\left(\underset{\text{Gorkov}}{\mathscr{G}_{\substack{m\\[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]}}}\frac{\partial}{\partial\delta_{m\downarrow\uparrow}(k)}\underset{\text{Gorkov}}{\mathscr{G}^{-1}_{\substack{m\\[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]}}}\right) &= -\frac{1}{\hbar}\frac{\begin{pmatrix}+\mathrm{i}\omega_k+(\epsilon_m(-\mathbf{k})-\mu)/\hbar & +\delta_{m\downarrow\uparrow}(k)\\ +\overline{\delta}_{m\downarrow\uparrow}(k) & +\mathrm{i}\omega_k-(\epsilon_m(\mathbf{k})-\mu)/\hbar\end{pmatrix}}{+\omega_k^2+\frac{\left(\epsilon_m(\mathbf{k})-\mu\right)^2}{\hbar^2}+|\delta_{m\downarrow\uparrow}(k)|^2}\cdot\begin{pmatrix}0 & -\hbar\\ 0 & 0\end{pmatrix}\\ &= +\frac{\begin{pmatrix}0 & +\mathrm{i}\omega_k+(\epsilon_m(-\mathbf{k})-\mu)/\hbar\\ 0 & \overline{\delta}_{m\downarrow\uparrow}(k)\end{pmatrix}}{+\omega_k^2+\frac{\left(\epsilon_m(\mathbf{k})-\mu\right)^2}{\hbar^2}+|\delta_{m\downarrow\uparrow}(k)|^2}\end{aligned}\tag{35.124}$$

which gives for the trace

$$\mathrm{Tr}_{2\times2}\left(\underset{\text{Gorkov}}{\mathscr{G}_{\substack{m\\[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]}}}\frac{\partial}{\partial\delta_{m\downarrow\uparrow}(k)}\underset{\text{Gorkov}}{\mathscr{G}^{-1}_{\substack{m\\[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]}}}\right) = +\frac{\overline{\delta}_{m\downarrow\uparrow}(k)}{\omega_k^2+\frac{\left(\epsilon_m(\mathbf{k})-\mu\right)^2}{\hbar^2}+|\delta_{m\downarrow\uparrow}(k)|^2}\tag{35.125}$$

Now we arrive at the final form of the gap-equations

$$\overline{\delta}_{n\downarrow\uparrow}(k') = + \sum_{\substack{k \in \mathrm{i}\Omega_{-1} \times \mathrm{Q} \\ \nu \in \{1,\ldots,rd\} \\ m \in \{1,2,3,\ldots\}}} \frac{\overline{\delta}_{m\downarrow\uparrow}(k)}{\omega_k^2 + \frac{\left(\epsilon_m(\mathbf{k}) - \mu\right)^2}{\hbar^2} + |\delta_{m\downarrow\uparrow}(k)|^2} \frac{2\omega_\nu(\mathbf{k}-\mathbf{k}')}{\omega_{k-k'}^2 + \omega_\nu^2(\mathbf{k}-\mathbf{k}')} \frac{|g_{mn\nu}(\mathbf{k}', \mathbf{k}-\mathbf{k}')|^2}{\hbar^3 \beta N_p}$$

36. Appendix - Proofs for Part V

Proof 36.1 of Theorem 29.80

We rewrite the action w.r.t. to the new fields

$$\begin{aligned}
S_{\mathrm{ph}}[\phi,\overline{\phi}] &= \sum \overline{\phi}_\nu(q)\left(-\mathrm{i}\omega_n + \omega_{\mathbf{q},\nu}\right)\phi_\nu(q) \\
&= \frac{1}{4}\sum_q \left(A_\nu - \Pi_\nu\right)(-q)\left[-\mathrm{i}\omega_n + \omega_\nu(\mathbf{q})\right]\left(A_\nu + \Pi_\nu\right)(q) \\
&= \frac{1}{4}\sum_q A_\nu(-q)\left[-\mathrm{i}\omega_n + \omega_\nu(\mathbf{q})\right]A_\nu(q) \\
&- \frac{1}{4}\sum_q \Pi_\nu(-q)\left[-\mathrm{i}\omega_n + \omega_\nu(\mathbf{q})\right]\Pi_\nu(+q) \\
&+ \frac{1}{4}\sum_q A_\nu(-q)\left[-\mathrm{i}\omega_n + \omega_\nu(\mathbf{q})\right]\Pi_\nu(q) \\
&- \frac{1}{4}\sum_q \Pi_\nu(-q)\left[-\mathrm{i}\omega_n + \omega_\nu(\mathbf{q})\right]A_\nu(q) \\
&\equiv \mathrm{I} + \mathrm{II} + \mathrm{III} + \mathrm{IV} \\
&= \dots
\end{aligned}$$

Now we will examine each term individually.

$$\mathrm{IV} = -\frac{1}{4}\sum_q A_\nu(-q)\left[+\mathrm{i}\omega_n + \omega_\nu(\mathbf{q})\right]\Pi_\nu(+q) \tag{36.1}$$

Therefore the terms proportional to $\omega_\nu(\mathbf{q})$ in III and IV will cancel out. Due to the symmetries $q \leftrightarrow -q$ there are more cancellations happening. This gives

$$\begin{aligned}
\dots &= \frac{1}{4}\sum_q A_\nu(-q)\left[\omega_\nu(\mathbf{q})\right]A_\nu(q) \\
&- \frac{1}{4}\sum_q \Pi_\nu(-q)\left[\omega_\nu(\mathbf{q})\right]\Pi_\nu(+q) \\
&+ \frac{1}{4}\sum_q A_\nu(-q)\left[-\mathrm{i}\omega_n\right]\Pi_\nu(q) \\
&- \frac{1}{4}\sum_q A_\nu(-q)\left[\mathrm{i}\omega_n\right]\Pi_\nu(+q) \\
&\equiv \widetilde{\mathrm{I}} + \widetilde{\mathrm{II}} + \widetilde{\mathrm{III}} + \widetilde{\mathrm{IV}} \\
&= \dots
\end{aligned}$$

Each term gets evaluated

$$\widetilde{\mathrm{I}} = \frac{1}{2} \sum_{q \in \Omega_{+1} \times \mathrm{Q}/\sim} A_\nu(-q) \left[\omega_\nu(\mathbf{q})\right] A_\nu(q) \tag{36.2}$$

$$\widetilde{\mathrm{II}} = -\frac{1}{2} \sum_{q \in \Omega_{+1} \times \mathrm{Q}/\sim} \Pi_\nu(-q) \left[\omega_\nu(\mathbf{q})\right] \Pi_\nu(+q) \tag{36.3}$$

$$\begin{aligned}\widetilde{\mathrm{III}} + \widetilde{\mathrm{IV}} &= -\frac{1}{2} \sum_q A_\nu(-q) \left[\mathrm{i}\omega_n\right] \Pi_\nu(q) \\ &= -\frac{1}{2} \sum_{q \in \Omega_{+1} \times \mathrm{Q}/\sim} A_\nu(-q) \left[\mathrm{i}\omega_n\right] \Pi_\nu(q) + A_\nu(+q) \left[-\mathrm{i}\omega_n\right] \Pi_\nu(-q)\end{aligned}$$

Now we focus on the terms that are proportional to Π and find by performing the integral

$$\begin{aligned}\widetilde{\mathrm{II}} + \widetilde{\mathrm{III}} + \widetilde{\mathrm{IV}} &= \sum_{q \in \Omega_{+1} \times \mathrm{Q}/\sim} \left\{ \Pi_\nu(-q) \frac{-\omega_\nu(\mathbf{q})}{2} \Pi_\nu(+q) + A_\nu(-q) \frac{-\mathrm{i}\omega_n}{2} \Pi_\nu(q) + A_\nu(+q) \frac{+\mathrm{i}\omega_n}{2} \Pi_\nu(-q) \right\} \\ &\equiv \sum_{q \in \Omega_{+1} \times \mathrm{Q}/\sim} -A_\nu(-q) \frac{-\mathrm{i}\omega_n}{2} \frac{2}{-\omega_\nu(\mathbf{q})} \frac{+\mathrm{i}\omega_n}{2} A_\nu(+q) \\ &\equiv \sum_{q \in \Omega_{+1} \times \mathrm{Q}/\sim} A_\nu(-q) \frac{\omega_n^2}{2\omega_\nu(\mathbf{q})} A_\nu(+q)\end{aligned}$$

and therefore

$$\begin{aligned}\ldots &= \sum_{q \in \Omega_{+1} \times \mathrm{Q}/\sim} A_\nu(-q) \left[\omega_\nu(\mathbf{q}) + \frac{\omega_n^2}{2\omega_\nu(\mathbf{q})}\right] A_\nu(+q) \\ &= \sum_{q \in \Omega_{+1} \times \mathrm{Q}/\sim} A_\nu(-q) \left[\frac{\omega_n^2 + \omega_\nu^2(\mathbf{q})}{2\omega_\nu(\mathbf{q})}\right] A_\nu(+q) \\ &= \sum_{q \in \Omega_{+1} \times \mathrm{Q}/\sim} A_\nu(-q) \left[-\frac{1}{\hbar} \mathscr{D}_{0,\nu}^{-1}(q)\right] A_\nu(+q)\end{aligned}$$

Proof 36.2 of Corollary 29.8 We compute

$$\begin{aligned}\left(\mathrm{P}_\zeta^2\,\psi\right)(x_1,\dots,x_n) &= \mathrm{P}_\zeta\,\frac{1}{N!}\sum_{\pi\in\mathrm{S}_N}\operatorname{sign}(\pi)^{1-\theta(\zeta)}\psi(x_{\pi(1)},\dots,x_{\pi(N)})\\ &= \frac{1}{N!^2}\sum_{\pi,\sigma\in\mathrm{S}_N}\operatorname{sign}(\pi)^{1-\theta(\zeta)}\operatorname{sign}(\sigma)^{1-\theta(\zeta)}\psi(x_{\sigma(\pi(1))},\dots,x_{\sigma(\pi(N))})\\ &= \frac{1}{N!^2}\sum_{\pi,\sigma\in\mathrm{S}_N}\operatorname{sign}(\sigma\circ\pi)^{1-\theta(\zeta)}\psi(x_{\sigma(\pi(1))},\dots,x_{\sigma(\pi(N))})\\ &= \dots\end{aligned}$$

Now we use, that for each $\pi\in\mathrm{S}_N$ one has $\mathrm{S}_N=\mathrm{S}_N\circ\pi$ (as a set). Hence we can write

$$\begin{aligned}\dots &= \frac{1}{N!^2}\sum_{\pi\in\mathrm{S}_N}\sum_{\tilde\sigma\in\mathrm{S}_N}\operatorname{sign}(\tilde\sigma)^{1-\theta(\zeta)}\psi(x_{\tilde\sigma(1)},\dots,x_{\tilde\sigma(N)})\\ &= \frac{1}{N!}\sum_{\sigma\in\mathrm{S}_N}\operatorname{sign}(\sigma)^{1-\theta(\zeta)}\psi(x_{\sigma(1)},\dots,x_{\sigma(N)})\\ &= \left(\mathrm{P}_\zeta\,\psi\right)(x_1,\dots,x_n)\end{aligned}$$

Note. Correct (x_n means x_N). The second equation sign uses $(\mathrm{P}_\zeta\,\phi)(x_1,\dots,x_N)=\frac{1}{N!}\sum_\sigma\operatorname{sign}(\sigma)^{1-\theta(\zeta)}\phi(x_{\sigma(1)},\dots)$ with $\phi(y_1,\dots,y_N)=\frac{1}{N!}\sum_\pi\dots\psi(y_{\pi(1)},\dots)$ and $y_l=x_{\sigma(l)}$, so $y_{\pi(l)}=x_{\sigma(\pi(l))}$. A shorter proof: P_ζ maps into $\mathscr{F}_\zeta^N$ and acts as the identity there (Lemma 29.9), hence $\mathrm{P}_\zeta^2=\mathrm{P}_\zeta$, cf. [38, Eq. (1.36)].

Proof 36.3 of Lemma 29.11

We have to show that the two expressions coincide. The wavefunction associated with Equation (29.10) is given as

$$(x_1,\dots,x_N|\psi\rangle=\prod_{j=1}^N\langle x_i|\psi_j\rangle\equiv\psi(x_1,\dots,x_N)\tag{36.4}$$

Therefore we obtain on the one hand

$$\begin{aligned}\left(\mathrm{P}_\zeta\,\psi\right)(x_1,\dots,x_N) &= \frac{1}{N!}\sum_{\pi\in\mathrm{S}_N}\operatorname{sign}(\pi)^{1-\theta(\zeta)}\psi(x_{\pi(1)},\dots,x_{\pi(N)})\\ &= \frac{1}{N!}\sum_{\pi\in\mathrm{S}_N}\operatorname{sign}(\pi)^{1-\theta(\zeta)}\prod_{j=1}^N\langle x_{\pi(j)}|\psi_j\rangle\\ &= \frac{1}{N!}\sum_{\pi\in\mathrm{S}_N}\operatorname{sign}(\pi)^{1-\theta(\zeta)}\prod_{j=1}^N\psi_j(x_{\pi(j)})\end{aligned}$$

and we obtain on the other hand with Equation (29.11)

$$(x_1, \dots, x_N | \, \mathrm{P}_\zeta \, |\psi\rangle = \frac{1}{N!} \sum_{\pi \in \mathrm{S}_N} \mathrm{sign}(\pi)^{1-\theta(\zeta)} \prod_{j=1}^{N} \psi_{\pi(j)}(x_j)$$

the two expressions coincide which can be seen by reordering the products and using $\mathrm{sign}(\sigma) = \mathrm{sign}(\sigma^{-1})$.

Note. In the first equation the factors are $\langle x_j | \psi_j \rangle$ (not $\langle x_i | \psi_j \rangle$). The reordering reads $\prod_j \psi_j(x_{\pi(j)}) = \prod_l \psi_{\pi^{-1}(l)}(x_l)$; then substitute $\pi \to \pi^{-1}$ in the sum.

Proof 36.4 of Lemma 29.14 We have to show, that

$$\forall \psi, \chi \in \mathscr{H}_N \, : \, \langle \psi | \, \mathrm{P}_\zeta \, \chi \rangle = \langle \mathrm{P}_\zeta \, \psi | \chi \rangle \tag{36.5}$$

It suffices to prove this identity for basis-elements. Therefore we compute on the one hand

$$\begin{aligned}
(i_1, \dots, i_N | \, \mathrm{P}_\zeta \, |j_1, \dots, j_N) &= \frac{1}{N!} \sum_{\pi \in \mathrm{S}_N} \mathrm{sign}(\pi)^{1-\theta(\zeta)} (i_1, \dots, i_N | j_{\pi(1)}, \dots, j_{\pi(N)}) \\
&= \frac{1}{N!} \sum_{\pi \in \mathrm{S}_N} \mathrm{sign}(\pi)^{1-\theta(\zeta)} \prod_{l=1}^{N} \langle i_l | j_{\pi(l)} \rangle \\
&= \frac{1}{N!} \sum_{\pi \in \mathrm{S}_N} \mathrm{sign}(\pi)^{1-\theta(\zeta)} \prod_{l=1}^{N} \delta_{i_l, j_{\pi(l)}}
\end{aligned}$$

and we obtain on the other hand

$$(i_1, \dots, i_N | \, \mathrm{P}_\zeta^\dagger \, |j_1, \dots, j_N) = \frac{1}{N!} \sum_{\pi \in \mathrm{S}_N} \mathrm{sign}(\pi)^{1-\theta(\zeta)} \prod_{l=1}^{N} \delta_{i_{\pi(l)}, j_l}$$

Just as in the prove of the Lemma before, the two expressions coincide, which can also be seen by expanding the products reordering the appearing factors and using $\mathrm{sign}(\sigma) = \mathrm{sign}(\sigma^{-1})$.

Note. The third line uses an orthonormal basis. For a general basis, keep $\langle i_l | j_{\pi(l)} \rangle$; the second expression is $(i | \, \mathrm{P}_\zeta^\dagger \, |j) = \overline{(j | \, \mathrm{P}_\zeta \, |i)} = \frac{1}{N!} \sum_\pi \mathrm{sign}(\pi)^{1-\theta(\zeta)} \prod_l \langle i_{\pi(l)} | j_l \rangle$, and relabeling $l \to \pi^{-1}(l)$, $\pi \to \pi^{-1}$ shows equality in the same way. It suffices to check basis elements because both sides are sesquilinear.

Proof 36.5 of Theorem 29.63 We adopt the more general notation from the earlier section. This yields for the Hamiltonian in the harmonic approximation

$$H \equiv \sum_{\lambda \in \mathscr{A}} \hbar\omega_\lambda b_\lambda^\dagger b_\lambda \tag{36.6}$$

in the grand-canonical Ensemble, we obtain, referring to an enumeration $\lambda_1, \lambda_2, \dots, \lambda_{rd_{\mathbf{x}}N_p}$ of $\mathscr{A}$, the identities

$$\langle b_\lambda^\dagger b_\lambda \rangle = \frac{\mathrm{Tr}_{\mathscr{H}}\left(\mathrm{e}^{-\beta H} b_\lambda^\dagger b_\lambda\right)}{\mathrm{Tr}_{\mathscr{H}}\left(\mathrm{e}^{-\beta H}\right)} = \frac{\sum_{n_{\lambda_1}=0}^\infty \sum_{n_{\lambda_2}=0}^\infty \cdots \sum_{n_{\lambda_{rd_{\mathbf{x}}N_p}}=0}^\infty \left\langle n_{\lambda_1}, \dots, n_{\lambda_{rd_{\mathbf{x}}N_p}} \mid \mathrm{e}^{-\beta H} b_\lambda^\dagger b_\lambda \mid n_{\lambda_1}, \dots, n_{\lambda_{rd_{\mathbf{x}}N_p}} \right\rangle}{\sum_{n_{\lambda_1}=0}^\infty \sum_{n_{\lambda_2}=0}^\infty \cdots \sum_{n_{\lambda_{rd_{\mathbf{x}}N_p}}=0}^\infty \left\langle n_{\lambda_1}, \dots, n_{\lambda_{rd_{\mathbf{x}}N_p}} \mid \mathrm{e}^{-\beta H} \mid n_{\lambda_1}, \dots, n_{\lambda_{rd_{\mathbf{x}}N_p}} \right\rangle} = \star$$

using now the hermiticity of the Hamiltonian, we see that we can replace $b_{\lambda_i}^\dagger b_{\lambda_i}$ by the numbers n_{λ_i} and factorize the expression, such that everything except for one pair of sums cancels out and we obtain

$$\star = \frac{\sum_{n_\lambda=0}^\infty \mathrm{e}^{-\beta\hbar\omega_\lambda n_\lambda} n_\lambda}{\sum_{n_\lambda=0}^\infty \mathrm{e}^{-\beta n_\lambda \hbar\omega_\lambda}} \equiv -\left(\frac{f'(x)}{f(x)}\right)_{|x=\beta\hbar\omega_\lambda}$$

We therefore examine the function

$$f(x) = \sum_{n_\lambda=0}^\infty \mathrm{e}^{-n_\lambda x} = \frac{1}{1-\mathrm{e}^{-x}}$$

and obtain the derivative

$$f'(x) = -\frac{\mathrm{e}^{-x}}{(1-\mathrm{e}^{-x})^2}$$

such that we obtain

$$\frac{-f'(x)}{f(x)} = \frac{\mathrm{e}^{-x}}{(1-\mathrm{e}^{-x})^2} \cdot \frac{1-\mathrm{e}^{-x}}{1} = \frac{\mathrm{e}^{-x}}{1-\mathrm{e}^{-x}} = \frac{1}{\mathrm{e}^{+x}-1} = \mathrm{B}_1(x)$$

Proof 36.6 of Lemma 31.5 As long as $m_{1,2,3} \neq \infty$ (or, equivalently $h, k, l \neq 0$) we can consider the three special vectors

$$\mathbf{T}_1 = m_1\mathbf{a}_1 - m_2\mathbf{a}_2, \quad \mathbf{T}_2 = m_2\mathbf{a}_2 - m_3\mathbf{a}_3, \quad \mathbf{T}_3 = m_3\mathbf{a}_3 - m_1\mathbf{a}_1. \tag{36.7}$$

According to the mnemonic

$$\text{Plane} = \text{Support-Vector} + c_1 \text{Directional-Vector-1} + c_2 \text{Directional-Vector-2} \quad c_i \in \mathbb{R} \tag{36.8}$$

we have to show that the scalar-product $\mathbf{T}_i \cdot \mathbf{G}$ vanishes.

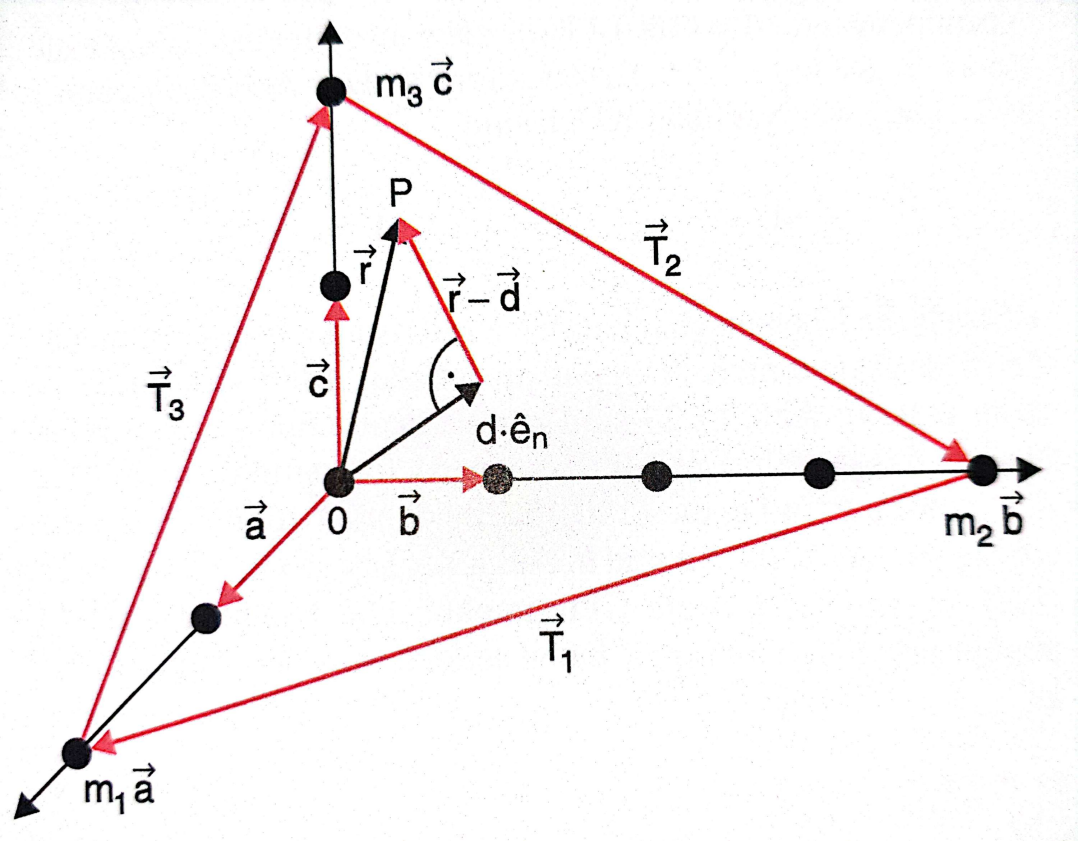


Figure 36.1.: Excerpt from Wolfang Demtröders Experimentalphysik 3.

And indeed, a straight-forward calculation yields

$$\begin{aligned}\mathbf{T}_1 \cdot \mathbf{G} &= \left(m_1\mathbf{a}_1 - m_2\mathbf{a}_2\right) \cdot \left(h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3\right) \\ &= 2\pi\left(m_1 h - m_2 k\right) \\ &= 0\end{aligned}$$

and analog for $\mathbf{T}_{1,2}$.

Now we consider the case that at least one of the m_i is equal to infinity. Without loss of generality, we consider $m_1 = \infty$ (equivalently one has $h = 0$). Then we consider $\widetilde{\mathbf{T}}_1 = \mathbf{a}_1$ and $\mathbf{T}_2 = m_2\mathbf{a}_2 - m_3\mathbf{a}_3$ as directional-vectors of the planes and the scalar-product vanishes again.

Now we consider the case that two of the m_i are equal to infinity. Without loss of generality, we consider $m_1 = m_2 = \infty$ (equivalently one has $h = k = 0$). Then we consider $\widetilde{\mathbf{T}}_1 = \mathbf{a}_1$ and $\widetilde{\mathbf{T}}_2 = \mathbf{a}_2$ as directional-vectors of the planes and the scalar-product vanishes again.

Adding Pictures.

Proof 36.7 of Lemma 30.4

We compute the matrix-elements to be

$$\begin{aligned}\langle \mathbf{k}_1\sigma_1, \mathbf{k}_2\sigma_2|V|\mathbf{k}_3\sigma_3, \mathbf{k}_4\sigma_4\rangle &= -|g|\delta_{\sigma_3\neq\sigma_4}\delta_{\sigma_1,\sigma_3}\delta_{\sigma_2,\sigma_4}\int \mathrm{d}^3\mathbf{r}\mathrm{d}^3\mathbf{r}'\delta(\mathbf{r}-\mathbf{r}')\psi^*_{\mathbf{k}_1}(\mathbf{r})\psi^*_{\mathbf{k}_2}(\mathbf{r}')\psi_{\mathbf{k}_3}(\mathbf{r})\psi_{\mathbf{k}_4}(\mathbf{r}')\\ &= -|g|\delta_{\sigma_3\neq\sigma_4}\delta_{\sigma_1,\sigma_3}\delta_{\sigma_2,\sigma_4}\int \mathrm{d}^3\mathbf{r}\psi^*_{\mathbf{k}_1}(\mathbf{r})\psi^*_{\mathbf{k}_2}(\mathbf{r})\psi_{\mathbf{k}_3}(\mathbf{r})\psi_{\mathbf{k}_4}(\mathbf{r}')\\ &= -\frac{|g|}{L^{d_\mathbf{x}}}\delta_{\sigma_3\neq\sigma_4}\delta_{\sigma_1,\sigma_3}\delta_{\sigma_2,\sigma_4}\delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4}\end{aligned}$$

Proof 36.8 of Theorem 30.5 We have computed the matrix-elements and will now insert them into the definition of the second quantized version of V. This yields

$$\begin{aligned}V^{2\mathrm{Q}} &= \frac{1}{2}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4}\sum_{\sigma_1,\sigma_2,\sigma_3,\sigma_4}\frac{-|g|}{L^{d_\mathbf{x}}}\delta_{\sigma_3\neq\sigma_4}\delta_{\sigma_1,\sigma_3}\delta_{\sigma_2,\sigma_4}\delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4}c^\dagger_{\mathbf{k}_1\sigma_1}c^\dagger_{\mathbf{k}_2\sigma_2}c_{\mathbf{k}_4\sigma_4}c_{\mathbf{k}_3\sigma_3}\\ &= \frac{-|g|}{2L^{d_\mathbf{x}}}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4}\sum_{\sigma_1,\sigma_2}\delta_{\sigma_1\neq\sigma_2}\delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4}c^\dagger_{\mathbf{k}_1\sigma_1}c^\dagger_{\mathbf{k}_2\sigma_2}c_{\mathbf{k}_4\sigma_2}c_{\mathbf{k}_3\sigma_1}\\ &= \frac{-|g|}{2L^{d_\mathbf{x}}}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4}\delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4}\left(c^\dagger_{\mathbf{k}_1\uparrow}c^\dagger_{\mathbf{k}_2\downarrow}c_{\mathbf{k}_4\downarrow}c_{\mathbf{k}_3\uparrow}+c^\dagger_{\mathbf{k}_1\downarrow}c^\dagger_{\mathbf{k}_2\uparrow}c_{\mathbf{k}_4\uparrow}c_{\mathbf{k}_3\downarrow}\right)\\ &= \frac{-|g|}{L^{d_\mathbf{x}}}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4}\delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4}c^\dagger_{\mathbf{k}_1\uparrow}c^\dagger_{\mathbf{k}_2\downarrow}c_{\mathbf{k}_4\downarrow}c_{\mathbf{k}_3\uparrow}\end{aligned}$$

Lastly we need to relabel the summation-indices to obtain the desired form of the Hamiltonian. For this we do the following manipulations

$$\begin{aligned}V^{2\mathrm{Q}} &= \frac{-|g|}{L^{d_\mathbf{x}}}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4}\delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4}c^\dagger_{\mathbf{k}_1\uparrow}c^\dagger_{\mathbf{k}_2\downarrow}c_{\mathbf{k}_4\downarrow}c_{\mathbf{k}_3\uparrow}\\ &\overset{k_3\leftrightarrow k_4}{=} \frac{-|g|}{L^{d_\mathbf{x}}}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4}\delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4}c^\dagger_{\mathbf{k}_1\uparrow}c^\dagger_{\mathbf{k}_2\downarrow}c_{\mathbf{k}_3\downarrow}c_{\mathbf{k}_4\uparrow}\\ &= \frac{-|g|}{L^{d_\mathbf{x}}}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_4}c^\dagger_{\mathbf{k}_1\uparrow}c^\dagger_{\mathbf{k}_2\downarrow}c_{\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_4\downarrow}c_{\mathbf{k}_4\uparrow}\\ &\overset{k_2\to-k_2}{=} \frac{-|g|}{L^{d_\mathbf{x}}}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_4}c^\dagger_{\mathbf{k}_1\uparrow}c^\dagger_{-\mathbf{k}_2\downarrow}c_{\mathbf{k}_1-\mathbf{k}_2-\mathbf{k}_4\downarrow}c_{\mathbf{k}_4\uparrow}\\ &\overset{k_2\equiv k,k_4\equiv k'}{=} \frac{-|g|}{L^{d_\mathbf{x}}}\sum_{\mathbf{k}_1,\mathbf{k},\mathbf{k}'}c^\dagger_{\mathbf{k}_1\uparrow}c^\dagger_{-\mathbf{k}\downarrow}c_{\mathbf{k}_1-\mathbf{k}-\mathbf{k}'\downarrow}c_{\mathbf{k}'\uparrow}\\ &\overset{k_1\equiv q}{=} \frac{-|g|}{L^{d_\mathbf{x}}}\sum_{\mathbf{q},\mathbf{k},\mathbf{k}'}c^\dagger_{\mathbf{q}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}c_{\mathbf{q}-\mathbf{k}-\mathbf{k}'\downarrow}c_{\mathbf{k}'\uparrow}\\ &\overset{q\to q+k}{=} \frac{-|g|}{L^{d_\mathbf{x}}}\sum_{\mathbf{q},\mathbf{k},\mathbf{k}'}c^\dagger_{\mathbf{q}+\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}c_{\mathbf{q}-\mathbf{k}'\downarrow}c_{\mathbf{k}'\uparrow}\end{aligned}$$

proving the theorem.

Proof 36.9 of Lemma 30.7 See Draft-Summary.

Proof 36.10 of Corollary 30.8

The First Identity

We have the notation

$$\langle \mathbf{x}|\mathbf{q}\rangle \equiv \frac{1}{\sqrt{L^{d_\mathbf{x}}}} \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{x}} \equiv \psi_\mathbf{q}(\mathbf{x}) \tag{36.9}$$

for the spatial part of wavefunctions. The only term that was not proven in the [Draft Summary] is the interaction-term.

Hence we compute

$$\begin{aligned}\int \mathrm{d}\mathbf{r}\, c_\uparrow^\dagger(\mathbf{r}) c_\downarrow^\dagger(\mathbf{r}) c_\downarrow(\mathbf{r}) c_\uparrow(\mathbf{r}) &= \sum_{\mathbf{k}_1,\ldots,\mathbf{k}_4} \int \mathrm{d}\mathbf{r}\, \overline{\psi}_{\mathbf{k}_1\uparrow}(\mathbf{r}) \overline{\psi}_{\mathbf{k}_2\downarrow}(\mathbf{r}) \psi_{\mathbf{k}_3\downarrow}(\mathbf{r}) \psi_{\mathbf{k}_4\uparrow}(\mathbf{r}) c_\uparrow^\dagger(\mathbf{k}_1) c_\downarrow^\dagger(\mathbf{k}_2) c_\downarrow(\mathbf{k}_3) c_\uparrow(\mathbf{k}_4) \\ &= \ldots\end{aligned}$$

the integral factor can[1] be simplified to

$$\int \mathrm{d}\mathbf{r}\, \overline{\psi}_{\mathbf{k}_1\uparrow}(\mathbf{r}) \overline{\psi}_{\mathbf{k}_2\downarrow}(\mathbf{r}) \psi_{\mathbf{k}_3\downarrow}(\mathbf{r}) \psi_{\mathbf{k}_4\uparrow}(\mathbf{r}) = \frac{1}{L^{2d_\mathbf{x}}} \int \mathrm{d}\mathbf{r}\, \mathrm{e}^{\mathrm{i}(\mathbf{k}_3+\mathbf{k}_4-(\mathbf{k}_1+\mathbf{k}_2))} = \frac{1}{L^{d_\mathbf{x}}} \delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4} \tag{36.10}$$

hence we obtain

$$\begin{aligned}\ldots &= \frac{1}{L^{d_\mathbf{x}}} \sum_{\mathbf{k}_1,\ldots,\mathbf{k}_3} c_\uparrow^\dagger(\mathbf{k}_1) c_\downarrow^\dagger(\mathbf{k}_2) c_\downarrow(\mathbf{k}_3) c_\uparrow(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3) \\ &\overset{\mathbf{k}_2\to-\mathbf{k}_2}{=} \frac{1}{L^{d_\mathbf{x}}} \sum_{\mathbf{k}_1,\ldots,\mathbf{k}_3} c_\uparrow^\dagger(\mathbf{k}_1) c_\downarrow^\dagger(-\mathbf{k}_2) c_\downarrow(\mathbf{k}_3) c_\uparrow(\mathbf{k}_1-(\mathbf{k}_2+\mathbf{k}_3)) \\ &\overset{\mathbf{k}_2\to\mathbf{k}}{=} \frac{1}{L^{d_\mathbf{x}}} \sum_{\mathbf{k}_1,\mathbf{k},\mathbf{k}_3} c_\uparrow^\dagger(\mathbf{k}_1) c_\downarrow^\dagger(-\mathbf{k}) c_\downarrow(\mathbf{k}_3) c_\uparrow(\mathbf{k}_1-(\mathbf{k}+\mathbf{k}_3)) \\ &\overset{\mathbf{k}_1\to\mathbf{k}_1+\mathbf{k}}{=} \frac{1}{L^{d_\mathbf{x}}} \sum_{\mathbf{k}_1,\mathbf{k},\mathbf{k}_3} c_\uparrow^\dagger(\mathbf{k}_1+\mathbf{k}) c_\downarrow^\dagger(-\mathbf{k}) c_\downarrow(\mathbf{k}_3) c_\uparrow(\mathbf{k}_1-\mathbf{k}_3) \\ &\overset{\mathbf{k}_1\equiv\mathbf{q}}{=} \frac{1}{L^{d_\mathbf{x}}} \sum_{\mathbf{q},\mathbf{k},\mathbf{k}_3} c_\uparrow^\dagger(\mathbf{k}+\mathbf{q}) c_\downarrow^\dagger(-\mathbf{k}) c_\downarrow(\mathbf{k}_3) c_\uparrow(\mathbf{q}-\mathbf{k}_3) \\ &\overset{\mathbf{k}_3\to-\mathbf{k}_3+\mathbf{q}}{=} \frac{1}{L^{d_\mathbf{x}}} \sum_{\mathbf{q},\mathbf{k},\mathbf{k}_3} c_\uparrow^\dagger(\mathbf{k}+\mathbf{q}) c_\downarrow^\dagger(-\mathbf{k}) c_\downarrow(\mathbf{q}-\mathbf{k}_3) c_\uparrow(\mathbf{k}_3) \\ &\overset{\mathbf{k}_3\equiv\mathbf{k}'}{=} \frac{1}{L^{d_\mathbf{x}}} \sum_{\mathbf{q},\mathbf{k},\mathbf{k}'} c_\uparrow^\dagger(\mathbf{k}+\mathbf{q}) c_\downarrow^\dagger(-\mathbf{k}) c_\downarrow(\mathbf{q}-\mathbf{k}') c_\uparrow(\mathbf{k}')\end{aligned}$$

[1] Cf. page 64 in Supermathematics.

The Second Identity

TBD.

Proof 36.11 of Corollary 30.12

See Waste-Folder 6, Topic 3 for a proof.

We compute with results from [Draft Summary]

$$S_{\text{int}}[\overline{\psi},\psi] \equiv \sum_{\omega_{n_1},\omega_{n_2},\omega_{n_3},\omega_{n_4}} \delta_{\omega_{n_1}+\omega_{n_2},\omega_{n_3}+\omega_{n_4}} \overline{\psi}(\omega_{n_1})\overline{\psi}(\omega_{n_2})\psi(\omega_{n_3})\psi(\omega_{n_4})$$
$$= \dots$$

now we change the enumeration of the second sum as $\omega_{n_2} \mapsto -\omega_{n_2}$ and obtain hence $\omega_{n_1} = \omega_{n_3} + \omega_{n_4} + \omega_{n_2}$ which gives

$$\dots = \sum_{\omega_{n_1},\omega_{n_2},\omega_{n_3},\omega_{n_4}} \delta_{\omega_{n_1}+\omega_{n_2},\omega_{n_3}+\omega_{n_4}} \overline{\psi}(\omega_{n_2}+\omega_{n_3}+\omega_{n_4})\overline{\psi}(\omega_{n_2})\psi(\omega_{n_3})\psi(\omega_{n_4})$$
$$= \dots$$

Now we shift the third summation according to $\omega_{n_3} \mapsto \omega_{n_3} - \omega_{n_4}$ and obtain finally

$$\dots = \sum_{\omega_{n_1},\omega_{n_2},\omega_{n_3},\omega_{n_4}} \delta_{\omega_{n_1}+\omega_{n_2},\omega_{n_3}+\omega_{n_4}} \overline{\psi}(\omega_{n_2}+\omega_{n_3})\overline{\psi}(\omega_{n_2})\psi(\omega_{n_3}-\omega_{n_4})\psi(\omega_{n_4})$$

Proof 36.12 of Lemma 30.14 See Supermathematics, equation (3.31) and See Waste-Folder 6, topic 5, page 6 for the boundary-conditions.

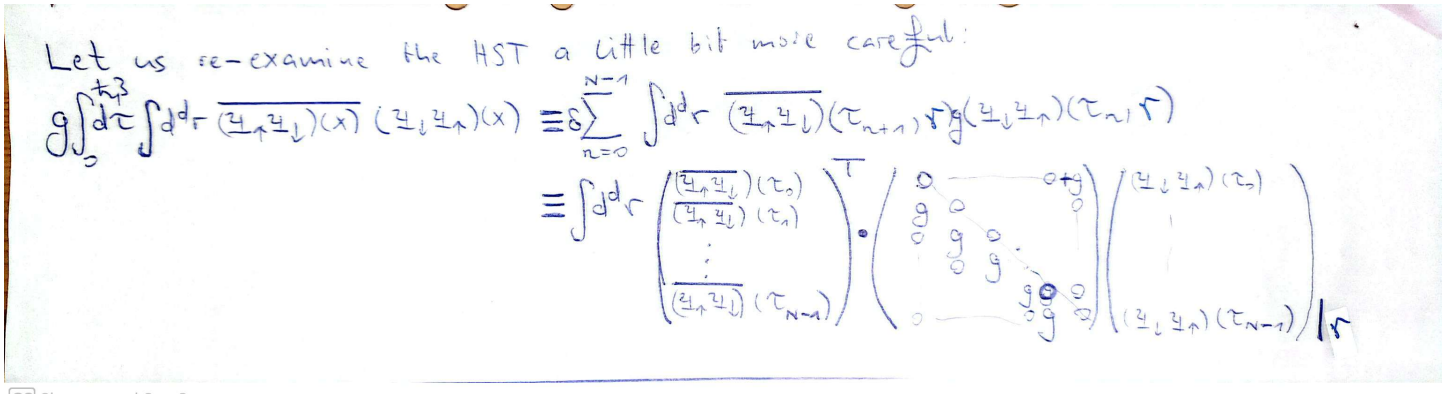


Figure 36.2.: Notes to clarify why periodic boundary-conditions emerge.

Proof 36.13 of Lemma 30.18

TBD

Proof 36.14 of Lemma 30.29

By direct computation, using the von Neumann series

$$\begin{aligned}\operatorname{Tr}\operatorname{Log}\mathscr{G}^{-1}_{\text{Gorkov}} &\equiv \operatorname{Tr}\operatorname{Log}\mathscr{G}^{-1}_{0\ \text{Gorkov}} + \operatorname{Tr}\operatorname{Log}\left(1+\mathscr{G}_{0\ \text{Gorkov}}\ V\right)^{-1}\\ &\equiv \text{const.} \quad + \quad \sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k}\operatorname{Tr}\left(\mathscr{G}_{0\ \text{Gorkov}}\ V\right)^{k}.\end{aligned}$$

Proof 36.15 of Theorem 30.30

TBD

Proof 36.16 of Corollary 30.22

TBD

Proof 36.17 of Theorem ?? (Linked-Cluster-Theorem)

TBUpdated: Ordering of the indices.

We rewrite the partition-function in its symmetrized form

With the expansion

$$\begin{aligned}\exp - S_{\text{int}}[\xi] &= \sum_{n=0}^{\infty} \frac{(-1/\hbar)^n}{n!} \prod_{\bullet=1}^{n} \int_0^{\hbar\beta} \mathrm{d}\tau_\bullet \, V(\xi(\tau_\bullet)) \\ &= \sum_{n=0}^{\infty} \frac{(-1/\hbar)^n}{n!} \prod_{\bullet=1}^{n} \oint V_{\alpha_1^\bullet,\ldots,\alpha_m^\bullet} \, \xi_{\alpha_1^\bullet}(\tau_\bullet) \cdots \xi_{\alpha_m^\bullet}(\tau_\bullet)\end{aligned}$$

one finds

$$\begin{aligned}\mathscr{G}_{\alpha,\alpha'}(\tau) &= \frac{-1}{\hbar} \langle \xi_\alpha(\tau) \xi_{\alpha'}(0) \rangle \\ &= \frac{-1}{\hbar} \frac{\displaystyle\sum_{n=0}^{\infty} \frac{(-1/\hbar)^n}{n!} \langle \xi_\alpha(\tau)\xi_{\alpha'}(0) \prod_{\bullet=1}^{n} \oint V_{\alpha_1^\bullet,\ldots,\alpha_m^\bullet} \, \xi_{\alpha_1^\bullet}(\tau_\bullet) \cdots \xi_{\alpha_m^\bullet}(\tau_\bullet) \rangle_0}{\displaystyle\sum_{n=0}^{\infty} \frac{(-1/\hbar)^n}{n!} \langle \prod_{\bullet=1}^{n} \oint V_{\alpha_1^\bullet,\ldots,\alpha_m^\bullet} \, \xi_{\alpha_1^\bullet}(\tau_\bullet) \cdots \xi_{\alpha_m^\bullet}(\tau_\bullet) \rangle_0}\end{aligned}$$

We will now examine the numerator of this expression and see that it factorizes into two factors, with one being equal to the denominator; This is what Alexander Altland called a „miraculous cancellation mechanism“. It follows by combinatorical counting

numerator

$$\begin{aligned}&= \sum_{n=0}^{\infty} \frac{(-1/\hbar)^n}{n!} \langle \xi_\alpha(\tau)\xi_{\alpha'}(0) \prod_{\bullet=1}^{n} \oint V_{\alpha_1^\bullet,\ldots,\alpha_m^\bullet} \, \xi_{\alpha_1^\bullet}(\tau_\bullet) \cdots \xi_{\alpha_m^\bullet}(\tau_\bullet) \rangle_0 \\ &= \sum_{n=0}^{\infty} \sum_{p=0}^{n} \frac{(-1/\hbar)^n}{(n-p)!p!} \langle \xi_\alpha(\tau)\xi_{\alpha'}(0) \prod_{\bullet=1}^{n-p} \oint V_{\alpha_1^\bullet,\ldots,\alpha_m^\bullet} \, \xi_{\alpha_1^\bullet}(\tau_\bullet) \cdots \xi_{\alpha_m^\bullet}(\tau_\bullet) \rangle_0^{\text{n.v.}} \langle \prod_{\bullet=1}^{p} \oint V_{\alpha_1^\bullet,\ldots,\alpha_m^\bullet} \, \xi_{\alpha_1^\bullet}(\tau_\bullet) \cdots \xi_{\alpha_m^\bullet}(\tau_\bullet) \rangle_0 \\ &= \sum_{n=0}^{\infty} \frac{(-1/\hbar)^n}{n!} \langle \xi_\alpha(\tau)\xi_{\alpha'}(0) \prod_{\bullet=1}^{n} \oint V_{\alpha_1^\bullet,\ldots,\alpha_m^\bullet} \, \xi_{\alpha_1^\bullet}(\tau_\bullet) \cdots \xi_{\alpha_m^\bullet}(\tau_\bullet) \rangle_0^{\text{n.v.}} \sum_{p=0}^{\infty} \frac{(-1/\hbar)^p}{p!} \langle \prod_{\bullet=1}^{p} \oint V_{\alpha_1^\bullet,\ldots,\alpha_m^\bullet} \, \xi_{\alpha_1^\bullet}(\tau_\bullet) \cdots \xi_{\alpha_m^\bullet}(\tau_\bullet) \rangle_0\end{aligned}$$

and it follows that

$$\mathscr{G}_{\alpha,\alpha'}(\tau) = -\frac{1}{\hbar} \sum_{n=0}^{\infty} \frac{(-1/\hbar)^n}{n!} \langle \xi_\alpha(\tau)\xi_{\alpha'}(0) \prod_{\bullet=1}^{n} \oint V_{\alpha_1^\bullet,\ldots,\alpha_m^\bullet} \, \xi_{\alpha_1^\bullet}(\tau_\bullet) \cdots \xi_{\alpha_m^\bullet}(\tau_\bullet) \rangle_0^{\text{n.v.}} \tag{36.11}$$

ToBeRedone with Graph Theory, Cf. the book from Salmhofer

Part VI.

"Experimental" (Work in Progresss)

37. Experimental: The Internal Energy using the full Bethe-Salpeter-Equation in the Tree-Level-Approximation

37.1. Correcting the Internal Energy for the Phononic Contribution

We will now elaborate how we can compute the correction-terms from the Bethe-Salpeter-equation in the specific heat calculation

$$\begin{aligned}\mathscr{G}^2_{0,\nu}(q)\hbar^2\left\langle\rho_\nu(q)\rho_\nu(-q)\right\rangle &= \frac{\mathscr{G}^2_{0,\nu}(q)}{\hbar\beta N_p}\sum_{\substack{\sigma,\sigma'\in\{\downarrow,\uparrow\}\\ k,k'\in \mathrm{i}\Omega_{-1}\times\mathbb{Q}\\ n,n',m,m'\in\{1,\dots,\infty\}}} g_{mn\nu}(\mathbf{k},\mathbf{q})g_{m'n'\nu}(\mathbf{k}',-\mathbf{q})\left\langle\overline{\psi}_{m\sigma}(k+q)\psi_{n\sigma}(k)\overline{\psi}_{m'\sigma'}(k'-q)\psi_{n'\sigma'}(k')\right\rangle\\ &= \frac{\mathscr{G}^2_{0,\nu}(q)}{\hbar\beta N_p}\sum_{\substack{\sigma,\sigma'\in\{\downarrow,\uparrow\}\\ k,k'\in \mathrm{i}\Omega_{-1}\times\mathbb{Q}\\ n,n',m,m'\in\{1,\dots,\infty\}}} g_{mn\nu}(\mathbf{k},\mathbf{q})g_{m'n'\nu}(\mathbf{k}',-\mathbf{q})\left\langle\psi_{n\sigma}(k)\psi_{n'\sigma'}(k')\overline{\psi}_{m'\sigma'}(k'-q)\overline{\psi}_{m\sigma}(k+q)\right\rangle\\ &= \dots\end{aligned} \tag{37.1}$$

We focus on the contribution that we neglected earlier (from the Bethe-Salpeter-equation TBReferenced and Equation Exp. Value as GF) and compute

$$\begin{aligned}&\left\langle\psi_{n\sigma}(k)\psi_{n'\sigma'}(k')\overline{\psi}_{m'\sigma'}(k'-q)\overline{\psi}_{m\sigma}(k+q)\right\rangle\\ &= \hbar^2\mathscr{G}\left(n\sigma k,\, n'\sigma'k' \mid m\sigma k+q,\, m'\sigma'k'-q\right)\\ &= \text{"Wick-Theorem-contributions"}\\ &- \hbar^2\sum_{\substack{\sigma_1,\sigma_2,\sigma_1',\sigma_2'\in\{\downarrow,\uparrow\}\\ n_1,n_2,n_1',n_2'\in\{1,\dots,\infty\}\\ k_1,k_2,k_1',k_2'\in \mathrm{i}\Omega_{-1}\times\mathbb{Q}}} \mathscr{G}^{\,0}_{\substack{n,n_1\\ \sigma,\sigma_1\\ k,k_1}}\mathscr{G}^{\,0}_{\substack{n',n_2\\ \sigma',\sigma_2\\ k',k_2}}V_{n_1,n_2,n_1',n_2'}\mathscr{G}^{\,0}_{\substack{n_1',m\\ \sigma_1',\sigma\\ k_1',k+q}}\mathscr{G}^{\,0}_{\substack{n_2',m'\\ \sigma_2',\sigma'\\ k_2',k'-q}}\end{aligned} \tag{37.2}$$

inserting this into the equation above yields

$$\begin{aligned}\dots &= -\hbar^2\frac{\mathscr{G}^2_{0,\nu}(q)}{\hbar\beta N_p}\sum_{\substack{\sigma,\sigma'\in\{\downarrow,\uparrow\}\\ k,k'\in \mathrm{i}\Omega_{-1}\times\mathbb{Q}\\ n,n',m,m'\in\{1,\dots,\infty\}}} g_{mn\nu}(\mathbf{k},\mathbf{q})g_{m'n'\nu}(\mathbf{k}',-\mathbf{q})\sum_{\substack{\sigma_1,\sigma_2,\sigma_1',\sigma_2'\in\{\downarrow,\uparrow\}\\ n_1,n_2,n_1',n_2'\in\{1,\dots,\infty\}\\ k_1,k_2,k_1',k_2'\in \mathrm{i}\Omega_{-1}\times\mathbb{Q}}} \mathscr{G}^{\,0}_{\substack{n,n_1\\ \sigma,\sigma_1\\ k,k_1}}\mathscr{G}^{\,0}_{\substack{n',n_2\\ \sigma',\sigma_2\\ k',k_2}}V^{\mathrm{as}}_{n_1,n_2,n_1',n_2'}\mathscr{G}^{\,0}_{\substack{n_1',m\\ \sigma_1',\sigma\\ k_1',k+q}}\mathscr{G}^{\,0}_{\substack{n_2',m'\\ \sigma_2',\sigma'\\ k_2',k'-q}}\\ &= \dots\end{aligned} \tag{37.3}$$

now we terminate the summations over $n_1, n_2, n_1', n_2', \sigma_1, \sigma_2, \sigma_1', \sigma_2'$ and k_1, k_2, k_1', k_2' and obtain

$$\ldots = \frac{-\hbar \mathscr{G}_{0,\nu}^2(q)}{\beta N_p} \sum_{\substack{\sigma,\sigma' \in \{\downarrow,\uparrow\} \\ k,k' \in \mathrm{i}\Omega_{-1}\times\mathbb{Q} \\ n,n',m,m' \in \{1,\ldots,\infty\}}} g_{mn\nu}(\mathbf{k},\mathbf{q}) g_{m'n'\nu}(\mathbf{k}',-\mathbf{q}) \mathscr{G}^{\ 0}_{\substack{n,n \\ \sigma,\sigma \\ k,k}} \mathscr{G}^{\ 0}_{\substack{n',n' \\ \sigma',\sigma' \\ k',k'}} V^{\mathrm{as}}_{\substack{n,n',m,m' \\ \sigma,\sigma',\sigma,\sigma' \\ k,k',k+q,k'-q}} \mathscr{G}^{\ 0}_{\substack{m,m \\ \sigma,\sigma \\ k+q,k+q}} \mathscr{G}^{\ 0}_{\substack{m',m' \\ \sigma',\sigma' \\ k'-q,k'-q}} \tag{37.4}$$

In order to get the total contribution, we sum over ν and q and multiply with $1/(\hbar\beta)$ obtain

"BS-Correction-Terms"

$$\begin{aligned} &= \frac{1}{\hbar\beta} \sum_{\substack{\nu \in \{1,\ldots,rd_{\mathbf{x}}\} \\ q \in \mathrm{i}\Omega_{+1}\times\mathbb{Q}}} \frac{-\hbar \mathscr{G}_{0,\nu}^2(q)}{\beta N_p} \sum_{\substack{\sigma,\sigma' \in \{\downarrow,\uparrow\} \\ k,k' \in \mathrm{i}\Omega_{-1}\times\mathbb{Q} \\ n,n',m,m' \in \{1,\ldots,\infty\}}} g_{mn\nu}(\mathbf{k},\mathbf{q}) g_{m'n'\nu}(\mathbf{k}',-\mathbf{q}) \mathscr{G}^{\ 0}_{\substack{n,n \\ \sigma,\sigma \\ k,k}} \mathscr{G}^{\ 0}_{\substack{n',n' \\ \sigma',\sigma' \\ k',k'}} V^{\mathrm{as}}_{\substack{n,n',m,m' \\ \sigma,\sigma',\sigma,\sigma' \\ k,k',k+q,k'-q}} \mathscr{G}^{\ 0}_{\substack{m,m \\ \sigma,\sigma \\ k+q,k+q}} \mathscr{G}^{\ 0}_{\substack{m',m' \\ \sigma',\sigma' \\ k'-q,k'-q}} \\ &= \frac{-1}{\beta^2 N_p} \sum_{\substack{\sigma,\sigma' \in \{\downarrow,\uparrow\} \\ \nu \in \{1,\ldots,rd_{\mathbf{x}}\} \\ q \in \mathrm{i}\Omega_{+1}\times\mathbb{Q} \\ k,k' \in \mathrm{i}\Omega_{-1}\times\mathbb{Q} \\ n,n',m,m' \in \{1,\ldots,\infty\}}} g_{mn\nu}(\mathbf{k},\mathbf{q}) g_{m'n'\nu}(\mathbf{k}',-\mathbf{q}) \mathscr{G}_{0,\nu}^2(q) \mathscr{G}^{\ 0}_{\substack{n,n \\ \sigma,\sigma \\ k,k}} \mathscr{G}^{\ 0}_{\substack{n',n' \\ \sigma',\sigma' \\ k',k'}} V^{\mathrm{as}}_{\substack{n,n',m,m' \\ \sigma,\sigma',\sigma,\sigma' \\ k,k',k+q,k'-q}} \mathscr{G}^{\ 0}_{\substack{m,m \\ \sigma,\sigma \\ k+q,k+q}} \mathscr{G}^{\ 0}_{\substack{m',m' \\ \sigma',\sigma' \\ k'-q,k'-q}} \end{aligned} \tag{37.5}$$

Now we use Equation (23.18) and compute the antisymmetrized part of the vertex as ...

$$\begin{aligned} &V^{\mathrm{as}}_{\alpha_1,\alpha_2;\alpha_3,\alpha_4} \\ &= \mathrm{AS}\, \frac{1}{\hbar\beta N_p} \sum_{\nu \in \{1,\ldots,rd_{\mathbf{x}}\}} \frac{\omega_\nu(\mathbf{k}_{\alpha_1} - \mathbf{k}_{\alpha_4})}{\omega^2_{\alpha_1-\alpha_4} + \omega^2_\nu(\mathbf{k}_{\alpha_1} - \mathbf{k}_{\alpha_4})} \frac{g_{m_{\alpha_1}m_{\alpha_4}\nu}(\mathbf{k}_{\alpha_4}, \mathbf{k}_{\alpha_1} - \mathbf{k}_{\alpha_4}) g^*_{m_{\alpha_3}m_{\alpha_2}\nu}(\mathbf{k}_{\alpha_2}, \mathbf{k}_{\alpha_1} - \mathbf{k}_{\alpha_4})}{\hbar^2} \delta_{k_{\alpha_3}+k_{\alpha_4},k_{\alpha_2}+k_{\alpha_1}} \delta_{\sigma_{\alpha_1},\sigma_{\alpha_4}} \delta_{\sigma_{\alpha_2},\sigma_{\alpha_3}} \\ &= \mathrm{AS}\, \frac{1}{\hbar\beta N_p} \sum_{\nu \in \{1,\ldots,rd_{\mathbf{x}}\}} \frac{\omega_\nu(\mathbf{k}_{\alpha_1} - \mathbf{k}_{\alpha_4})}{\omega^2_{\alpha_1-\alpha_4} + \omega^2_\nu(\mathbf{k}_{\alpha_1} - \mathbf{k}_{\alpha_4})} \frac{g_{m_{\alpha_1}m_{\alpha_4}\nu}(\mathbf{k}_{\alpha_4}, \mathbf{k}_{\alpha_1} - \mathbf{k}_{\alpha_4}) g_{m_{\alpha_2}m_{\alpha_3}\nu}(\mathbf{k}_{\alpha_2} + \mathbf{k}_{\alpha_1} - \mathbf{k}_{\alpha_4}, -\mathbf{k}_{\alpha_1} + \mathbf{k}_{\alpha_4})}{\hbar^2} \delta_{k_{\alpha_3}+k_{\alpha_4},k_{\alpha_2}+k_{\alpha_1}} \delta_{\sigma_{\alpha_1},\sigma_{\alpha_4}} \delta_{\sigma_{\alpha_2},\sigma_{\alpha_3}} \end{aligned} \tag{37.6}$$

37.2. Correcting the Internal Energy for the Interacting Contribution

TBD.

38. Experimental: Feynman-Diagramology

In quantum field theory, there are *four* famous theorems about "Feynman-diagrams", of which three are never proven in the generality in which one claims their applicability. Those are …

- The partition-function is the sum of all "diagrams" without "external vertices".
- The free energy is the sum of all "connected diagrams" without "external vertices".
- The self-energy is the sum of all "one-particle-irreducible two-point[1] diagrams".
- The n-body Green-functions are computed as sums of all "connected diagrams" with n "external vertices" (a.k.a. "Linked Cluster Theorem").

It should be emphasized at this point, that the entire Feynman-diagrammatic-machinery lacks mathematical precision (at least in the context of condensed matter theory). We will fix this here.

Note on the update. The first statement is proven in Corollary 38.48, the second one in Corollary 38.51. The fourth statement holds in the following precise form: the n-body Green-functions are the sums of all diagrams *without vacuum components* (Corollary 38.52). These diagrams are connected for $n = 1$ (Corollary 38.53), but in general not for $n \geq 2$, where only the connected (cumulant) Green-functions are sums of connected diagrams. The third statement (self-energy) is not yet proven here.

38.1. Graph Theory

38.1.1. Fundamentals

Definition 38.1 A *statistical pre-graph* is a quintuple

$$g = (V, H, \partial, \epsilon, \tau), \tag{38.1}$$

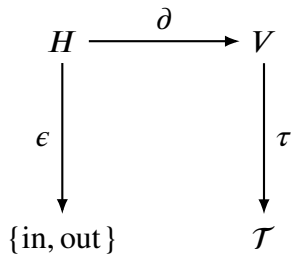
where

- $V = \{v_1, v_2, \dots, v_{|V|}\}$ is a finite set of elements which we call *vertices*,
- $H = \{h_1, h_2, \dots, h_{|H|}\}$ is a finite set of elements which we call *oriented half-edges*,
- $(\partial, \epsilon) : H \to V \times \{\text{in}, \text{out}\}$ assigns to each half-edge its *associated vertex* and *direction*,
- $\tau : V \to \mathcal{T}$ assigns each vertex a *type* from a finite set of *vertex-types*.

Remark 38.1.2 Instead of laboriously defining the set of half-edges and their image under the map ∂, one often simply draws the half-graph as below.

[1] I.e. diagrams with two external legs.

Remark 38.1.1 The diagram elucidates the definitions.



Definition 38.2 For a vertex $v \in V$, its *valency* is defined by

$$\mathrm{val}(v) = \left|\partial^{-1}(v)\right|. \tag{38.2}$$

Fact 38.3 Vertices of valency 0 will never appear in the physical theory. Vertices of valency 1, and 2 and higher are usually denoted as ...

- A vertex v with $\mathrm{val}(v) = 1$ is attached to exactly one half-edge. These are "*source vertices*" or "*external vertices*", whereas we will clarify this distinction later on, when we introduce the underlying symbols. All remaining edges are called *internal edges*.
- A vertex v with $\mathrm{val}(v) = 2$ is (depending on the context) called a *mass* or a *potential* or an *impurity vertex* or a *one-body interaction-vertex*.
- A vertex v with $\mathrm{val}(v) = 4$ is called a *two-body interaction-vertex*.
- A vertex v with $\mathrm{val}(v) = 6$ is called a *three-body interaction-vertex*.
- ...
- A vertex v with $\mathrm{val}(v) \geq 2$ can (more generally) be called a *many-body interaction-vertex* or (inclusively) *internal vertex*

Notation 38.4 The table summarizes the symbols that we will use to denote the different types of vertices and their properties.

Symbol(v)	$\tau(v)$	$\left(\epsilon \circ \partial^{-1}\right)(v)$	$\lvert\partial^{-1}(v)\rvert$
$\bullet$	external vertex	{in}, {out}	1
$\times$	source vertex	{out}	1
$\circ$	drain / sink vertex	{in}	1
$\boxed{m}$	mass vertex	{in, out}	2
$\boxed{p}$	potential vertex	{in, out}	2
$\boxed{\mathrm{imp}}$	impurity vertex	{in, out}	2
ෆෆෆ	interaction vertex		3, 4, 5 ...
∿∿∿	interaction vertex		3, 4, 5 ...

Examples:

Some **common examples** that one might be anticipating, if one has already seen some so-called "Feynman-diagrams", are the following:

a) Two vertices, one with outgoing one with incoming half-edge (valency 1 respectively). Cf. TBDrawn 1

b) Three vertices, one with outgoing one with incoming half-edge (valency 1 respectively) and one with two half-edges, one incoming and one outgoing (valency 2). Cf. TBDrawn 1

c) Three vertices, one with outgoing one with incoming half-edge (valency 1 respectively) and one with two half-edges, two incoming and two outgoing (valency 4). Cf. TBDrawn 1

d) Four vertices, one with outgoing one with incoming half-edge (valency 1 respectively) and one with two half-edges, two incoming and two outgoing (valency 4), and one with two half-edges, one incoming and one outgoing (valency 2). Cf. TBDrawn 1

Other, more **exotic examples**, that will however also become relevant, are the following:

a) Four vertices, two with outgoing two with incoming half-edges (valency 1 respectively). Cf. TBDrawn 2

b) Three vertices, one with outgoing one with incoming half-edges (valency 1 respectively) and one with three half-edges ...
   - three incoming, Cf. TBDrawn 2
   - two incoming and one outgoing, Cf. TBDrawn 2
   - one incoming and two outgoing, Cf. TBDrawn 2
   - three outgoing. Cf. TBDrawn 2

c) Three vertices, one with outgoing one with incoming half-edge (valency 1 respectively) and one with two half-edges, two incoming and two outgoing (valency 4). Cf. TBDrawn 2

We now extend the definition above.

Definition 38.5 A *statistical graph* is a statistical pre-graph $g = (V, H, \partial, \epsilon, \tau)$ equipped with an involution

$$\iota : H \to H,$$

that we call *pairing*, satisfying

$$\iota^2 = \mathrm{id}_H, \qquad \epsilon \neq \epsilon \circ \iota \tag{38.3}$$

Remark 38.5.1 *Correction note.* The second condition in Equation (38.3) is meant pointwise, $\epsilon(\iota(h)) \neq \epsilon(h)$ for all $h \in H$, i.e. every half-edge is glued to a half-edge of the opposite direction. As an inequality of maps, $\epsilon \neq \epsilon \circ \iota$ would only require this for a single half-edge. The following Remarks, Lemma 38.6 and Corollary 38.7 use the pointwise condition.

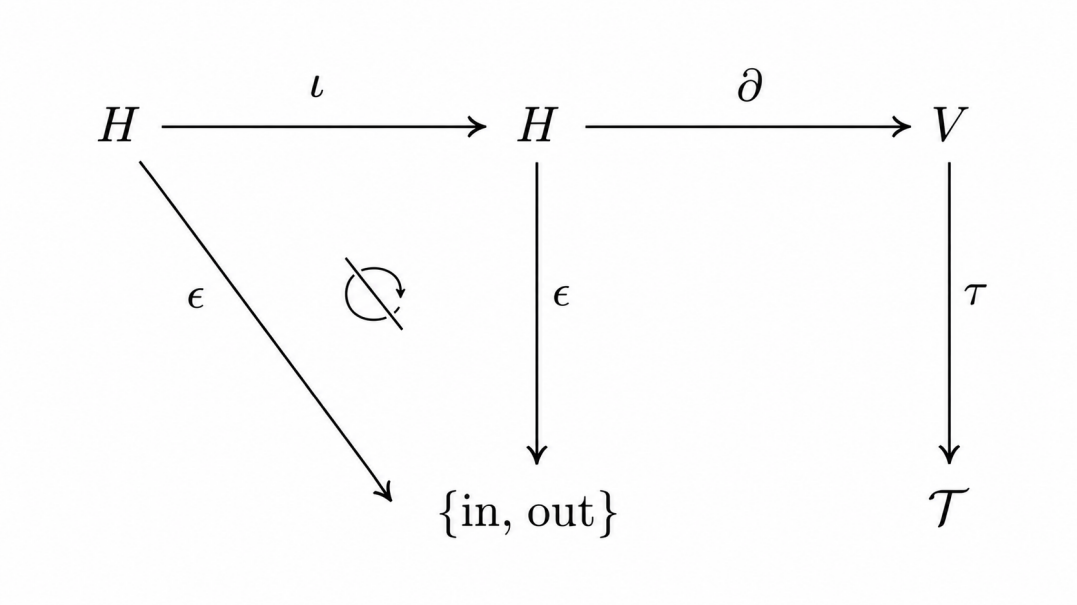
Remark 38.5.2 We will notate the statistical graph as a sextuple $G = (V, H, \partial, \epsilon, \tau, \iota)$.

Remark 38.5.3 The involution tells us which half-edges are *glued* together to form a so-called "edge" (to be defined cleanly below). The condition $\iota^2 = \mathrm{id}_H$ means that if $\iota(h) = h'$, then h is said to be *glued* to h'.

Remark 38.5.4 Notice that the second conditions prohibits a half-edge from being glued to itself.

Remark 38.5.5 Notice further that it might not be always possible to find a pairing for a given statistical pre-graph. In that case, we say that the statistical pre-graph is *unpairable*.

Remark 38.5.6 Notice that the definition implies that one finds the following diagram



Lemma 38.6 Let

$$g = (V, H, \partial, \epsilon, \tau) \tag{38.4}$$

be a statistical pregraph, and define

$$H_{\text{in}}(g) := \{h \in H \mid \epsilon(h) = \text{in}\}, \qquad H_{\text{out}}(g) := \{h \in H \mid \epsilon(h) = \text{out}\}. \tag{38.5}$$

A pairing of g exists if and only if

$$\left|H_{\text{in}}(g)\right| = \left|H_{\text{out}}(g)\right|. \tag{38.6}$$

Proof 38.6 Suppose first that a pairing ι exists. Since every incoming half-edge is paired with an outgoing half-edge, the restriction

$$\iota|_{H_{\text{in}}(g)} : H_{\text{in}}(g) \to H_{\text{out}}(g) \tag{38.7}$$

is a bijection. Therefore the two sets have equal cardinality. Conversely, suppose that the two sets have equal cardinality. Since they are finite, there exists a bijection

$$b : H_{\text{out}}(g) \longrightarrow H_{\text{in}}(g). \tag{38.8}$$

Define $\iota : H \to H$ by

$$\iota(h) := \begin{cases} b(h) & \text{if } h \in H_{\text{out}}(g), \\ b^{-1}(h) & \text{if } h \in H_{\text{in}}(g). \end{cases} \tag{38.9}$$

Then $\iota^2 = \mathrm{id}_H$, and ι exchanges incoming and outgoing half-edges. Hence ι is a pairing of g.

Corollary 38.7 The number of pairings of a statistical pregraph g is

$$n_{\text{pairs}}(g) = \begin{cases} \left|H_{\text{in}}(g)\right|! & \text{if } \left|H_{\text{in}}(g)\right| = \left|H_{\text{out}}(g)\right|, \\ 0 & \text{otherwise.} \end{cases} \tag{38.10}$$

Proof 38.7 If the cardinalities differ, no pairing exists by Lemma 38.6.

Suppose that both sets have cardinality m. Every pairing is uniquely determined by its restriction to a bijection

$$H_{\text{out}}(g) \longrightarrow H_{\text{in}}(g), \tag{38.11}$$

and every such bijection defines a pairing. Since there are $m!$ bijections between two sets of cardinality m, one obtains

$$n_{\text{pairs}}(g) = m!. \tag{38.12}$$

Notation 38.8 For a given statistical pre-graph $g = (V, H, \partial, \epsilon, \tau)$, we denote the set of all statistical graphs that can be constructed from g by equipping it with a pairing ι as $C(g)$, i.e.

$$C(g) \quad = \quad \{(V, H, \partial, \epsilon, \tau, \iota) \mid \iota \text{ is a pairing on } H\} \quad \equiv \quad \bigcup_{j=1}^{n_{\text{pairs}}} \{G_j(g)\}. \tag{38.13}$$

Remark 38.8.1 If no such pairing exists, then we say that the statistical pre-graph is *unpairable* and we set $C(g) = \emptyset$. Oftentimes we also call $\emptyset$ the *null-graph*

Definition 38.9 Let $G = (V, H, \partial, \epsilon, \tau, \iota)$ be a statistical graph. We define a relation $\sim_\iota$ on H by

$$h \sim_\iota h' \quad \Longleftrightarrow \quad h' \in \{h, \iota(h)\}. \tag{38.14}$$

Remark 38.9.1 Notice that this implies that half-edges that were glued together are equivalent under this relation.

Definition 38.10 For a statistical graph, we define the *set of edges* as the quotient

$$E(G) := H/\sim_\iota = \{\{h, \iota(h)\} \mid h \in H\}. \tag{38.15}$$

An element

$$e = [h]_{\sim_\iota} = \{h, \iota(h)\} \in E(G) \tag{38.16}$$

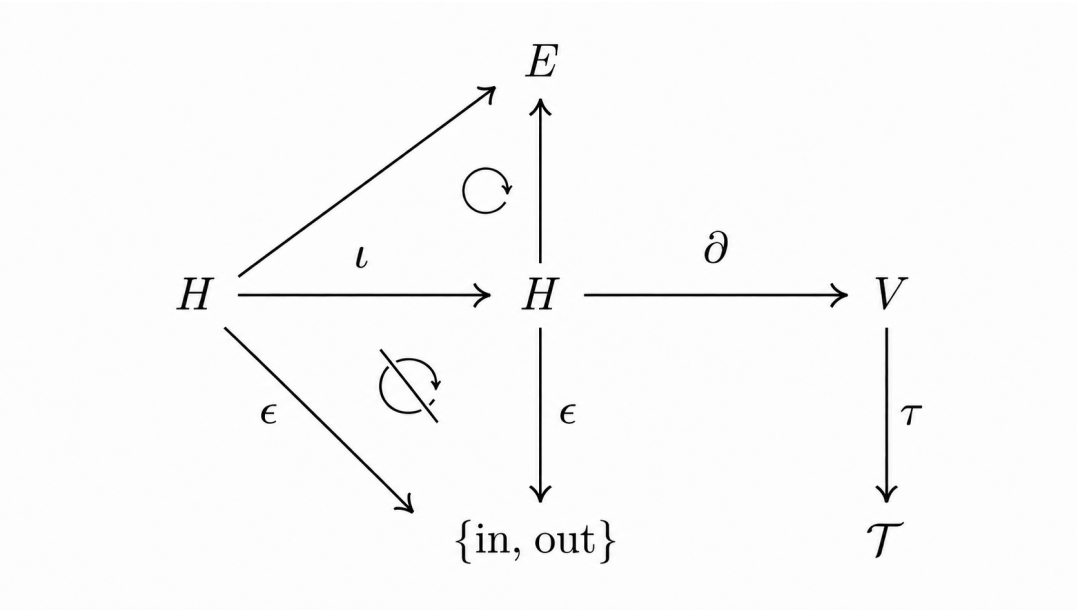
is called an *edge* of G.

Lemma 38.11 Notice that one finds that

$$\forall e \in E(G) : \ \iota(e) = e. \tag{38.17}$$

Proof 38.11 Follows from set-parenthesis allowing the rearrangement of the order, without changing the set.

Remark 38.11.1 Notice that the definition implies that one finds the following diagram



TBD: Re-creating this picture as a tikzpicture.

Definition 38.12 Let

$$G = (V, H, \partial, \epsilon, \tau, \iota) \tag{38.18}$$

be a statistical graph and let $E(G) = H/\sim_\iota$ be its set of edges. For every edge $e \in E(G)$, there are unique half-edges $h_{\text{out}}(e), h_{\text{in}}(e) \in H$ satisfying

$$\epsilon\left(h_{\text{out}}(e)\right) = \text{out}, \qquad \epsilon\left(h_{\text{in}}(e)\right) = \text{in}\,. \tag{38.19}$$

Definition 38.13 Let $G = (V, H, \partial, \epsilon, \tau, \iota)$ be a statistical graph. Two vertices $v, w \in V$ are *adjacent* if and only if there exists two half-edges $h_{\text{in}}, h_{\text{out}} \in H$ such that

$$\partial(h_{\text{in}}) = v, \text{ and } \big(\partial\circ\iota\big)(h_{\text{out}}) = w \qquad \text{or} \qquad \partial(h_{\text{out}}) = w, \text{ and } \big(\partial\circ\iota\big)(h_{\text{in}}) = v. \tag{38.20}$$

Remark 38.13.1 *Correction note.* As written, the two half-edges h_{in} and h_{out} are unrelated, so the condition does not express that v and w are joined by an edge. The intended definition is: v and w are adjacent if and only if there is a half-edge $h \in H$ with $\partial(h) = v$ and $\partial(\iota(h)) = w$, i.e. if and only if there is an edge $e \in E(G)$ with $\{s_G(e), t_G(e)\} = \{v, w\}$ (cf. Definition 38.16).

Definition 38.14 We define the maps

$$s_G, t_G \,:\, E(G) \longrightarrow V \tag{38.21}$$

by

$$s_G(e) := \partial\left(h_{\text{out}}(e)\right), \qquad t_G(e) := \partial\left(h_{\text{in}}(e)\right). \tag{38.22}$$

Definition 38.15 We then define the *Feynman-map* by

$$\text{Feynman} \,:\, G = (V, H, \partial, \epsilon, \tau, \iota) \mapsto \Gamma(G) := \left(V, E(G), s_G, t_G, \tau\right). \tag{38.23}$$

We call $\Gamma(G)$ the *statistical Feynman-diagram associated with* G.

Remark 38.15.1 If we combine every vertex with its type and define

$$\mathcal{V} := \{(v, \tau(v)) \,|\, v \in V\}\,, \tag{38.24}$$

then we may equivalently write the statistical Feynman-diagram as

$$\Gamma = (\mathcal{V}, E, s, t). \tag{38.25}$$

Definition 38.16 Let

$$\Gamma = (V, E, s, t, \tau) \tag{38.26}$$

be a statistical Feynman-diagram. We call two vertices $v, w \in V$ *adjacent* if there exists an edge $e \in E$ such that

$$\big(s(e), t(e)\big) = \{v, w\} \tag{38.27}$$

Remark 38.16.1 *Correction note.* On the left-hand side the set $\{s(e), t(e)\}$ is meant (an ordered pair cannot equal a set), i.e. v and w are adjacent if $\{s(e), t(e)\} = \{v, w\}$ for some $e \in E$. For $v = w$ this means that e is a self-loop at v.

Remark 38.16.2 The Feynman-map acts elementwise on the set of statistical graphs generated by a pregraph g. Thus,

$$C(g) = \big\{G_i(g)\big\}_{i=1}^{n_{\text{pairs}}(g)} \overset{\text{Feynman}}{\mapsto} \big\{\Gamma_i(g) := \text{Feynman}\,\big(G_i(g)\big)\big\}_{i=1}^{n_{\text{pairs}}(g)}. \tag{38.28}$$

Hence every pairing of g first gives a statistical graph and subsequently a labelled statistical Feynman-diagram. Only after passing to isomorphism classes will diagrams that differ merely by a structure-preserving relabelling be identified.

So far we have only been considering Feynman-diagrams that originate from a single pre-graph.

Definition 38.17 Let

$$\Gamma_1 = (V_1, E_1, s_1, t_1, \tau_1), \qquad \Gamma_2 = (V_2, E_2, s_2, t_2, \tau_2) \tag{38.29}$$

be two statistical Feynman-diagrams with

$$V_1 \cap V_2 = \emptyset, \qquad E_1 \cap E_2 = \emptyset. \tag{38.30}$$

We define their *disjoint union* by

$$\Gamma_1 \sqcup \Gamma_2 := \left(V_1 \sqcup V_2, E_1 \sqcup E_2, s_{1\sqcup 2}, t_{1\sqcup 2}, \tau_{1\sqcup 2}\right), \tag{38.31}$$

where

$$s_{1\sqcup 2}(e) := \begin{cases} s_1(e) & \text{if } e \in E_1, \\ s_2(e) & \text{if } e \in E_2, \end{cases} \qquad t_{1\sqcup 2}(e) := \begin{cases} t_1(e) & \text{if } e \in E_1, \\ t_2(e) & \text{if } e \in E_2, \end{cases} \tag{38.32}$$

and

$$\tau_{1\sqcup 2}(v) := \begin{cases} \tau_1(v) & \text{if } v \in V_1, \\ \tau_2(v) & \text{if } v \in V_2. \end{cases} \tag{38.33}$$

Definition 38.18 A non-empty statistical Feynman-diagram

$$\Gamma = (V, E, s, t, \tau) \tag{38.34}$$

is called *connected* if there do not exist two non-empty statistical Feynman-diagrams Γ_1 and Γ_2 such that

$$\Gamma = \Gamma_1 \sqcup \Gamma_2. \tag{38.35}$$

If such a decomposition exists, then Γ is called *disconnected*.

Definition 38.19 Let

$$\Gamma = (V, E, s, t, \tau) \tag{38.36}$$

be a statistical Feynman-diagram. A *walk of length* $n \in \mathbb{N}_0$ from $u \in V$ to $v \in V$ is a finite sequence

$$\left(v_0, e_1, v_1, e_2, \ldots, e_n, v_n\right) \tag{38.37}$$

satisfying

$$v_0 = u, \qquad v_n = v, \tag{38.38}$$

and, for every $l \in \{1, \dots, n\}$,

$$\left\{ s(e_l), t(e_l) \right\} = \left\{ v_{l-1}, v_l \right\}. \tag{38.39}$$

For $n = 0$, the one-element sequence (u) is called the *trivial walk* from u to itself. A walk is called a *path* if its vertices $v_0, \dots, v_n$ are pairwise distinct, except that the trivial path of length zero is allowed.

Definition 38.20 Let

$$\Gamma = (V, E, s, t, \tau) \tag{38.40}$$

be a statistical Feynman-diagram. For $u, v \in V$, we define

$$u \sim_\Gamma v \quad \Longleftrightarrow \quad \text{there exists a finite walk in } \Gamma \text{ from } u \text{ to } v. \tag{38.41}$$

Notation 38.21 For every $v \in V$, we denote its equivalence class under $\sim_\Gamma$ by

$$C_v(\Gamma) := [v]_{\sim_\Gamma} = \left\{ u \in V \,\middle|\, u \sim_\Gamma v \right\}. \tag{38.42}$$

Theorem 38.22 The relation $\sim_\Gamma$ defined in Equation (38.41) is an equivalence relation on the vertex set V of a statistical Feynman-diagram

$$\Gamma = (V, E, s, t, \tau). \tag{38.43}$$

Proof 38.22 We verify the three defining properties.

Reflexivity: For every $u \in V$, the trivial walk (u) is a walk from u to itself. Hence

$$u \sim_\Gamma u. \tag{38.44}$$

Symmetry: Suppose that $u \sim_\Gamma v$. Then there exists a walk

$$(v_0, e_1, v_1, \dots, e_n, v_n) \tag{38.45}$$

with $v_0 = u$ and $v_n = v$. Since walks may traverse edges in either direction, the reversed sequence

$$(v_n, e_n, v_{n-1}, \dots, e_1, v_0) \tag{38.46}$$

is a walk from v to u. Therefore

$$v \sim_\Gamma u. \tag{38.47}$$

Transitivity: Suppose that $u \sim_\Gamma v$ and $v \sim_\Gamma w$. Concatenating a walk from u to v with a walk from v to w gives a finite walk from u to w. Hence

$$u \sim_\Gamma w. \tag{38.48}$$

Thus $\sim_\Gamma$ is reflexive, symmetric, and transitive.

Corollary 38.23 The relation $\sim_\Gamma$ induces a partition of the vertex set V into equivalence classes:

$$V/\sim_\Gamma = \{C_i\}_{i\in I}, \tag{38.49}$$

where $I \subseteq V$ may be chosen to contain exactly one representative from each equivalence class.

Proof 38.23 Since $\sim_\Gamma$ is an equivalence relation, its equivalence classes are non-empty, pairwise disjoint, and their union is V.

Notation 38.24 For every equivalence class $C_i \in V/\sim_\Gamma$, define

$$E_i := \{e \in E \mid s(e) \in C_i \text{ and } t(e) \in C_i\}. \tag{38.50}$$

We denote the corresponding statistical *Feynman-subdiagram* by

$$\Gamma_i := (C_i, E_i, s_i, t_i, \tau_i), \tag{38.51}$$

where

$$s_i := s|_{E_i}, \qquad t_i := t|_{E_i}, \qquad \tau_i := \tau|_{C_i}. \tag{38.52}$$

Theorem 38.25 Every statistical Feynman-diagram

$$\Gamma = (V, E, s, t, \tau) \tag{38.53}$$

admits a unique decomposition into connected components:

$$\Gamma = \bigsqcup_{i\in I} \Gamma_i, \tag{38.54}$$

where the vertex set of Γ_i is the equivalence class C_i under $\sim_\Gamma$.

Proof 38.25 The equivalence classes $\{C_i\}_{i\in I}$ form a partition of V. Moreover, the endpoints of every edge $e \in E$ are adjacent and therefore belong to the same equivalence class. Consequently, the sets $\{E_i\}_{i\in I}$ form a partition of E. The restrictions s_i, t_i, and τ_i therefore reconstruct s, t, and τ under the disjoint union. Hence

$$\Gamma = \bigsqcup_{i\in I} \Gamma_i. \tag{38.55}$$

Each Γ_i is connected because any two vertices in C_i are joined by a finite walk. Such a walk only visits vertices of C_i (all of them are equivalent to its starting point) and therefore only uses edges of E_i. If $\Gamma_i = \Gamma_a \sqcup \Gamma_b$ with non-empty Γ_a, Γ_b, a walk from a vertex of Γ_a to a vertex of Γ_b would need an edge with one endpoint in each part, and such edges do not exist in a disjoint union. Finally, in any decomposition of Γ into connected components, two vertices belong to the same component if and only if they are connected by a finite walk. Thus the vertex sets of the components must be precisely the equivalence classes C_i. The decomposition is therefore unique up to the ordering of its components.

[Maybe we will add things here later on.] [2]

Definition 38.26 Let

$$\Gamma_i = (V_i, E_i, s_i, t_i, \tau_i), \qquad i \in \{1, 2\}, \tag{38.56}$$

be two statistical Feynman-diagrams. An *isomorphism*

$$\varphi : \Gamma_1 \longrightarrow \Gamma_2 \tag{38.57}$$

is a pair of bijections

$$\varphi = (\varphi_V, \varphi_E), \qquad \varphi_V : V_1 \longrightarrow V_2, \qquad \varphi_E : E_1 \longrightarrow E_2, \tag{38.58}$$

satisfying

$$\tau_1 = \tau_2 \circ \varphi_V, \tag{38.59}$$

together with

$$\varphi_V \circ s_1 = s_2 \circ \varphi_E, \qquad \varphi_V \circ t_1 = t_2 \circ \varphi_E. \tag{38.60}$$

[2] Cf. Book Graph Theory from Robin J. Wilson or arXiv:1301.6918v1.
Might be later relevant:
- matrix-representations of graphs
- adjacency matrices
- vector-space of a Graph
- Cf. page 42 in the book of Salmhofer.
- page 110, 111 in Negele, Orland: Definition of a Tree-Diagram.
- page 110: reference to SSB and their implications for expectation-values.
- Definition of a pairing from Etingof.
- Cf. also Mahan page 85 for a decomposition of graphs.
- Cf. also Peskin page 305 for some nice pictures of Feynman-Diagrams.

If such an isomorphism exists, we call Γ_1 and Γ_2 *isomorphic* and write

$$\Gamma_1 \cong \Gamma_2. \tag{38.61}$$

An isomorphism from a statistical Feynman-diagram Γ to itself is called an *automorphism*[3] of Γ.

Remark 38.26.1 Every isomorphism preserves adjacency. Indeed, if an edge $e \in E_1$ connects two vertices $v, w \in V_1$, then $\varphi_E(e) \in E_2$ connects $\varphi_V(v)$ and $\varphi_V(w)$ with the same orientation. The converse is generally false: preservation of adjacency alone does not preserve the number of parallel edges or distinguish different permutations of edges. This is why an isomorphism consists of both a vertex bijection φ_V and an edge bijection φ_E.

Notation 38.27 For a statistical Feynman-diagram

$$\Gamma = (V, E, s, t, \tau), \tag{38.62}$$

we denote its set of automorphisms by

$$\mathrm{Aut}(\Gamma) := \left\{ \varphi = (\varphi_V, \varphi_E) \,\middle|\, \varphi : \Gamma \longrightarrow \Gamma \text{ is an isomorphism} \right\}. \tag{38.63}$$

Lemma 38.28 The set of automorphisms $\mathrm{Aut}(\Gamma)$ forms a group under composition of maps.

Proof 38.28 Let

$$\varphi = (\varphi_V, \varphi_E), \qquad \Psi = (\psi_V, \psi_E) \tag{38.64}$$

be two elements of $\mathrm{Aut}(\Gamma)$. Define their composition componentwise by

$$\varphi \circ \Psi := \left(\varphi_V \circ \psi_V, \varphi_E \circ \psi_E \right). \tag{38.65}$$

Since compositions of bijections are bijections, both components of $\varphi \circ \Psi$ are bijective. Moreover,

$$\tau = \tau \circ \left(\varphi_V \circ \psi_V \right), \tag{38.66}$$

and

$$\left(\varphi_V \circ \psi_V \right) \circ s = s \circ \left(\varphi_E \circ \psi_E \right), \qquad \left(\varphi_V \circ \psi_V \right) \circ t = t \circ \left(\varphi_E \circ \psi_E \right). \tag{38.67}$$

Hence $\varphi \circ \Psi \in \mathrm{Aut}(\Gamma)$. Composition is associative because composition of maps is associative. The identity element is

[3] Cf. also 01-Feynman-Diagrams (Michael Polyak Notes), under Equation (18).

$$\mathrm{id}_\Gamma := \left(\mathrm{id}_V, \mathrm{id}_E\right). \tag{38.68}$$

Finally, if $\varphi = (\varphi_V, \varphi_E) \in \mathrm{Aut}(\Gamma)$, then

$$\varphi^{-1} := \left(\varphi_V^{-1}, \varphi_E^{-1}\right) \tag{38.69}$$

also preserves τ, s, and t, and therefore belongs to $\mathrm{Aut}(\Gamma)$. Thus every element has an inverse, and $\mathrm{Aut}(\Gamma)$ is a group.

Lemma 38.29 Isomorphism defines an equivalence relation on every collection of statistical Feynman-diagrams. Explicitly, define

$$\Gamma_1 \sim_{\mathrm{iso}} \Gamma_2 \quad \Longleftrightarrow \quad \Gamma_1 \cong \Gamma_2. \tag{38.70}$$

Then $\sim_{\mathrm{iso}}$ is an equivalence relation.

Proof 38.29 The relation is reflexive because

$$\left(\mathrm{id}_V, \mathrm{id}_E\right) \tag{38.71}$$

is an isomorphism from every statistical Feynman-diagram to itself. It is symmetric because, if

$$\varphi = (\varphi_V, \varphi_E) : \Gamma_1 \to \Gamma_2 \tag{38.72}$$

is an isomorphism, then

$$\varphi^{-1} = \left(\varphi_V^{-1}, \varphi_E^{-1}\right) : \Gamma_2 \to \Gamma_1 \tag{38.73}$$

is also an isomorphism. Finally, it is transitive because the componentwise composition of an isomorphism from Γ_1 to Γ_2 with an isomorphism from Γ_2 to Γ_3 is an isomorphism from Γ_1 to Γ_3.

Remark 38.29.1 Let

$$\left\{\Gamma_i(g)\right\}_{i=1}^{n_{\mathrm{pairs}}(g)} \tag{38.74}$$

be the family of labelled statistical Feynman-diagrams generated by a pregraph g. Its quotient under diagram isomorphism is

$$\left\{\Gamma_i(g)\right\}_{i=1}^{n_{\mathrm{pairs}}(g)} \Big/ \sim_{\mathrm{iso}} = \left\{[\Gamma_j(g)]_{\mathrm{iso}}\right\}_{j \in \widetilde{I}}, \tag{38.75}$$

where

$$[\Gamma_j(g)]_{\mathrm{iso}} := \left\{\Gamma_i(g) \,\middle|\, \Gamma_i(g) \cong \Gamma_j(g)\right\}, \tag{38.76}$$

and $\widetilde{I}$ contains one representative index from each isomorphism class.

38.1.2. These Wicked Diagrams...

We now define a mapping that associates a given statistical pre-graph with a set of statistical graphs, and consequently a set of statistical Feynman-diagrams.

Theorem 38.30 Let

$$g = (V, H, \partial, \epsilon, \tau) \tag{38.77}$$

be a statistical pregraph. Considering all pairings of g gives the sequence

$$g \mapsto C(g) = \left\{G_i(g)\right\}_{i=1}^{n_{\text{pairs}}(g)} \overset{\text{Feynman}}{\mapsto} \mathcal{D}_{\text{lab}}(g) := \left\{\Gamma_i(g)\right\}_{i=1}^{n_{\text{pairs}}(g)}, \tag{38.78}$$

where

$$\Gamma_i(g) := \text{Feynman}\left(G_i(g)\right). \tag{38.79}$$

Thus, the number of labelled statistical Feynman-diagrams generated from g, counted before passing to isomorphism classes, is

$$\left|\mathcal{D}_{\text{lab}}(g)\right| = |C(g)| = n_{\text{pairs}}(g). \tag{38.80}$$

Explicitly,

$$n_{\text{pairs}}(g) = \begin{cases} \left|H_{\text{in}}(g)\right|! & \text{if } \left|H_{\text{in}}(g)\right| = \left|H_{\text{out}}(g)\right|, \\ 0 & \text{otherwise.} \end{cases} \tag{38.81}$$

Graphical Examples

TBD.

Remark 38.30.1 We illustrate the construction with a single internal vertex v with two incoming half-edges $h_1^{\text{in}}, h_2^{\text{in}}$ and two outgoing half-edges $h_1^{\text{out}}, h_2^{\text{out}}$ (a two-body interaction vertex).

1. *Without external vertices.* By Corollary 38.7 there are $2! = 2$ pairings, namely ι_1: $h_1^{\text{out}} \leftrightarrow h_1^{\text{in}}$, $h_2^{\text{out}} \leftrightarrow h_2^{\text{in}}$, and ι_2: $h_1^{\text{out}} \leftrightarrow h_2^{\text{in}}$, $h_2^{\text{out}} \leftrightarrow h_1^{\text{in}}$. Both Feynman-diagrams consist of v and two edges from v to v (Figure 38.1 (a)), so they are isomorphic. This diagram has $|\operatorname{Aut}| = 2$: the identity and the exchange of the two self-loops.
2. *With two external vertices.* Adding an external vertex x with one outgoing half-edge and an external vertex y with one incoming half-edge (of different types) gives $|H_{\text{in}}| = |H_{\text{out}}| = 3$, hence $3! = 6$ pairings. They fall into two isomorphism classes:
   (b) x is joined directly to y, and v carries two self-loops. These are 2 pairings, $|\operatorname{Aut}| = 2$, and the diagram is disconnected.

(c) $x \to v$, $v \to y$ and one self-loop at v. These are 4 pairings (the half-edge of x can be glued to either incoming half-edge of v, and either outgoing half-edge of v can be glued to y), $|\operatorname{Aut}| = 1$, and the diagram is connected.

In all three cases the number of pairings in an isomorphism class equals $4/|\operatorname{Aut}|$, where $4 = 2! \cdot 2!$ is the number of relabellings of the legs of v. This is no coincidence but the orbit-stabilizer theorem, see Lemma 38.44 and Theorem 38.46. The values of these diagrams for a two-body interaction are computed in Remark 38.53.1.

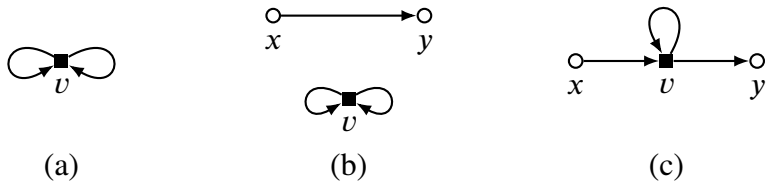


Figure 38.1.: The Feynman-diagrams of Remark 38.30.1. External vertices are drawn as circles, the internal vertex v as a square, and every edge points from its outgoing to its incoming half-edge.

In the next sections, we will use the above definitions to formulate the diagrammatic expansion of the partition function, the free energy, and the Green-functions. We will also discuss how to compute the self-energy and the vertex functions using Feynman-diagrams. For simplicity, we will focus on systems with particle-number preserving interactions for the beginning.

38.2. Pure Systems

Notation 38.31 We use the notation of Notation 16.24. Thus

$$S[\psi, \overline{\psi}] = S_0[\psi, \overline{\psi}] + S_{\text{int}}[\psi, \overline{\psi}] \quad \text{with} \quad S_0[\psi, \overline{\psi}] = \psi^\dagger A \psi \tag{38.82}$$

and

$$C(i|i') := \left\langle \psi_i \overline{\psi}_{i'} \right\rangle_0 = A^{-1}_{ii'} \tag{38.83}$$

denotes the *free covariance*.

Remark 38.31.1 Notice that the free covariance is merely (in the physics notation) the Green-function. One has by Equation (16.29),

$$C(i|i') \equiv -c\, \mathscr{G}_0(i|i'). \tag{38.84}$$

Remark 38.31.2 The letter C is used here only to keep the diagrammatic combinatorics separate from the conventional Green-function prefactors. The edges of a diagram naturally carry the covariance $C = A^{-1}$; after the conventional normalization one rewrites them as free Green-functions.

Notation 38.32 We consider an index-set $\mathscr{V} = \{1, \dots, n_{\text{int}}\}$ for our interactions and we write the interaction as a finite sum of ordered monomials

$$S_{\text{int}}[\psi, \overline{\psi}] = \sum_{\nu \in \mathscr{V}} M_\nu[\psi, \overline{\psi}] \tag{38.85}$$

where every M_ν is an ordered sum of monomials with degree $d_\nu + d'_\nu$ in the generators of $\mathscr{P}_\zeta$. If

$$\begin{aligned} M_\nu[\psi, \overline{\psi}] &\equiv \sum_{\substack{1 \le j_1 < \dots < j_{d_\nu} \le D \\ 1 \le j'_1 < j'_2 < \dots < j'_{d'_\nu} \le D}} \overline{\psi}(j_1) \cdots \overline{\psi}(j_{d_\nu}) m_\nu(j_1, \dots, j_{d_\nu}, j'_1, \dots j'_{d_\nu}) \, \psi(j'_{d'_\nu}) \cdots \psi(j'_1) \\ &= \frac{1}{d_\nu! \, d'_\nu!} \sum_{\substack{1 \le j_1 < \dots < j_{d_\nu} \le D \\ 1 \le j'_1 < j'_2 < \dots < j'_{d_\nu} \le D}} \overline{\psi}(j_1) \cdots \overline{\psi}(j_{d_\nu}) m_\nu(j_1, \dots, j_{d_\nu}, j'_1, \dots j'_{d_\nu}) \, \psi(j'_{d'_\nu}) \cdots \psi(j'_1) \end{aligned} \tag{38.86}$$

whereas the coefficients $m_\nu(j_1, \dots, j_{d_\nu}, j'_1, \dots j'_{d_\nu})$ are allowed to be ...

- complex numbers (simple case),
- elements in a polynomial algebra (general, and more complicated case).

Remark 38.32.1 *Correction note on Equation (38.86).* The two lines are not consistent as written.

1. The prefactor $1/(d_\nu! \, d'_\nu!)$ belongs to *unrestricted* sums over all $(j_1, \dots, j_{d_\nu}) \in \{1, \dots, D\}^{d_\nu}$ and $(j'_1, \dots, j'_{d'_\nu}) \in \{1, \dots, D\}^{d'_\nu}$ with ζ-symmetric coefficients, see Equation (38.97). For $\zeta = -1$ and ζ-symmetric coefficients, the unrestricted sum equals $d_\nu! \, d'_\nu!$ times the ordered sum (all orderings of pairwise distinct indices give the same term, coinciding indices give zero), which is exactly the content of the second line.
2. For $\zeta = +1$ the strict orderings $j_1 < j_2 < \dots$ exclude repeated indices such as $\overline{\psi}(j)^2$. The unrestricted form avoids this.
3. The number of primed indices is d'_ν: in the summation conditions and in the arguments of m_ν, j'_{d_ν} has to read $j'_{d'_\nu}$.

In Subsection 38.2.1 we use the unrestricted, ζ-symmetric form.

Definition 38.33 For fixed *external indices*

$$(I \,|\, I') = (i_1, \dots, i_n \,|\, i'_n, \dots, i'_1) \tag{38.87}$$

we consider the ordered monomial

$$X_{(I|I')}[\psi, \overline{\psi}] := \psi_{i_1} \cdots \psi_{i_n} \overline{\psi}_{i'_1} \cdots \overline{\psi}_{i'_n}. \tag{38.88}$$

Fact 38.34 When it comes to the computation of ...

- partition-functions,

- free energies,
- Green-functions,

... we encounter the problem of computing the expectation-value of a polynomial expression of the form

$$P[\psi,\overline{\psi}] \equiv \left(X_{(I|I')}\mathrm{e}^{-S_{\mathrm{int}}}\right)[\psi,\overline{\psi}] = \left(\sum_{k=0}^{\infty}\frac{(-1)^k}{k!}X_{(I|I')}S_{\mathrm{int}}^k.\right)[\psi,\overline{\psi}] \tag{38.89}$$

and since with Equation (38.85) one has

$$S_{\mathrm{int}}^k[\psi,\overline{\psi}] = \left(\sum_{\nu\in\mathscr{V}}M_\nu[\psi,\overline{\psi}]\right)^k = \sum_{\nu_1,\ldots,\nu_k\in\mathscr{V}}M_{\nu_1}[\psi,\overline{\psi}]\cdots M_{\nu_k}[\psi,\overline{\psi}] \tag{38.90}$$

The goal is now to map polynomial expressions of the form

$$\left(X_{(I|I')}M_{\nu_1}\cdots M_{\nu_k}\right)[\psi,\overline{\psi}] \tag{38.91}$$

to pre-graphs (and therefore, subsequently, to Feynman-diagrams). We seek to do so, as we will encounter such polynomial expressions in the perturbative expansion of the partition function, the free energy, and the Green-functions. The following translation-key will allow us to do so. To this end, we now use Equation (38.86) and obtain the frighteningly long expression

$$\begin{aligned}
&\left(X_{(I|I')}M_{\nu_1}\cdots M_{\nu_k}\right)[\psi,\overline{\psi}]\\
&= \psi_{i_1}\cdots\psi_{i_n}\overline{\psi}_{i'_1}\cdots\overline{\psi}_{i'_n}\prod_{l=1}^{k}\frac{1}{d_{\nu_l}!\,d'_{\nu_l}!}\sum_{\substack{1\le j_{1,l}<\ldots<j_{d_{\nu_l},l}\le D\\ 1\le j'_{1,l}<j'_{2,l}<\ldots<j'_{d_{\nu_l},l}\le D}}\overline{\psi}(j_{1,l})\cdots\overline{\psi}(j_{d_{\nu_l},l})m_{\nu_l}(j_{1,l},\ldots,j_{d_{\nu_l},l},j'_{1,l},\ldots j'_{d_{\nu_l},l})\,\psi(j'_{d'_{\nu_l},l})\cdots\psi(j'_{1,l})\\
&= \sum_{\substack{1\le j_{1,1}<\ldots<j_{d_{\nu_1},1}\le D\\ 1\le j'_{1,1}<j'_{2,1}<\ldots<j'_{d_{\nu_1},1}\le D\\ \vdots\\ 1\le j_{1,k}<\ldots<j_{d_{\nu_k},k}\le D\\ 1\le j'_{1,k}<j'_{2,l}<\ldots<j'_{d_{\nu_k},k}\le D}}\psi_{i_1}\cdots\psi_{i_n}\overline{\psi}_{i'_1}\cdots\overline{\psi}_{i'_n}\prod_{l=1}^{k}\overline{\psi}(j_{1,l})\cdots\overline{\psi}(j_{d_{\nu_l},l})\frac{m_{\nu_l}(j_{1,l},\ldots,j_{d_{\nu_l},l},j'_{1,l},\ldots j'_{d_{\nu_l},l})}{d_{\nu_l}!\,d'_{\nu_l}!}\psi(j'_{d'_{\nu_l},l})\cdots\psi(j'_{1,l})\\
&= \sum_{\substack{1\le j_{1,1}<\ldots<j_{d_{\nu_1},1}\le D\\ 1\le j'_{1,1}<j'_{2,1}<\ldots<j'_{d_{\nu_1},1}\le D\\ \vdots\\ 1\le j_{1,k}<\ldots<j_{d_{\nu_k},k}\le D\\ 1\le j'_{1,k}<j'_{2,l}<\ldots<j'_{d_{\nu_k},k}\le D}}\left(\prod_{l=1}^{k}\frac{m_{\nu_l}(j_{1,l},\ldots,j_{d_{\nu_l},l},j'_{1,l},\ldots j'_{d_{\nu_l},l})}{d_{\nu_l}!\,d'_{\nu_l}!}\right)\psi_{i_1}\cdots\psi_{i_n}\overline{\psi}_{i'_1}\cdots\overline{\psi}_{i'_n}\prod_{l=1}^{k}\overline{\psi}(j_{1,l})\cdots\overline{\psi}(j_{d_{\nu_l},l})\psi(j'_{d'_{\nu_l},l})\cdots\psi(j'_{1,l})\\
&= \ldots
\end{aligned} \tag{38.92}$$

TBImplemented: A potential sign-factor that originates from commuting the m_ν.

Remark 38.34.1 *On the sign-factor from commuting the m_ν.* Moving a coefficient m_{ν_l} to the left past generators produces a sign only if m_{ν_l} is odd. If the m_ν are complex numbers or even elements (e.g. polynomials in bosonic fields or even products of Graßmann-variables), no sign arises, and the third equality in Equation (38.92) holds as

written. If some m_{ν_l} were odd (as for Graßmann-valued external sources), moving it past the q generators in front of it would produce the factor ζ^q; this case is excluded in Notation 38.37. Moreover, Equation (38.92) inherits the issues of Remark 38.32.1, and the summation conditions contain index typos ($j_{d_{\nu_1},l}$ should read $j_{d_{\nu_1},1}$, $j'_{2,l}$ in the k-th row should read $j'_{2,k}$, and the last primed index of vertex l is $j'_{d'_{\nu_l},l}$).

Remark 38.34.2 Notice that we have now for each monomial appearing in the sum of Equation (38.92) in total ...

- $N_{\text{tot}} \equiv 2n + \sum_{l=1}^{k}(d_{\nu_l} + d'_{\nu_l})$ variables
- $N_{\text{non-conj}} \equiv n + \sum_{l=1}^{k} d'_{\nu_l}$ are non-conjugated variables
- $N_{\text{conj}} \equiv n + \sum_{l=1}^{k} d_{\nu_l}$ are conjugated variables

Definition 38.35 We define *the pregraph associated to the polynomial expression in Equation* (38.92) as the statistical pre-graph with ...

- n external vertices with an outgoing half-edge
- n external vertices with an incoming half-edge
- k internal vertices of type $\nu_1, \dots, \nu_k$, where the vertex of type ν_l carries d_{ν_l} incoming half-edges and d'_{ν_l} outgoing half-edges, for $l = 1, \dots, k$.

Remark 38.35.1 In order to identify diagrams that differ only by a relabelling of the internal vertices and their half-edges, while keeping the external indices fixed, we give the external vertices pairwise distinct types. The half-edges then correspond one-to-one to the factors of the monomials in Equation (38.92): outgoing half-edges to ψ-factors and incoming half-edges to $\overline{\psi}$-factors, see Definition 38.38.

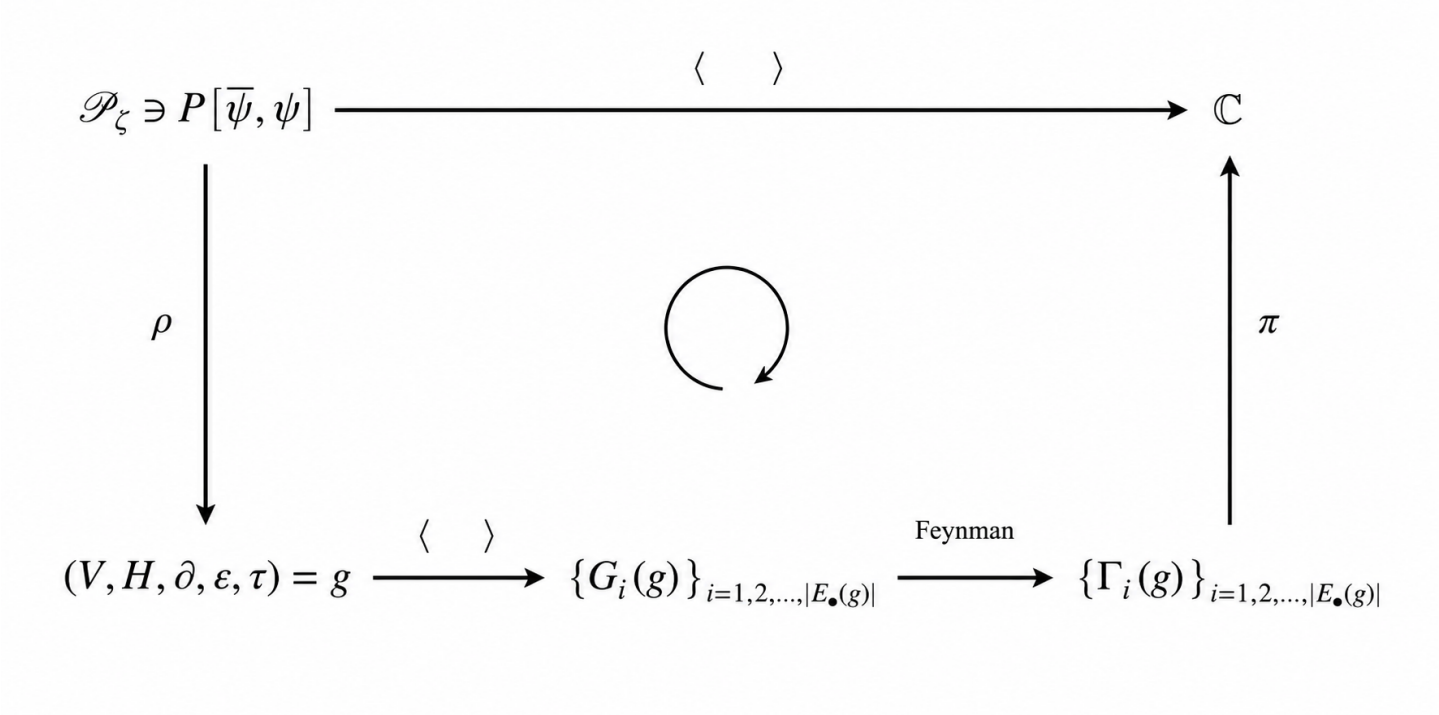


Figure 38.2.: TBD: Implementing this as a tikzpicture.

Fact 38.36 Notice that we can rewrite the polynomial expression in Equation (38.92) as

$$\begin{aligned}
\dots &= \sum_{\substack{1\le j_{1,1}<\dots<j_{d_{\nu_1},1}\le D\\ 1\le j'_{1,1}<j'_{2,1}<\dots<j'_{d_{\nu_1},1}\le D\\ \vdots\\ 1\le j_{1,k}<\dots<j_{d_{\nu_k},k}\le D\\ 1\le j'_{1,k}<j'_{2,l}<\dots<j'_{d_{\nu_k},k}\le D}} \left(\prod_{l=1}^{k}\frac{m_{\nu_l}(j_{1,l},\dots,j_{d_{\nu_l},l},j'_{1,l},\dots j'_{d_{\nu_l},l})}{d_{\nu_l}!\,d'_{\nu_l}!}\right)\psi_{i_1}\cdots\psi_{i_n}\overline{\psi}_{i'_1}\cdots\overline{\psi}_{i'_n}\prod_{l=1}^{k}\overline{\psi}(j_{1,l})\cdots\overline{\psi}(j_{d_{\nu_l},l})\psi(j'_{d'_{\nu_l},l})\cdots\psi(j'_{1,l})\\
&= \sum_{\substack{1\le j_{1,1}<\dots<j_{d_{\nu_1},1}\le D\\ 1\le j'_{1,1}<j'_{2,1}<\dots<j'_{d_{\nu_1},1}\le D\\ \vdots\\ 1\le j_{1,k}<\dots<j_{d_{\nu_k},k}\le D\\ 1\le j'_{1,k}<j'_{2,l}<\dots<j'_{d_{\nu_k},k}\le D}} \left(\prod_{l=1}^{k}\frac{m_{\nu_l}(j_{1,l},\dots,j_{d_{\nu_l},l},j'_{1,l},\dots j'_{d_{\nu_l},l})}{d_{\nu_l}!\,d'_{\nu_l}!}\right)\psi_{i_1}\cdots\psi_{i_n}\overline{\psi}_{i'_1}\cdots\overline{\psi}_{i'_n}\left(\prod_{l=1}^{k}\overline{\psi}(j_{1,l})\cdots\overline{\psi}(j_{d_{\nu_l},l})\right)\left(\prod_{l=1}^{k}\psi(j'_{d'_{\nu_l},l})\cdots\psi(j'_{1,l})\right)\\
&= \dots
\end{aligned} \tag{38.93}$$

in order to get all the conjugated variables to the right and all the not-conjugated variables to the left, we need to apply the commutation-relations. This gives for $\psi(j'_{d'_{\nu_1},1})$ the prefactor $\zeta^{n+\sum_{l=1}^{k}d_{\nu_l}}$ this gives in total (applying the same scheme to all of the other variables) the prefactor

$$\zeta^{d'_{\nu_1}\left(n+\sum_{l=1}^{k}d_{\nu_l}\right)+d'_{\nu_2}\left(n+\sum_{l=1}^{k}d_{\nu_l}\right)+\dots+d'_{\nu_k}\left(n+\sum_{l=1}^{k}d_{\nu_l}\right)}=\zeta^{\sum_{\bar{l}=1}^{k}d'_{\nu_{\bar{l}}}\left(n+\sum_{l=1}^{k}d_{\nu_l}\right)} \tag{38.94}$$

such that

$$\dots=\zeta^{\sum_{\bar{l}=1}^{k}d'_{\nu_{\bar{l}}}\left(n+\sum_{l=1}^{k}d_{\nu_l}\right)}\sum_{\substack{1\le j_{1,1}<\dots<j_{d_{\nu_1},1}\le D\\ 1\le j'_{1,1}<j'_{2,1}<\dots<j'_{d_{\nu_1},1}\le D\\ \vdots\\ 1\le j_{1,k}<\dots<j_{d_{\nu_k},k}\le D\\ 1\le j'_{1,k}<j'_{2,l}<\dots<j'_{d_{\nu_k},k}\le D}}\left(\prod_{l=1}^{k}\frac{m_{\nu_l}(j_{1,l},\dots,j_{d_{\nu_l},l},j'_{1,l},\dots j'_{d_{\nu_l},l})}{d_{\nu_l}!\,d'_{\nu_l}!}\right)\left[\psi_{i_1}\cdots\psi_{i_n}\left(\prod_{l=1}^{k}\psi(j'_{d'_{\nu_l},l})\cdots\psi(j'_{1,l})\right)\overline{\psi}_{i'_1}\cdots\overline{\psi}_{i'_n}\left(\prod_{l=1}^{k}\overline{\psi}(j_{1,l})\cdots\overline{\psi}(j_{d_{\nu_l},l})\right)\right] \tag{38.95}$$

Remark 38.36.1 *Correction note on the Fact above.* The step from the first to the second line performs the regrouping

$$\prod_{l}\left(\overline{\psi}\text{-block}_l\ \psi\text{-block}_l\right)\longrightarrow\left(\prod_{l}\overline{\psi}\text{-block}_l\right)\left(\prod_{l}\psi\text{-block}_l\right)$$

without a sign. For $\zeta=-1$ this is not correct: moving the ψ-block of vertex l past the $\overline{\psi}$-blocks of the vertices $l'>l$ produces $\zeta^{d'_{\nu_l}d_{\nu_{l'}}}$. The total prefactor is therefore

$$\zeta^{\sum_{l<l'}d'_{\nu_l}d_{\nu_{l'}}+\left(\sum_{l=1}^{k}d'_{\nu_l}\right)\left(n+\sum_{l=1}^{k}d_{\nu_l}\right)}$$

instead of the exponent stated above. In the next subsection this reordering is not needed at all: Wick's theorem in pair form (Lemma 38.40) assigns the sign directly to every pairing (Equation (38.102)), and for number-conserving vertices it is given by the loop rule (Corollary 38.47).

38.2.1. "Experimental Section": The Diagrammatic Expansions

TBD.

In this subsection we prove the diagrammatic expansions announced at the beginning of this chapter, in the setting of Notation 38.31. The strategy is the following:

1. Wick's theorem in a *pair form* assigns a sign to every pairing of a pregraph. This makes the explicit reordering of the generators in the Facts above unnecessary.
2. The expectation-value of a polynomial expression is the sum of *amplitudes* over all pairings of the associated pregraph (labelled expansion).
3. The relabellings of the internal vertices and of their half-edges form a group. Its orbits on the set of pairings are the isomorphism classes of Feynman-diagrams, and its stabilizers are their automorphism groups.
4. The orbit-stabilizer theorem produces the *symmetry factors* $1/|\operatorname{Aut}(\Gamma)|$.
5. The exponential formula yields the free energy, and the factorization of vacuum components yields the linked-cluster theorem for Green-functions.

Notation 38.37 Throughout this subsection we assume the following.

1. We write $\psi(j) \equiv \psi_j$ and $\overline{\psi}(j) \equiv \overline{\psi}_j$ for $j \in \{1, \dots, D\}$, A is invertible, $C(i|i') = A^{-1}_{ii'} = \langle \psi_i \overline{\psi}_{i'} \rangle_0$, and $\langle \cdot \rangle_0$ is normalized, $\langle 1 \rangle_0 = 1$. For $\pi \in \mathrm{S}_M$ we write $s_\zeta(\pi) := \operatorname{sign}(\pi)^{1-\theta(\zeta)}$. For arbitrary generators $y_1, \dots, y_M$ (each of them a ψ or a $\overline{\psi}$) one then has

$$y_{\pi(1)} \cdots y_{\pi(M)} = s_\zeta(\pi)\, y_1 \cdots y_M, \tag{38.96}$$

   and the signs of successive reorderings multiply.

2. Every interaction monomial is given in the *symmetric normal form*

$$M_\nu[\psi, \overline{\psi}] = \frac{1}{d_\nu!\, d'_\nu!} \sum_{j_1, \dots, j_{d_\nu}=1}^{D} \sum_{j'_1, \dots, j'_{d'_\nu}=1}^{D} \overline{\psi}(j_1) \cdots \overline{\psi}(j_{d_\nu})\, m_\nu(j_1, \dots, j_{d_\nu} \mid j'_1, \dots, j'_{d'_\nu})\, \psi(j'_{d'_\nu}) \cdots \psi(j'_1) \tag{38.97}$$

   with *unrestricted* sums and $d_\nu + d'_\nu \geq 1$. The coefficients m_ν are complex numbers (or, more generally, even elements that commute with all generators), and they are ζ-*symmetric*: for all $\alpha \in \mathrm{S}_{d_\nu}$ and $\beta \in \mathrm{S}_{d'_\nu}$

$$m_\nu(j_{\alpha(1)}, \dots, j_{\alpha(d_\nu)} \mid j'_{\beta(1)}, \dots, j'_{\beta(d'_\nu)}) = s_\zeta(\alpha)\, s_\zeta(\beta)\, m_\nu(j_1, \dots, j_{d_\nu} \mid j'_1, \dots, j'_{d'_\nu}). \tag{38.98}$$

3. For $\zeta = -1$ every $d_\nu + d'_\nu$ is even, i.e. every M_ν is even and commutes with all generators.
4. The interaction carries a formal coupling λ, $S_{\mathrm{int}} \to \lambda S_{\mathrm{int}}$, and identities between infinite series are identities of formal power series in λ, i.e. of the coefficients of every power λ^K. For fixed K all sums below are finite. The relation to the integrals themselves is as in Fact 16.26.

Remark 38.37.1 Every polynomial interaction can be brought into this form. If

$$M = \sum_{j, j'} \overline{\psi}(j_1) \cdots \overline{\psi}(j_d)\, c(j \mid j')\, \psi(j'_{d'}) \cdots \psi(j'_1)$$

with arbitrary coefficients c, then replacing c by its ζ-symmetrization

$$c^{\mathrm{sym}}(j_1,\dots,j_d \mid j'_1,\dots,j'_{d'}) = \frac{1}{d!\,d'!}\sum_{\alpha,\beta} s_\zeta(\alpha)\,s_\zeta(\beta)\,c(j_{\alpha(1)},\dots,j_{\alpha(d)} \mid j'_{\beta(1)},\dots,j'_{\beta(d')})$$

does not change M by Equation (38.96), and one sets $m := d!\,d'!\,c^{\mathrm{sym}}$. For example, the two-body interaction $\frac{1}{2}\sum \overline{\psi}(j_1)\overline{\psi}(j_2)V(j_1j_2|j'_1j'_2)\psi(j'_2)\psi(j'_1)$ with $V(j_2j_1|j'_2j'_1) = V(j_1j_2|j'_1j'_2)$ has $d = d' = 2$ and

$$m(j_1j_2 \mid j'_1j'_2) = V(j_1j_2 \mid j'_1j'_2) + \zeta\, V(j_1j_2 \mid j'_2j'_1), \tag{38.99}$$

i.e. the direct term plus ζ times the exchange term (for fermions: the antisymmetrized vertex).

Definition 38.38 Let $(I|I') = (i_1,\dots,i_n \mid i'_n,\dots,i'_1)$ be external indices as in Definition 38.33, $k \in \mathbb{N}_0$ and $\nu = (\nu_1,\dots,\nu_k) \in \mathscr{V}^k$. The *labelled pregraph* $g = g(I|I';\nu)$ is the statistical pregraph with

- external vertices $x_1,\dots,x_n,y_1,\dots,y_n$ and internal vertices $v_1,\dots,v_k$,
- half-edges h^x_a attached to x_a with direction out, h^y_b attached to y_b with direction in, and $h^{\mathrm{in}}_{l,r}$ $(r = 1,\dots,d_{\nu_l})$ resp. $h^{\mathrm{out}}_{l,r}$ $(r = 1,\dots,d'_{\nu_l})$ attached to v_l with direction in resp. out,
- types $\tau(x_a) = (\mathrm{ext},\mathrm{out},a)$ and $\tau(y_b) = (\mathrm{ext},\mathrm{in},b)$, which are pairwise distinct, and $\tau(v_l) = \nu_l$.

This is the pregraph of Definition 38.35, with external vertices of pairwise distinct types. Every half-edge corresponds to one factor of the product

$$Y := X_{(I|I')}\prod_{l=1}^{k}\overline{\psi}(j_{1,l})\cdots\overline{\psi}(j_{d_{\nu_l},l})\,\psi(j'_{d'_{\nu_l},l})\cdots\psi(j'_{1,l}), \tag{38.100}$$

namely $h^x_a \leftrightarrow \psi_{i_a}$, $h^y_b \leftrightarrow \overline{\psi}_{i'_b}$, $h^{\mathrm{in}}_{l,r} \leftrightarrow \overline{\psi}(j_{r,l})$ and $h^{\mathrm{out}}_{l,r} \leftrightarrow \psi(j'_{r,l})$. Thus outgoing half-edges correspond to ψ-factors and incoming half-edges to $\overline{\psi}$-factors. We denote by $\ell(h) \in \{1,\dots,D\}$ the index of the factor of h (its *label*) and by $p(h)$ the position of this factor in Y.

Definition 38.39 Let $G \in C(g)$ be a statistical graph with pairing ι, $N := |E(G)|$, and let $e_1,\dots,e_N$ be an enumeration of $E(G)$. Let $\rho_G \in \mathrm{S}_{2N}$ be the permutation with

$$\big(\rho_G(1),\rho_G(2),\dots,\rho_G(2N)\big) = \big(p(h_{\mathrm{out}}(e_1)),p(h_{\mathrm{in}}(e_1)),\dots,p(h_{\mathrm{out}}(e_N)),p(h_{\mathrm{in}}(e_N))\big)\,.$$

We define the *sign* $\sigma(G) := s_\zeta(\rho_G)$ and the *amplitude*

$$\mathcal{A}(G) := \sigma(G)\sum_{\text{internal labels}}\prod_{l=1}^{k} m_{\nu_l}(j_{1,l},\dots,j_{d_{\nu_l},l} \mid j'_{1,l},\dots,j'_{d'_{\nu_l},l})\prod_{e\in E(G)} C\left(\ell(h_{\mathrm{out}}(e)) \,\middle|\, \ell(h_{\mathrm{in}}(e))\right), \tag{38.101}$$

where the sum runs over all $j_{r,l}, j'_{r,l} \in \{1,\dots,D\}$, while the external labels i_a, i'_b are fixed.

Remark 38.39.1 The sign $\sigma(G)$ does not depend on the enumeration of the edges: changing it permutes blocks of length two, which changes ρ_G by an even permutation. By Equation (38.96), $\sigma(G)$ is the sign in

$$Y = \sigma(G) \prod_{e \in E(G)} \left(\psi_{h_{\mathrm{out}}(e)} \, \overline{\psi}_{h_{\mathrm{in}}(e)} \right), \tag{38.102}$$

where ψ_h resp. $\overline{\psi}_h$ denotes the factor of h, and the order of the (even) pairs is irrelevant. In words: $\sigma(G)$ is the sign that arises when Y is reordered such that every ψ-factor is directly followed by the $\overline{\psi}$-factor it is paired with. Every edge contributes the covariance $C = \langle \psi \, \overline{\psi} \rangle_0$ of its pair.

Lemma 38.40 (*Wick's theorem in pair form.*) Let $Y = y_1 \cdots y_M$ be a product of generators with fixed labels in arbitrary order, containing N_ψ factors ψ and $N_{\overline{\psi}}$ factors $\overline{\psi}$. If $N_\psi \neq N_{\overline{\psi}}$, then $\langle Y \rangle_0 = 0$. If $N_\psi = N_{\overline{\psi}} = N$, then

$$\langle Y \rangle_0 = \sum_{\iota} s_\zeta(\rho_\iota) \prod_{(\psi_a, \overline{\psi}_b) \text{ paired by } \iota} C(a \mid b),$$

where the sum runs over the $N!$ bijections ι between the ψ-factors and the $\overline{\psi}$-factors, and ρ_ι is defined as in Definition 38.39 (list the positions of every ψ-factor followed by the position of its partner).

Proof 38.40 *Unequal numbers.* For $\varphi \in \mathbb{R}$ the substitution $\psi_j \mapsto \mathrm{e}^{\mathrm{i}\varphi} \psi_j$, $\overline{\psi}_j \mapsto \mathrm{e}^{-\mathrm{i}\varphi} \overline{\psi}_j$ leaves $S_0 = \psi^\dagger A \psi$ and the integration measure invariant (for complex variables because $\overline{\psi}$ is the complex conjugate of ψ, for Graßmann-variables because the Berezin-measure acquires the factor $\mathrm{e}^{-\mathrm{i}\varphi D} \mathrm{e}^{\mathrm{i}\varphi D} = 1$). Hence $\langle Y \rangle_0 = \mathrm{e}^{\mathrm{i}\varphi(N_\psi - N_{\overline{\psi}})} \langle Y \rangle_0$ for all φ, i.e. $\langle Y \rangle_0 = 0$.

Equal numbers. Let $\psi_{a_1}, \dots, \psi_{a_N}$ and $\overline{\psi}_{b_1}, \dots, \overline{\psi}_{b_N}$ be the ψ- resp. $\overline{\psi}$-factors of Y in their order of appearance, and $Y_0 := \psi_{a_1} \cdots \psi_{a_N} \overline{\psi}_{b_N} \cdots \overline{\psi}_{b_1}$. By Equation (38.96), $Y = s_\zeta(\rho_0) Y_0$ for the reordering permutation ρ_0, and by Theorem 16.22

$$\langle Y_0 \rangle_0 = \sum_{\pi \in \mathrm{S}_N} s_\zeta(\pi) \prod_{r=1}^{N} C(a_r \mid b_{\pi(r)}).$$

Let ι_π pair ψ_{a_r} with $\overline{\psi}_{b_{\pi(r)}}$; then $\pi \mapsto \iota_\pi$ is a bijection onto all pairings. Moving all ψ's to the left (keeping their order), reordering the $\overline{\psi}$'s and reversing them gives

$$\prod_{r=1}^{N} \left(\psi_{a_r} \overline{\psi}_{b_{\pi(r)}} \right) = \zeta^{\frac{N(N-1)}{2}} \psi_{a_1} \cdots \psi_{a_N} \, \overline{\psi}_{b_{\pi(1)}} \cdots \overline{\psi}_{b_{\pi(N)}} = \zeta^{\frac{N(N-1)}{2}} s_\zeta(\pi) \, \psi_{a_1} \cdots \psi_{a_N} \, \overline{\psi}_{b_1} \cdots \overline{\psi}_{b_N} = s_\zeta(\pi) \, Y_0,$$

using $\zeta^2 = 1$. Hence $Y = s_\zeta(\rho_0) s_\zeta(\pi) \prod_r (\psi_{a_r} \overline{\psi}_{b_{\pi(r)}})$, i.e. $s_\zeta(\rho_{\iota_\pi}) = s_\zeta(\rho_0) s_\zeta(\pi)$, and

$$\langle Y \rangle_0 = s_\zeta(\rho_0) \langle Y_0 \rangle_0 = \sum_{\pi} s_\zeta(\rho_{\iota_\pi}) \prod_{r=1}^{N} C(a_r \mid b_{\pi(r)}).$$

Lemma 38.41 (*Labelled expansion.*) With $g = g(I \mid I'; \nu)$,

$$\left\langle X_{(I \mid I')} M_{\nu_1} \cdots M_{\nu_k} \right\rangle_0 = \prod_{l=1}^{k} \frac{1}{d_{\nu_l}! \, d'_{\nu_l}!} \sum_{G \in C(g)} \mathcal{A}(G),$$

where the sum is empty (and the left-hand side vanishes) if g is unpairable.

Proof 38.41 We insert Equation (38.97) for every M_{ν_l} and move the coefficients m_{ν_l} to the front, which produces no sign as they are complex numbers or even. This gives $X\,M_{\nu_1}\cdots M_{\nu_k} = \prod_l (d_{\nu_l}!\,d'_{\nu_l}!)^{-1}\sum_{\text{labels}}\prod_l m_{\nu_l}(\dots)\,Y$. For fixed labels we apply Lemma 38.40 to Y. Under the correspondence of Definition 38.38, the bijections between the ψ-factors and the $\overline{\psi}$-factors are precisely the pairings of g (Lemma 38.6), and the sign of a pairing is $\sigma(G)$. Interchanging the finite sums yields the claim.

Notation 38.42 Let $k_\mu := |\{l \mid \nu_l = \mu\}|$ for $\mu \in \mathscr{V}$. We denote by $\mathfrak{G}(g)$ the group of all bijections $\gamma : H \to H$ that fix every external half-edge and for which there is a bijection γ_V of the internal vertices with $\tau\circ\gamma_V = \tau$, such that γ maps the incoming (outgoing) half-edges of every internal vertex v onto the incoming (outgoing) half-edges of $\gamma_V(v)$. Thus $\mathfrak{G}(g)$ consists of the permutations of the internal vertices of equal type combined with permutations of the incoming and of the outgoing half-edges at every internal vertex, and

$$|\mathfrak{G}(g)| = \prod_{\mu\in\mathscr{V}} k_\mu!\,\left(d_\mu!\,d'_\mu!\right)^{k_\mu}.$$

$\mathfrak{G}(g)$ acts on the pairings by $\iota \mapsto \gamma\iota\gamma^{-1}$; this is again a pairing, since γ preserves the directions. We write $\gamma\cdot G$ for the corresponding statistical graph.

Lemma 38.43 (*Invariance of the amplitude.*) For all $\gamma \in \mathfrak{G}(g)$ and $G \in C(g)$ one has $\mathcal{A}(\gamma\cdot G) = \mathcal{A}(G)$.

Proof 38.43 Let γ map the vertex v_l to $v_{l'} = \gamma_V(v_l)$, with $\gamma(h^{\text{in}}_{l,r}) = h^{\text{in}}_{l',\alpha_l(r)}$ and $\gamma(h^{\text{out}}_{l,r}) = h^{\text{out}}_{l',\beta_l(r)}$ for permutations α_l, β_l. The edges of $G' := \gamma\cdot G$ are $\gamma(e) = \{\gamma(h),\gamma(\iota(h))\}$ for $e = \{h,\iota(h)\} \in E(G)$, with $h_{\text{out}}(\gamma(e)) = \gamma(h_{\text{out}}(e))$ and $h_{\text{in}}(\gamma(e)) = \gamma(h_{\text{in}}(e))$.

Sign. Let π_γ be the permutation of positions induced by γ, $p(\gamma(h)) = \pi_\gamma(p(h))$. Then $\rho_{G'} = \pi_\gamma\circ\rho_G$, hence $\sigma(G') = s_\zeta(\pi_\gamma)\sigma(G)$. The permutation π_γ permutes the factors within the blocks of the internal vertices (by α_l, β_l) and permutes whole blocks of equal length. The latter costs no sign, since the blocks are even for $\zeta = -1$ (Notation 38.37, 3.). Hence $s_\zeta(\pi_\gamma) = \prod_l s_\zeta(\alpha_l)s_\zeta(\beta_l)$.

Sum. We substitute the internal summation labels by $\widetilde{\ell}(h) := \ell(\gamma(h))$; this is a bijective substitution of the dummy variables, and the external labels are unaffected since γ fixes the external half-edges. Then

$$\prod_{e'\in E(G')} C\left(\ell(h_{\text{out}}(e'))\,\middle|\,\ell(h_{\text{in}}(e'))\right) = \prod_{e\in E(G)} C\left(\widetilde{\ell}(h_{\text{out}}(e))\,\middle|\,\widetilde{\ell}(h_{\text{in}}(e))\right).$$

The coefficient of the vertex $v_{l'}$ has the arguments $\ell(h^{\text{in}}_{l',r}) = \widetilde{\ell}(h^{\text{in}}_{l,\alpha_l^{-1}(r)})$ (and analogously for the outgoing half-edges), so by Equation (38.98) and $\tau(v_{l'}) = \tau(v_l)$ the product of the coefficients acquires the factor $\prod_l s_\zeta(\alpha_l)s_\zeta(\beta_l)$. Thus the sum in Equation (38.101) for G' equals $\prod_l s_\zeta(\alpha_l)s_\zeta(\beta_l)$ times the sum for G.

Together, $\mathcal{A}(G') = \left(\prod_l s_\zeta(\alpha_l)s_\zeta(\beta_l)\right)^2\mathcal{A}(G) = \mathcal{A}(G)$.

Lemma 38.44 (*Orbits and stabilizers.*) Let $G, G' \in C(g)$ with pairings ι, ι'.

1. $\Gamma(G) \cong \Gamma(G')$ if and only if $G' = \gamma \cdot G$ for some $\gamma \in \mathfrak{G}(g)$.
2. The stabilizer of G in $\mathfrak{G}(g)$ is isomorphic to $\mathrm{Aut}(\Gamma(G))$.

Proof 38.44 *(i), "⇒".* Let $\varphi = (\varphi_V, \varphi_E) : \Gamma(G) \to \Gamma(G')$ be an isomorphism. Every half-edge is $h_{\mathrm{out}}(e)$ or $h_{\mathrm{in}}(e)$ for exactly one edge e of G, and likewise for G'. Hence

$$\gamma(h_{\mathrm{out}}(e)) := h_{\mathrm{out}}(\varphi_E(e)), \qquad \gamma(h_{\mathrm{in}}(e)) := h_{\mathrm{in}}(\varphi_E(e))$$

defines a bijection $\gamma : H \to H$ that preserves the directions, and $\partial \circ \gamma = \varphi_V \circ \partial$ follows from $\varphi_V \circ s = s \circ \varphi_E$ and $\varphi_V \circ t = t \circ \varphi_E$. Since $\tau \circ \varphi_V = \tau$ and the external vertices have pairwise distinct types, φ_V fixes every external vertex, so γ fixes every external half-edge (each external vertex carries exactly one half-edge). Internal vertices are mapped to internal vertices of the same type, and γ maps the incoming (outgoing) half-edges of v onto those of $\varphi_V(v)$. Hence $\gamma \in \mathfrak{G}(g)$. Finally, γ maps the ι-pair $\{h_{\mathrm{out}}(e), h_{\mathrm{in}}(e)\}$ onto the ι'-pair $\{h_{\mathrm{out}}(\varphi_E(e)), h_{\mathrm{in}}(\varphi_E(e))\}$, i.e. $\gamma\iota = \iota'\gamma$.

(i), "⇐". Let $\iota' = \gamma\iota\gamma^{-1}$, and extend γ_V by the identity on the external vertices. Then

$$\varphi_E(\{h, \iota(h)\}) := \{\gamma(h), \gamma(\iota(h))\} = \{\gamma(h), \iota'(\gamma(h))\}$$

defines a bijection $E(G) \to E(G')$. Since γ preserves the directions and $\partial \circ \gamma = \gamma_V \circ \partial$, one has $\gamma_V \circ s = s \circ \varphi_E$ and $\gamma_V \circ t = t \circ \varphi_E$, and $\tau \circ \gamma_V = \tau$. Hence (γ_V, φ_E) is an isomorphism $\Gamma(G) \to \Gamma(G')$.

(ii). For $G' = G$ both constructions are mutually inverse: γ is determined by φ_E, as every half-edge is determined by its edge and its direction, and γ_V is determined by γ, as every vertex carries at least one half-edge (Notation 38.37, 2.). Both constructions are compatible with composition, hence they define a group isomorphism between the stabilizer of G and $\mathrm{Aut}(\Gamma(G))$.

Definition 38.45 For a multiplicity function $\mathbf{k} = (k_\mu)_{\mu \in \mathscr{V}} \in \mathbb{N}_0^{\mathscr{V}}$, let $\nu(\mathbf{k})$ list every μ exactly k_μ times (in a fixed order of $\mathscr{V}$), and $g_{\mathbf{k}} := g(I|I'; \nu(\mathbf{k}))$. We denote by $\mathfrak{D}(I|I')$ the set of isomorphism classes of the statistical Feynman-diagrams $\Gamma(G)$, $G \in C(g_{\mathbf{k}})$, $\mathbf{k} \in \mathbb{N}_0^{\mathscr{V}}$, and by $k(\Gamma)$ the number of internal vertices. For $[\Gamma] \in \mathfrak{D}(I|I')$ we set $\mathcal{A}(\Gamma) := \mathcal{A}(G)$ for any such G with $\Gamma(G) \cong \Gamma$. This is well-defined: the multiplicities k_μ are isomorphism invariants (as τ is preserved), and for fixed $\mathbf{k}$ one uses Lemmas 38.43 and 38.44. For $n = 0$ we write $\mathfrak{D}_{\mathrm{vac}}$ and call its elements *vacuum diagrams*; $\mathfrak{D}_{\mathrm{vac}}$ contains the empty diagram ($\mathbf{k} = 0$) with amplitude 1.

Theorem 38.46 (*Feynman-diagrammatic expansion.*) Under the assumptions of Notation 38.37,

$$\left\langle X_{(I|I')}\, \mathrm{e}^{-\lambda S_{\mathrm{int}}} \right\rangle_0 = \sum_{[\Gamma] \in \mathfrak{D}(I|I')} \frac{(-\lambda)^{k(\Gamma)}}{|\operatorname{Aut}(\Gamma)|}\, \mathcal{A}(\Gamma). \tag{38.103}$$

Proof 38.46 By the exponential series and Equation (38.85),

$$\left\langle X\, \mathrm{e}^{-\lambda S_{\mathrm{int}}} \right\rangle_0 = \sum_{k=0}^{\infty} \frac{(-\lambda)^k}{k!} \sum_{\nu \in \mathscr{V}^k} \left\langle X\, M_{\nu_1} \cdots M_{\nu_k} \right\rangle_0 .$$

The M_ν are even and hence commute, so the summand depends only on the multiplicities $\mathbf{k}$ of ν, and there are $k!/\prod_\mu k_\mu!$ tuples with given multiplicities. With Lemma 38.41 and Notation 38.42,

$$\left\langle X\, \mathrm{e}^{-\lambda S_{\mathrm{int}}} \right\rangle_0 = \sum_{\mathbf{k}} \frac{(-\lambda)^{|\mathbf{k}|}}{\prod_\mu k_\mu!\,(d_\mu!\,d'^{\,}_\mu!)^{k_\mu}} \sum_{G \in C(g_{\mathbf{k}})} \mathcal{A}(G) = \sum_{\mathbf{k}} \frac{(-\lambda)^{|\mathbf{k}|}}{|\mathfrak{G}(g_{\mathbf{k}})|} \sum_{G \in C(g_{\mathbf{k}})} \mathcal{A}(G),$$

where $|\mathbf{k}| = \sum_\mu k_\mu$. By Lemma 38.43, $\mathcal{A}$ is constant on the $\mathfrak{G}(g_{\mathbf{k}})$-orbits. By the orbit-stabilizer theorem and Lemma 38.44 (ii), an orbit O has $|O| = |\mathfrak{G}(g_{\mathbf{k}})|/|\operatorname{Aut}(\Gamma_O)|$ elements, where $\Gamma_O = \Gamma(G)$ for any $G \in O$. Therefore

$$\frac{1}{|\mathfrak{G}(g_{\mathbf{k}})|} \sum_{G \in C(g_{\mathbf{k}})} \mathcal{A}(G) = \sum_O \frac{\mathcal{A}(\Gamma_O)}{|\operatorname{Aut}(\Gamma_O)|},$$

and by Lemma 38.44 (i) the orbits correspond bijectively to the isomorphism classes in $\mathfrak{D}(I|I')$ with internal vertex multiplicities $\mathbf{k}$. Summing over $\mathbf{k}$ yields the claim.

Corollary 38.47 (*Loop rule.*) Assume $d_\nu = d'_\nu$ for all ν. For $G \in C(g)$ join, at every internal vertex v_l, the incoming half-edge $h^{\mathrm{in}}_{l,r}$ with the outgoing half-edge $h^{\mathrm{out}}_{l,r}$ ($r = 1, \dots, d_{\nu_l}$) to a *segment*. Following edges and segments alternately, the half-edges decompose into $L(G)$ closed loops and n open lines, the a-th of which starts at x_a and ends at $y_{\pi_G(a)}$ for a permutation $\pi_G \in \mathrm{S}_n$. Then

$$\sigma(G) = \zeta^{L(G)}\, \zeta^{\frac{n(n-1)}{2}}\, s_\zeta(\pi_G).$$

Proof 38.47 *Decomposition.* For an outgoing half-edge h, $\iota(h)$ is incoming. If $\iota(h) = h^{\mathrm{in}}_{l,r}$, its successor is $h^{\mathrm{out}}_{l,r}$; if $\iota(h) = h^y_b$, the line ends. The successor map is injective, and the half-edges h^x_a have no predecessor. Hence the outgoing half-edges decompose into n chains starting at the x_a and ending at distinct y_b, and into cycles.

Sign. The block of v_l in Equation (38.100) is nested, $\overline{\psi}_1 \cdots \overline{\psi}_d \psi_d \cdots \psi_1 = \prod_r (\overline{\psi}_r \psi_r)$ (the innermost pair is even and can be moved to the front, then induction), i.e. it is the product of the even segment factors $(\overline{\psi}_r \psi_r)$. For a closed loop with segments $s_1, \dots, s_q$ in cyclic order (the outgoing half-edge of s_t is paired with the incoming half-edge of s_{t+1}), moving $\overline{\psi}_{s_1}$ to the end past $2q-1$ odd factors gives

$$\prod_{t=1}^{q} \left(\overline{\psi}_{s_t} \psi_{s_t}\right) = \zeta \prod_{t=1}^{q} \left(\psi_{s_t} \overline{\psi}_{s_{t+1}}\right), \qquad s_{q+1} := s_1.$$

For the a-th open line with segments $s_1, \dots, s_q$ ($q \geq 0$) and segment product L_a, regrouping gives $\psi_{i_a} L_a \overline{\psi}_{i'_{\pi(a)}} = (\psi_{i_a} \overline{\psi}_{s_1})(\psi_{s_1} \overline{\psi}_{s_2}) \cdots (\psi_{s_q} \overline{\psi}_{i'_{\pi(a)}})$ without sign. As the L_a are even, the computation in the proof of Lemma 38.40 yields

$$\prod_{a=1}^{n} \left(\psi_{i_a} L_a \overline{\psi}_{i'_{\pi(a)}}\right) = \left(\prod_a L_a\right) \zeta^{\frac{n(n-1)}{2}}\, \psi_{i_1} \cdots \psi_{i_n}\, \overline{\psi}_{i'_{\pi(1)}} \cdots \overline{\psi}_{i'_{\pi(n)}} = \zeta^{\frac{n(n-1)}{2}}\, s_\zeta(\pi)\, X_{(I|I')} \prod_a L_a.$$

Since all segment factors are even, $Y = X_{(I|I')} \prod_a L_a \prod_{\mathrm{loops}} \prod_t (\overline{\psi}_{s_t} \psi_{s_t})$. Inserting both identities and comparing with Equation (38.102) gives the claim.

Corollary 38.48 (*Partition-function.*) The partition-function of Notation 16.24 is

$$Z = Z_0 \sum_{[\Gamma]\in\mathfrak{D}_{\mathrm{vac}}} \frac{(-\lambda)^{k(\Gamma)}}{|\operatorname{Aut}(\Gamma)|}\,\mathcal{A}(\Gamma),$$

the sum of all vacuum diagrams (including the empty one). For number-conserving vertices, $\sigma = \zeta^L$ by Corollary 38.47.

Proof 38.48 $Z = \int \mathrm{d}_\zeta(\overline{\psi},\psi)\,\mathrm{e}^{-S_0-\lambda S_{\mathrm{int}}} = Z_0\langle \mathrm{e}^{-\lambda S_{\mathrm{int}}}\rangle_0$, and Theorem 38.46 with $n=0$.

Lemma 38.49 (*Isomorphisms and components.*)

1. Every isomorphism $\varphi:\Gamma\to\Gamma'$ maps every connected component of Γ isomorphically onto a connected component of Γ'.
2. If $\Gamma = \bigsqcup_c \Gamma_c^{\sqcup n_c}$ is the disjoint union of n_c copies of pairwise non-isomorphic connected diagrams Γ_c, then $|\operatorname{Aut}(\Gamma)| = \prod_c n_c!\,|\operatorname{Aut}(\Gamma_c)|^{n_c}$.
3. If $\Gamma = \Gamma_1\sqcup\Gamma_2$ and every automorphism of Γ maps Γ_1 onto Γ_1, then $\operatorname{Aut}(\Gamma)\cong\operatorname{Aut}(\Gamma_1)\times\operatorname{Aut}(\Gamma_2)$.

Proof 38.49 (i) Since φ preserves s and t, it maps walks to walks, $(v_0,e_1,v_1,\dots)\mapsto(\varphi_V(v_0),\varphi_E(e_1),\varphi_V(v_1),\dots)$, and so does φ^{-1}. Hence $u\sim_\Gamma v$ if and only if $\varphi_V(u)\sim_{\Gamma'}\varphi_V(v)$, i.e. φ_V maps the equivalence classes C_i onto equivalence classes, and φ_E maps the corresponding edge sets E_i onto each other (Theorem 38.25). (ii) By (i), an automorphism permutes the connected components and maps every copy of Γ_c to a copy of Γ_c. Fixing an identification of every copy with Γ_c, the automorphisms correspond bijectively to a permutation of the n_c copies for every c, together with an automorphism of Γ_c for every copy. (iii) The map $\varphi\mapsto(\varphi|_{\Gamma_1},\varphi|_{\Gamma_2})$ is a group isomorphism.

Lemma 38.50 (*Multiplicativity.*) Let $\Gamma\in\mathfrak{D}(I|I')$ decompose as $\Gamma=\Gamma_1\sqcup\Gamma_2$, where Γ_2 contains no external vertex. Then $k(\Gamma)=k(\Gamma_1)+k(\Gamma_2)$ and $\mathcal{A}(\Gamma)=\mathcal{A}(\Gamma_1)\,\mathcal{A}(\Gamma_2)$, where $\Gamma_1\in\mathfrak{D}(I|I')$ and $\Gamma_2\in\mathfrak{D}_{\mathrm{vac}}$.

Proof 38.50 Choose a labelled representative G. Its internal vertices split into those of Γ_1 and those of Γ_2, and ι maps the half-edges of Γ_i to half-edges of Γ_i. Renaming the internal vertices does not change amplitudes (proof of Lemma 38.43), so the restrictions of G are labelled representatives of Γ_1 and Γ_2. The vertex blocks of Γ_2 in Equation (38.100) are even and can be moved to the right end without a sign, $Y=Y_1Y_2$. As the pairs of Γ_1 only involve factors of Y_1, Equation (38.102) gives $\sigma(G)=\sigma(G_1)\sigma(G_2)$. The sum over the labels and the products of coefficients and covariances factorize.

Corollary 38.51 (*Free energy: connected vacuum diagrams.*) Let $\mathfrak{D}_{\mathrm{vac}}^{\mathrm{conn}}\subset\mathfrak{D}_{\mathrm{vac}}$ be the isomorphism classes of non-empty connected vacuum diagrams. Then

$$\ln\frac{Z}{Z_0} = \sum_{[\Gamma]\in\mathfrak{D}_{\mathrm{vac}}^{\mathrm{conn}}} \frac{(-\lambda)^{k(\Gamma)}}{|\operatorname{Aut}(\Gamma)|}\,\mathcal{A}(\Gamma).$$

Consequently, for $\Omega = -\frac{1}{\beta}\ln Z$ and $\Omega_0 = -\frac{1}{\beta}\ln Z_0$, the difference $\Omega - \Omega_0$ is $-\frac{1}{\beta}$ times the sum of all connected vacuum diagrams.

Proof 38.51 By Theorem 38.25, every vacuum diagram is, uniquely up to the order, a disjoint union of connected vacuum diagrams, and every non-empty connected vacuum diagram contains at least one internal vertex. Hence the isomorphism classes of vacuum diagrams correspond bijectively to the multiplicity functions (n_c) with finite support on $\mathfrak{D}^{\mathrm{conn}}_{\mathrm{vac}}$ (by Lemma 38.49 (i), isomorphic diagrams have the same multiplicities). Let $w(\Gamma) := (-\lambda)^{k(\Gamma)}\mathcal{A}(\Gamma)$, which is multiplicative by Lemma 38.50. With Lemma 38.49 (ii),

$$\sum_{[\Gamma]\in\mathfrak{D}_{\mathrm{vac}}} \frac{w(\Gamma)}{|\operatorname{Aut}(\Gamma)|} = \sum_{(n_c)} \prod_c \frac{1}{n_c!}\left(\frac{w(\Gamma_c)}{|\operatorname{Aut}(\Gamma_c)|}\right)^{n_c} = \exp\left(\sum_{[\Gamma_c]\in\mathfrak{D}^{\mathrm{conn}}_{\mathrm{vac}}} \frac{w(\Gamma_c)}{|\operatorname{Aut}(\Gamma_c)|}\right).$$

These rearrangements are identities of formal power series: for every power λ^K only the finitely many diagrams with K internal vertices contribute, and $w(\Gamma_c) \in \lambda\,\mathbb{C}[[\lambda]]$ for connected Γ_c. Since exp and ln are mutually inverse bijections between $\lambda\,\mathbb{C}[[\lambda]]$ and $1 + \lambda\,\mathbb{C}[[\lambda]]$, Corollary 38.48 yields the claim.

Corollary 38.52 (*Linked-cluster theorem.*) Let $\mathfrak{D}^{\mathrm{lin}}(I|I') \subset \mathfrak{D}(I|I')$ be the isomorphism classes of diagrams without vacuum components, i.e. every connected component contains at least one external vertex. Then

$$\left\langle X_{(I|I')}\right\rangle = \frac{\left\langle X_{(I|I')}\,\mathrm{e}^{-\lambda S_{\mathrm{int}}}\right\rangle_0}{\left\langle \mathrm{e}^{-\lambda S_{\mathrm{int}}}\right\rangle_0} = \sum_{[\Gamma]\in\mathfrak{D}^{\mathrm{lin}}(I|I')} \frac{(-\lambda)^{k(\Gamma)}}{|\operatorname{Aut}(\Gamma)|}\,\mathcal{A}(\Gamma),$$

and $\mathcal{G}(i_1,\dots,i_n \mid i'_n,\dots,i'_1) = (-\frac{1}{c})^n\langle X_{(I|I')}\rangle$ by Equation (16.33).

Proof 38.52 The first equality is $\langle X\rangle = \frac{1}{Z}\int X\mathrm{e}^{-S} = \frac{Z_0}{Z}\langle X\mathrm{e}^{-\lambda S_{\mathrm{int}}}\rangle_0$. For $\Gamma \in \mathfrak{D}(I|I')$, let Γ_{lin} be the union of the connected components that contain an external vertex, and Γ_{vac} the union of the remaining ones; this decomposition is unique by Theorem 38.25. Every automorphism fixes the external vertices (pairwise distinct types), hence by Lemma 38.49 (i) maps the component of every external vertex onto itself, i.e. Γ_{lin} onto Γ_{lin}, and Lemma 38.49 (iii) gives $\operatorname{Aut}(\Gamma) \cong \operatorname{Aut}(\Gamma_{\mathrm{lin}}) \times \operatorname{Aut}(\Gamma_{\mathrm{vac}})$. Conversely, every pair consisting of a diagram in $\mathfrak{D}^{\mathrm{lin}}(I|I')$ and a vacuum diagram gives a diagram in $\mathfrak{D}(I|I')$ (the union of the pairings is a pairing of the combined pregraph), and isomorphisms preserve the decomposition. Hence $[\Gamma] \mapsto ([\Gamma_{\mathrm{lin}}], [\Gamma_{\mathrm{vac}}])$ is a bijection $\mathfrak{D}(I|I') \to \mathfrak{D}^{\mathrm{lin}}(I|I')\times\mathfrak{D}_{\mathrm{vac}}$. With Lemma 38.50, Theorem 38.46 factorizes into the sum over $\mathfrak{D}^{\mathrm{lin}}(I|I')$ times the sum over $\mathfrak{D}_{\mathrm{vac}}$, and the latter is $\langle \mathrm{e}^{-\lambda S_{\mathrm{int}}}\rangle_0$ (Corollary 38.48), which is invertible in $\mathbb{C}[[\lambda]]$.

Corollary 38.53 (*Two-point function: connected diagrams.*) Assume $d_\nu = d'_\nu$ for all ν. Then every connected component of a diagram in $\mathfrak{D}^{\mathrm{lin}}(I|I')$ contains as many vertices x_a as vertices y_b. In particular, for $n = 1$ every diagram in $\mathfrak{D}^{\mathrm{lin}}(i|i')$ is connected, and

$$\mathcal{G}(i \mid i') = -\frac{1}{c}\sum_{\substack{[\Gamma]\in\mathfrak{D}(i|i')\\ \Gamma\text{ connected}}} \frac{(-\lambda)^{k(\Gamma)}}{|\operatorname{Aut}(\Gamma)|}\,\mathcal{A}(\Gamma), \qquad \sigma = \zeta^L.$$

Proof 38.53 A connected component K consists of whole vertices with all their half-edges, and ι maps half-edges of K to half-edges of K. By Lemma 38.6, K has as many outgoing as incoming half-edges, i.e. $|\{x_a \in$

$K\}| + \sum_{v\in K \text{ internal}} d'_{\tau(v)} = |\{y_b \in K\}| + \sum_{v\in K \text{ internal}} d_{\tau(v)}$, and $d = d'$ gives the first claim. For $n = 1$ the component of x_1 contains y_1, and all other components are vacuum components. Finally, $\zeta^{n(n-1)/2} s_\zeta(\pi_G) = 1$ for $n = 1$.

Remark 38.53.1 *Example.* For the two-body vertex (38.99) we evaluate the diagrams of Figure 38.1 with the loop rule.

1. Diagram (a), represented by ι_1: every segment closes on itself, so $L = 2$, $\sigma = 1$, and $|\operatorname{Aut}| = 2$. By Corollary 38.51, the first-order contribution to $\ln(Z/Z_0)$ is

$$-\frac{\lambda}{2} \sum_{j_1, j_2, j'_1, j'_2} \big(V(j_1 j_2 | j'_1 j'_2) + \zeta V(j_1 j_2 | j'_2 j'_1)\big)\, C(j'_1 | j_1)\, C(j'_2 | j_2),$$

   i.e. the Hartree- and the Fock-term, which the ζ-symmetric vertex combines into a single diagram.

2. Diagram (b) contains a vacuum component and therefore cancels in the Green-function (Corollary 38.52).

3. Diagram (c), represented by $h^x \leftrightarrow h_1^{\text{in}}$, $h_1^{\text{out}} \leftrightarrow h^y$, $h_2^{\text{out}} \leftrightarrow h_2^{\text{in}}$: one open line and one closed loop, so $\sigma = \zeta$, and $|\operatorname{Aut}| = 1$. Hence, to first order,

$$\langle \psi_i \overline{\psi}_{i'} \rangle = C(i|i') - \lambda \sum_{j_1, j_2, j'_1, j'_2} \big(\zeta V(j_1 j_2 | j'_1 j'_2) + V(j_1 j_2 | j'_2 j'_1)\big)\, C(i|j_1)\, C(j'_2 | j_2)\, C(j'_1 | i') + \mathcal{O}(\lambda^2),$$

   where the first term is the Hartree-term (with the sign ζ of its closed loop) and the second one is the Fock-term.

A direct computation of $\langle M \rangle_0$ and $\langle \psi_i \overline{\psi}_{i'} M \rangle_0$ with Lemma 38.40 confirms both results.

Remark 38.53.2 *What is not covered here.*

1. For $n \geq 2$ the diagrams of $\mathfrak{D}^{\text{lin}}(I|I')$ need not be connected (e.g. products of two two-point functions). The connected (cumulant) Green-functions are the sums of the connected diagrams. This follows from the generating functional $\ln Z[j, \bar{j}]$ (Notation 16.27) by the exponential formula, with the sources as additional vertices of valency one; since the sources are odd for $\zeta = -1$, this requires an extension of the sign book-keeping above.

2. The statement that the self-energy is the sum of the one-particle-irreducible two-point diagrams additionally requires the decomposition of connected two-point diagrams into chains of one-particle-irreducible parts, together with the corresponding factorization of the automorphism groups (Dyson-equation).

3. Mixed systems (several fields of different statistics) can be treated in the same way, with one type of edge per field and the pair-statistics of Definition 8.12 in the sign rule.

39. Experimental: Logarithm of a Grassmann-Polynomial

We start from

$$\log(1+\eta) = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} \eta^n \tag{39.1}$$

This gives therefore

$$\partial_\eta \log(1+\eta) = \sum_{n=1}^{\infty} (-1)^{n+1} \eta^{n-1} = \dots \tag{39.2}$$

now shifting the index as $m = n - 1$ gives

$$\dots = \sum_{m=0}^{\infty} (-1)^m \eta^m \tag{39.3}$$

Notice that this is exactly the expression for the geometric series as

$$(1+\eta)^{-1} = \sum_{m=0}^{\infty} (-1)^m \eta^m \tag{39.4}$$

Therefore we see that

$$\partial_\eta \log(1+\eta) = (1+\eta)^{-1}. \tag{39.5}$$

40. Experimental: The Grand Potential of Interacting Mixed Systems

40.1. The EPW-System

Proof 40.1 of Theorem 24.15

The grand canonical potential $\Omega(\mu, T, V)$ obeys the equation[1]

$$\Omega - \Omega_0 = -\frac{1}{\beta} \operatorname{Log} \frac{Z}{Z_0} = -\frac{1}{\beta} \times \text{„all connected diagrams“} \tag{40.1}$$

Thus we compute the connected diagrams of the system.

Computing the connected Diagrams through a Series-Expansion

We can therefore simply compute the partition-function in a perturbative expansion, take from the appearing Feynman-diagrams the connected ones and add the expression for the non-interacting grand canonical potential on top of it.

$$\begin{aligned}
&\frac{Z}{Z_0} \\
&= \langle \exp -S_{\text{int}}[\overline{\chi}, \chi] \rangle_0 \\
&= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \langle S_{\text{int}}^n[\overline{\chi}, \chi] \rangle_0 \\
&= 1 + 0 \\
&+ \frac{1}{2} \sum_{\substack{\tau_1,\tau_2 \in [0,\hbar\beta] \\ \mu,\mu' \in \{\downarrow,\uparrow\} \\ \mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}' \in \mathrm{Q} \\ m,m',n,n' \in \{1,2,\dots\} \\ \nu,\nu' \in \{1,2,\dots,rd_{\mathbf{x}}\}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q}) g_{m'n'\nu'}(\mathbf{k}',\mathbf{q}')}{\hbar^2 N_p} \left\langle \left(\phi_{\mathbf{q}\nu}(\tau_1) + \overline{\phi}_{-\mathbf{q}\nu}(\tau_1) \right) \overline{\psi}_{\mathbf{k}+\mathbf{q}m\mu}(\tau_1) \psi_{\mathbf{k}n\mu}(\tau_1) \left(\phi_{\mathbf{q}'\nu'}(\tau_2) + \overline{\phi}_{-\mathbf{q}'\nu'}(\tau_2) \right) \overline{\psi}_{\mathbf{k}'+\mathbf{q}'m'} \right.
\\
&= \dots
\end{aligned}$$

We now factorize and compute the correlators

[1] See also Mahan 3.6.1 for an expansion of the thermodynamic potential.

$$
\begin{aligned}
&\left\langle \left(\phi_{\mathbf{q}\nu}(\tau_1)+\overline{\phi}_{-\mathbf{q}\nu}(\tau_1)\right)\overline{\psi}_{\mathbf{k}+\mathbf{q}m\mu}(\tau_1)\psi_{\mathbf{k}n\mu}(\tau_1)\left(\phi_{\mathbf{q}'\nu'}(\tau_2)+\overline{\phi}_{-\mathbf{q}'\nu'}(\tau_2)\right)\overline{\psi}_{\mathbf{k}'+\mathbf{q}'m'\mu'}(\tau_2)\psi_{\mathbf{k}'n'\mu'}(\tau_2)\right\rangle_0 \\
&= \left\langle \overline{\psi}_{\mathbf{k}+\mathbf{q}m\mu}(\tau_1)\psi_{\mathbf{k}n\mu}(\tau_1)\overline{\psi}_{\mathbf{k}'+\mathbf{q}'m'\mu'}(\tau_2)\psi_{\mathbf{k}'n'\mu'}(\tau_2)\right\rangle_0 \left\langle \left(\phi_{\mathbf{q}\nu}(\tau_1)+\overline{\phi}_{-\mathbf{q}\nu}(\tau_1)\right)\left(\phi_{\mathbf{q}'\nu'}(\tau_2)+\overline{\phi}_{-\mathbf{q}'\nu'}(\tau_2)\right)\right\rangle_0 \\
&= -\hbar\left\langle \overline{\psi}_{\mathbf{k}+\mathbf{q}m\mu}(\tau_1)\psi_{\mathbf{k}n\mu}(\tau_1)\overline{\psi}_{\mathbf{k}'+\mathbf{q}'m'\mu'}(\tau_2)\psi_{\mathbf{k}'n'\mu'}(\tau_2)\right\rangle_0 \mathscr{D}^{\ 0}_{\substack{\mathbf{q},-\mathbf{q}'\\ \nu,\nu'}}(\tau_1-\tau_2) \\
&= +\hbar\left\langle \psi_{\mathbf{k}n\mu}(\tau_1)\psi_{\mathbf{k}'n'\mu'}(\tau_2)\overline{\psi}_{\mathbf{k}+\mathbf{q}m\mu}(\tau_1)\overline{\psi}_{\mathbf{k}'+\mathbf{q}'m'\mu'}(\tau_2)\right\rangle_0 \mathscr{D}^{\ 0}_{\substack{\mathbf{q},-\mathbf{q}'\\ \nu,\nu'}}(\tau_1-\tau_2) \\
&= +\hbar^3\left(\mathscr{G}^{\ 0}_{\substack{\mathbf{k},\mathbf{k}'+\mathbf{q}'\\ n,m'\\ \mu,\mu'}}(\tau_1-\tau_2)\mathscr{G}^{\ 0}_{\substack{\mathbf{k}',\mathbf{k}+\mathbf{q}\\ n',m\\ \mu',\mu}}(\tau_2-\tau_1)-\mathscr{G}^{\ 0}_{\substack{\mathbf{k},\mathbf{k}+\mathbf{q}\\ n,m\\ \mu,\mu}}(\tau_1-\tau_1)\mathscr{G}^{\ 0}_{\substack{\mathbf{k}',\mathbf{k}'+\mathbf{q}'\\ n',m'\\ \mu',\mu'}}(\tau_2-\tau_2)\right)\mathscr{D}^{\ 0}_{\substack{\mathbf{q},-\mathbf{q}'\\ \nu,\nu'}}(\tau_1-\tau_2)
\end{aligned}
$$

Reinserting this in the equation above yields

$$
\begin{aligned}
\ldots &= 1 \\
&+\frac{\hbar}{2N_p}\sum\!\!\!\!\!\!\int_{\substack{\tau_1,\tau_2\in[0,\hbar\beta]\\ \mu\in\{\downarrow,\uparrow\}\\ \mathbf{k},\mathbf{k}',\mathbf{q}\in\mathrm{Q}\\ m,n\in\{1,2,\ldots\}\\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} g_{mn\nu}(\mathbf{k},\mathbf{q})g_{nm\nu}(\mathbf{k}',-\mathbf{q})\mathscr{G}^{\ 0}_{\substack{\mathbf{k},\mathbf{k}'-\mathbf{q}\\ n,n\\ \mu,\mu}}(\tau_1-\tau_2)\mathscr{G}^{\ 0}_{\substack{\mathbf{k}',\mathbf{k}+\mathbf{q}\\ m,m\\ \mu,\mu}}(\tau_2-\tau_1)\mathscr{D}^{\ 0}_{\mathbf{q}\nu}(\tau_1-\tau_2) \\
&-\frac{\hbar}{2N_p}\sum\!\!\!\!\!\!\int_{\substack{\tau_1,\tau_2\in[0,\hbar\beta]\\ \mu,\mu'\in\{\downarrow,\uparrow\}\\ \mathbf{k},\mathbf{k}',\mathbf{q}\in\mathrm{Q}\\ m,m'\in\{1,2,\ldots\}\\ \nu,\nu'\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} g_{mm\nu}(\mathbf{k},\mathbf{q})g_{m'm'\nu'}(\mathbf{k}',-\mathbf{q})\mathscr{G}^{\ 0}_{\substack{\mathbf{k},\mathbf{k}+\mathbf{q}\\ m,m\\ \mu,\mu}}(\tau_1-\tau_1)\mathscr{G}^{\ 0}_{\substack{\mathbf{k}',\mathbf{k}'-\mathbf{q}\\ m',m'\\ \mu',\mu'}}(\tau_2-\tau_2)\mathscr{D}^{\ 0}_{\mathbf{q},\nu}(\tau_1-\tau_2)
\end{aligned}
$$

This can be simplified by using the Kronecker-relation for the delta-functions

$$
\begin{aligned}
\ldots &= 1+\frac{\hbar}{2N_p}\sum\!\!\!\!\!\!\int_{\substack{\tau_1,\tau_2\in[0,\hbar\beta]\\ \mu\in\{\downarrow,\uparrow\}\\ \mathbf{k}',\mathbf{q}\in\mathrm{Q}\\ m,n\in\{1,2,\ldots\}\\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} g_{mn\nu}(\mathbf{k}'-\mathbf{q},\mathbf{q})g^*_{mn\nu}(\mathbf{k}'-\mathbf{q},+\mathbf{q})\mathscr{G}_{\substack{\mathbf{k}'-\mathbf{q},\mathbf{k}'-\mathbf{q}\\ n,n\\ \mu,\mu}}(\tau_1-\tau_2)\mathscr{G}_{\substack{\mathbf{k}',\mathbf{k}'\\ m,m\\ \mu,\mu}}(\tau_2-\tau_1)\mathscr{D}^{\ 0}_{\mathbf{q}\nu}(\tau_1-\tau_2) \\
&-\frac{\hbar}{2N_p}\sum\!\!\!\!\!\!\int_{\substack{\tau_1,\tau_2\in[0,\hbar\beta]\\ \mu,\mu'\in\{\downarrow,\uparrow\}\\ \mathbf{k},\mathbf{k}'\in\mathrm{Q}\\ m,m'\in\{1,2,\ldots\}\\ \nu,\nu'\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} g_{mm\nu}(\mathbf{k},0)g_{m'm'\nu'}(\mathbf{k}',0)\mathscr{G}_{\substack{\mathbf{k},\mathbf{k}\\ m,m\\ \mu,\mu}}(\tau_1-\tau_1)\mathscr{G}_{\substack{\mathbf{k}',\mathbf{k}'\\ m',m'\\ \mu',\mu'}}(\tau_2-\tau_2)\mathscr{D}^{\ 0}_{\mathbf{q}=0,\nu}(\tau_1-\tau_2)=\ldots
\end{aligned}
$$

Now using the hermiticity of g and changing summation $\mathbf{q}\mapsto-\mathbf{q}$ and simplifying the notation we obtain

$$\ldots = 1 + \frac{\hbar}{2N_p} \sum\!\!\!\!\!\!\int_{\substack{\tau_1,\tau_2 \in [0,\hbar\beta] \\ \mu \in \{\downarrow,\uparrow\} \\ \mathbf{k}',\mathbf{q} \in \mathrm{Q} \\ m,n \in \{1,2,\ldots\} \\ \nu \in \{1,2,\ldots,rd_{\mathbf{x}}\}}} |g_{mn\nu}(\mathbf{k}'+\mathbf{q},-\mathbf{q})|^2 \mathscr{G}^{\,0}_{n,\mu}(\mathbf{k}'+\mathbf{q},\tau_1-\tau_2)\mathscr{G}^{\,0}_{m,\mu}(\mathbf{k}',\tau_2-\tau_1)\mathscr{D}^{0}_{\nu}(\mathbf{q},\tau_1-\tau_2)$$

$$- \frac{\hbar}{2N_p} \sum\!\!\!\!\!\!\int_{\substack{\tau_1,\tau_2 \in [0,\hbar\beta] \\ \mu,\mu' \in \{\downarrow,\uparrow\} \\ \mathbf{k},\mathbf{k}' \in \mathrm{Q} \\ m,m' \in \{1,2,\ldots\} \\ \nu,\nu' \in \{1,2,\ldots,rd_{\mathbf{x}}\}}} g_{mm\nu}(\mathbf{k},0) g_{m'm'\nu'}(\mathbf{k}',0) \mathscr{G}^{\,0}_{m,\mu}(\mathbf{k},\tau_1-\tau_1)\mathscr{G}^{\,0}_{m',\mu'}(\mathbf{k}',\tau_2-\tau_2)\mathscr{D}^{0}_{\nu}(\mathbf{q}=0,\tau_1-\tau_2) = \ldots$$

ToBeUpdated, because one of the terms doesn't neccessarily vanish.[2]

[See Waste-Folder 1, topic 18 for the final expressions.]

Remark: Notice that one could also use now

$$|g_{mn\nu}(\mathbf{k}'+\mathbf{q},-\mathbf{q})| = |g_{nm\nu}(\mathbf{k}',\mathbf{q})| \tag{40.2}$$

[2] Cf. the GPAW-documentation:
For the three translational modes at $\mathbf{q} = 0$ *the matrix elements* $g_{mn\nu}(\mathbf{k},\mathbf{q}) = 0$*, as a consequence of the acoustic sum rule.*
See `https://gpaw.readthedocs.io/documentation/elph/elph.html`. See further Felicianos article:
In the case of the three translational modes at $|\mathbf{q}| = 0$ *we set the matrix elements* $g_{mn\nu}(\mathbf{k},\mathbf{q})$ *to zero, as a consequence of the acoustic sum rule (...).*

41. Experimental: The Self-Energy Correction of the EPy3W-System

41.1. Example: A Spin-Independent-Interaction between an Electron-Gas and an interacting Phonon-Gas

We consider the model from Definition 8.39 and compute the self-energy correction that originates from the coupling between phonon-phonon-interactions and electron-phonon-interactions.

Theorem 41.1 The self-energy correction due to the phonon-phonon-interactions reads

$$TBD \tag{41.1}$$

41.2. Self Energy of a Spin-Independent-Interaction between an Electron-Gas and an interacting Phonon-Gas

Proof 41.1 of Theorem 41.1

Notice first, that going over to the field-integral-description of the problem gives the action

$$\begin{aligned} S[\chi,\overline{\chi}] = &\quad S_{\text{el}}[\psi,\overline{\psi}] &+ &\quad S_{\text{ph}}[\phi,\overline{\phi}] &+ \left(S_{\text{el-ph-int}} + S_{\text{ph-ph-int}}\right)[\chi,\overline{\chi}] \\ = &\sum\!\!\!\!\!\!\int \overline{\psi}_{m\mathbf{k}\sigma}(\tau)\left(\partial_\tau + \frac{\epsilon_{m\mathbf{k}\sigma}-\mu}{\hbar}\right)\psi_{m\mathbf{k}\sigma}(\tau) &+ &\sum\!\!\!\!\!\!\int \overline{\phi}_{\mathbf{q}\nu}(\tau)\left(\partial_\tau + \omega_{\mathbf{q},\nu}\right)\phi_{\mathbf{q}\nu}(\tau) &+ \left(S_{\text{el-ph-int}} + S_{\text{ph-ph-int}}\right)[\chi,\overline{\chi}] \end{aligned} \tag{41.2}$$

with interaction-terms

$$S_{\text{el-ph-int}}[\chi,\overline{\chi}] = \sum\!\!\!\!\!\!\int \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\hbar\sqrt{N_p}}\left(\phi_{\mathbf{q}\nu}(\tau) + \overline{\phi}_{-\mathbf{q}\nu}(\tau)\right)\overline{\psi}_{\mathbf{k}+\mathbf{q}m\sigma}(\tau)\psi_{\mathbf{k}n\sigma}(\tau) \tag{41.3}$$

and

$$S_{\text{ph-ph-int}}[\chi,\overline{\chi}] = \sum\!\!\!\!\!\!\int \frac{\Phi_{\nu\nu'\nu''}}{\hbar}(\mathbf{q},\mathbf{q}',\mathbf{q}'')\left(\phi_{\mathbf{q}\nu}(\tau) + \overline{\phi}_{-\mathbf{q}\nu}(\tau)\right)\left(\phi_{\mathbf{q}'\nu'}(\tau) + \overline{\phi}_{-\mathbf{q}'\nu'}(\tau)\right)\left(\phi_{\mathbf{q}'\nu'}(\tau) + \overline{\phi}_{-\mathbf{q}'\nu'}(\tau)\right) \tag{41.4}$$

We will now determine the self-energy of the electronic system.

We will use the following trick: Inverting the Dyson-equation with the von Neumann series on the one hand, and re-expressing the imaginary-time-Green-function with help of the field integral on the other hand, gives the two equations

$$\mathscr{G}_{\alpha,\alpha'}(\mathrm{i}\omega_n) = \sum_{n=0}^{\infty} \left[\left(\mathscr{G}_0 \cdot \Sigma \right)^n (\mathrm{i}\omega_n) \cdot \mathscr{G}_0(\mathrm{i}\omega_n) \right]_{\alpha,\alpha'} \tag{41.5}$$

$$\mathscr{G}_{\alpha,\alpha'}(\mathrm{i}\omega_n) = \int_0^{\hbar\beta} \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\omega_n\tau}\, \mathscr{G}_{\alpha,\alpha'}(\tau) = \frac{-1}{\hbar} \int_0^{\hbar\beta} \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\omega_n\tau} \left\langle \psi_\alpha(\tau)\overline{\psi}_{\alpha'}(0) \right\rangle \tag{41.6}$$

The self-energy of the electronic Green-function is known to be given as the sum of all the connected irreducible diagrams of the interaction

$$\Sigma(\mathrm{i}\omega_n) = \sum_{j=0}^{\infty} \Sigma^{(j)}(\mathrm{i}\omega_n) \approx 0 + \Sigma^{(2)}(\mathrm{i}\omega_n) + 0 + \mathcal{O}(\mathrm{V}^4), \tag{41.7}$$

whereas the first contribution will turn out to vanish since the interaction can be expanded as a sum of monomials of creation- and annihilation-operators with uneven degree, and whereas we obtain for the second contribution a decomposition as

$$\Sigma^{(2)}(\mathrm{i}\omega_n) = \Sigma^{(2)}_{g\text{-}g}(\mathrm{i}\omega_n) + \Sigma^{(2)}_{g\text{-}\Phi}(\mathrm{i}\omega_n) \tag{41.8}$$

whereas the Φ-Φ-contribution vanishes due to the linked cluster theorem. In the earlier theorem, we have already determined the g-g-contribution, and due to the linearity of matrix-multiplication, we therefore only need to consider those terms in the series expansion, that contribute to the self-energy contribution that we are interested in. Inserting this in the upper-equation above and keeping the first non-vanishing terms yields the sets of equations

$$\mathscr{G}_{\alpha,\alpha'}(\mathrm{i}\omega_n) = \mathscr{G}_{\substack{0 \\ \alpha,\alpha'}}(\mathrm{i}\omega_n) + \left(\mathscr{G}_0 \cdot \Sigma^{(2)} \cdot \mathscr{G}_0 \right)_{\alpha,\alpha'} (\mathrm{i}\omega_n) \tag{41.9}$$

$$\mathscr{G}_{\alpha,\alpha'}(\mathrm{i}\omega_n) = \frac{-1}{\hbar} \int_0^{\hbar\beta} \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\omega_n\tau} \left\langle \psi_\alpha(\tau)\overline{\psi}_{\alpha'}(0) \right\rangle \tag{41.10}$$

The lower equation can be calculated explicitly with help of the Wick-theorem, linked-cluster-theorem, and the residue-theorem, and then, by comparing the first non-vanishing coefficients with the upper-equation, we can conclude what $\Sigma^{(2)}(\mathrm{i}\omega_n)$ must be.

Fact 1: The action, corresponding to this system, is given by the equation above.

Fact 2: The electronic Green-function is written in second order perturbation-theory as

$$\begin{aligned} \mathscr{G}_{\substack{b,b' \\ \mathbf{p},\mathbf{p}' \\ \sigma,\sigma'}}(\tau) &= \mathscr{G}^{(0)}_{\substack{b,b' \\ \mathbf{p},\mathbf{p}' \\ \sigma,\sigma'}}(\tau) + \mathscr{G}^{(1)}_{\substack{b,b' \\ \mathbf{p},\mathbf{p}' \\ \sigma,\sigma'}}(\tau) + \mathscr{G}^{(2)}_{\substack{b,b' \\ \mathbf{p},\mathbf{p}' \\ \sigma,\sigma'}}(\tau) + \dots \\ &= \mathscr{G}_{\substack{0 \\ b,b' \\ \mathbf{p},\mathbf{p}' \\ \sigma,\sigma'}}(\tau) + \quad 0 \quad + \mathscr{G}^{(2)}_{\substack{b,b' \\ \mathbf{p},\mathbf{p}' \\ \sigma,\sigma'}}(\tau) + \dots \end{aligned}$$

The second contribution decomposes as

$$\mathscr{G}^{(2)}_{\substack{b,b'\\ \mathbf{p},\mathbf{p}'\\ \sigma,\sigma'}}(\tau) \equiv \mathscr{G}^{(2)}_{\substack{g\text{-}g\\ b,b'\\ \mathbf{p},\mathbf{p}'\\ \sigma,\sigma'}}(\tau) + \mathscr{G}^{(2)}_{\substack{g\text{-}\Phi\\ b,b'\\ \mathbf{p},\mathbf{p}'\\ \sigma,\sigma'}}(\tau) \tag{41.11}$$

and the second contribution gives

$$\mathscr{G}^{(2)}_{\substack{g\text{-}\Phi\\ b,b'\\ \mathbf{p},\mathbf{p}'\\ \sigma,\sigma'}}(\tau) = \frac{1}{2!}\oint\!\!\!\!\!\!\sum_{\substack{\tau_1,\tau_2\in(0,\hbar\beta)\\ \mu\in\{\downarrow,\uparrow\}\\ m,n\in\{1,2,\dots\}\\ \nu,\kappa,\kappa',\kappa''\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ \mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}',\mathbf{q}''\in\mathrm{Q}}} -\frac{1}{\hbar}\frac{g_{mn\nu}(\mathbf{k},\mathbf{k}')\Phi_{\kappa,\kappa',\kappa''}(\mathbf{q},\mathbf{q}',\mathbf{q}'')}{\hbar^2\sqrt{N_p}}\left\langle \psi_{\mathbf{p}b\sigma}(\tau)\overline{\psi}_{\mathbf{p}'b'\sigma'}(0)A_\nu(\tau_1,\mathbf{k}')\overline{\psi}_{m\mu}(\tau_1,\mathbf{k}+\mathbf{k}')\psi_{n\mu}(\tau_1,\mathbf{k})A_\kappa(\tau_2,\mathbf{q})A_{\kappa'}(\tau_2,\mathbf{q}')A_{\kappa''}(\tau_2,\mathbf{q}'')\right\rangle_0 \tag{41.12}$$

whereas we introduced

$$A_\nu(\tau_1,\mathbf{k}') \equiv \phi_\nu(\tau_1,\mathbf{k}') + \overline{\phi}_\nu(\tau_1,-\mathbf{k}') \tag{41.13}$$

Now we compute the correlator as

$$\begin{aligned}
&\left\langle \psi_{\mathbf{p}b\sigma}(\tau)\overline{\psi}_{\mathbf{p}'b'\sigma'}(0)A_\nu(\tau_1,\mathbf{k}')\overline{\psi}_{m\mu}(\tau_1,\mathbf{k}+\mathbf{k}')\psi_{n\mu}(\tau_1,\mathbf{k})A_\kappa(\tau_2,\mathbf{q})A_{\kappa'}(\tau_2,\mathbf{q}')A_{\kappa''}(\tau_2,\mathbf{q}'')\right\rangle_0\\
&= \left\langle \psi_{\mathbf{p}b\sigma}(\tau)\psi_{n\mu}(\tau_1,\mathbf{k})\overline{\psi}_{\mathbf{p}'b'\sigma'}(0)\overline{\psi}_{m\mu}(\tau_1,\mathbf{k}+\mathbf{k}')\right\rangle_0 \left\langle A_\nu(\tau_1,\mathbf{k}')A_\kappa(\tau_2,\mathbf{q})A_{\kappa'}(\tau_2,\mathbf{q}')A_{\kappa''}(\tau_2,\mathbf{q}'')\right\rangle_0\\
&\equiv \left\langle \psi_{A_1}\psi_{A_2}\overline{\psi}_{B_1}\overline{\psi}_{B_2}\right\rangle_0 \langle A_1A_2A_3A_4\rangle_0\\
&\overset{\mathrm{LCT}}{=} -\left\langle \psi_{A_1}\overline{\psi}_{B_2}\right\rangle_0\left\langle \psi_{A_2}\overline{\psi}_{B_1}\right\rangle_0\Big[\langle A_1A_2\rangle_0\langle A_3A_4\rangle_0 + \langle A_1A_3\rangle_0\langle A_2A_4\rangle_0 + \langle A_1A_4\rangle_0\langle A_2A_3\rangle_0\Big]\\
&= -(-\hbar)^4\mathscr{G}_{\substack{0\\ \mathbf{p},\mathbf{k}+\mathbf{k}'\\ b,m\\ \sigma,\mu}}(\tau-\tau_1)\mathscr{G}_{\substack{0\\ \mathbf{k},\mathbf{p}'\\ n,b'\\ \mu,\sigma'}}(\tau_1-0)\Big[\mathscr{D}_{\substack{0\\ \nu,\kappa\\ \mathbf{k}',-\mathbf{q}}}(\tau_1-\tau_2)\mathscr{D}_{\substack{0\\ \kappa',\kappa''\\ \mathbf{q}',-\mathbf{q}''}}(0) + \mathscr{D}_{\substack{0\\ \nu,\kappa'\\ \mathbf{k}',-\mathbf{q}'}}(\tau_1-\tau_2)\mathscr{D}_{\substack{0\\ \kappa,\kappa''\\ \mathbf{q},-\mathbf{q}''}}(0) + \mathscr{D}_{\substack{0\\ \nu,\kappa''\\ \mathbf{k}',-\mathbf{q}''}}(\tau_1-\tau_2)\mathscr{D}_{\substack{0\\ \kappa,\kappa'\\ \mathbf{q},-\mathbf{q}'}}(0)\Big]
\end{aligned} \tag{41.14}$$

Plugging this back into Equation (41.12) yields

$$\begin{aligned}
\mathscr{G}^{(2)}_{\substack{g\text{-}\Phi\\ b,b'\\ \mathbf{p},\mathbf{p}'\\ \sigma,\sigma'}}(\tau) &= \frac{1}{2!}\oint\!\!\!\!\!\!\sum_{\substack{\tau_1,\tau_2\in(0,\hbar\beta)\\ \mu\in\{\downarrow,\uparrow\}\\ m,n\in\{1,2,\dots\}\\ \nu,\kappa,\kappa',\kappa''\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ \mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}',\mathbf{q}''\in\mathrm{Q}}} -\frac{1}{\hbar}\frac{g_{mn\nu}(\mathbf{k},\mathbf{k}')\Phi_{\kappa,\kappa',\kappa''}(\mathbf{q},\mathbf{q}',\mathbf{q}'')}{\hbar^2\sqrt{N_p}}\left\langle \psi_{\mathbf{p}b\sigma}(\tau)\overline{\psi}_{\mathbf{p}'b'\sigma'}(0)A_\nu(\tau_1,\mathbf{k}')\overline{\psi}_{m\mu}(\tau_1,\mathbf{k}+\mathbf{k}')\psi_{n\mu}(\tau_1,\mathbf{k})A_\kappa(\tau_2,\mathbf{q})A_{\kappa'}(\tau_2,\mathbf{q}')A_{\kappa''}(\tau_2,\mathbf{q}'')\right\rangle_0\\
&= \frac{1}{2!}\oint\!\!\!\!\!\!\sum_{\substack{\tau_1,\tau_2\in(0,\hbar\beta)\\ \mu\in\{\downarrow,\uparrow\}\\ m,n\in\{1,2,\dots\}\\ \nu,\kappa,\kappa',\kappa''\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ \mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}',\mathbf{q}''\in\mathrm{Q}}} -\hbar\frac{g_{mn\nu}(\mathbf{k},\mathbf{k}')\Phi_{\kappa,\kappa',\kappa''}(\mathbf{q},\mathbf{q}',\mathbf{q}'')}{\sqrt{N_p}}\mathscr{G}_{\substack{0\\ \mathbf{p},\mathbf{k}+\mathbf{k}'\\ b,m\\ \sigma,\mu}}(\tau-\tau_1)\mathscr{G}_{\substack{0\\ \mathbf{k},\mathbf{p}'\\ n,b'\\ \mu,\sigma'}}(\tau_1-0)\Big[\mathscr{D}_{\substack{0\\ \nu,\kappa\\ \mathbf{k}',-\mathbf{q}}}(\tau_1-\tau_2)\mathscr{D}_{\substack{0\\ \kappa',\kappa''\\ \mathbf{q}',-\mathbf{q}''}}(0) + \mathscr{D}_{\substack{0\\ \nu,\kappa'\\ \mathbf{k}',-\mathbf{q}'}}(\tau_1-\tau_2)\mathscr{D}_{\substack{0\\ \kappa,\kappa''\\ \mathbf{q},-\mathbf{q}''}}(0) + \mathscr{D}_{\substack{0\\ \nu,\kappa''\\ \mathbf{k}',-\mathbf{q}''}}(\tau_1-\tau_2)\mathscr{D}_{\substack{0\\ \kappa,\kappa'\\ \mathbf{q},-\mathbf{q}'}}(0)\Big]\\
&= \frac{1}{2!}\oint\!\!\!\!\!\!\sum_{\substack{\tau_1,\tau_2\in(0,\hbar\beta)\\ \mu\in\{\downarrow,\uparrow\}\\ m,n\in\{1,2,\dots\}\\ \nu,\kappa,\kappa',\kappa''\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ \mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}',\mathbf{q}''\in\mathrm{Q}}} -\hbar\frac{g_{mn\nu}(\mathbf{k},\mathbf{k}')}{\sqrt{N_p}}\mathscr{G}_{\substack{0\\ \mathbf{p},\mathbf{k}+\mathbf{k}'\\ b,m\\ \sigma,\mu}}(\tau-\tau_1)\mathscr{G}_{\substack{0\\ \mathbf{k},\mathbf{p}'\\ n,b'\\ \mu,\sigma'}}(\tau_1-0)\mathscr{D}_{\substack{0\\ \nu,\kappa\\ \mathbf{k}',-\mathbf{q}}}(\tau_1-\tau_2)\mathscr{D}_{\substack{0\\ \kappa',\kappa''\\ \mathbf{q}',-\mathbf{q}''}}(0)\Big[\Phi_{\kappa,\kappa',\kappa''}(\mathbf{q},\mathbf{q}',\mathbf{q}'') + \Phi_{\kappa',\kappa,\kappa''}(\mathbf{q}',\mathbf{q},\mathbf{q}'') + \Phi_{\kappa'',\kappa,\kappa'}(\mathbf{q}'',\mathbf{q},\mathbf{q}')\Big]
\end{aligned} \tag{41.15}$$

Now we compute the Fourier-Matsubara-transform.

Proof 41.2

We will now focus on the temporal components of the Hartree-contribution to the Green-function. For this we consider the function

$$\widetilde{\mathscr{G}}(\tau) = \iint_{[0,\hbar\beta]^2} \mathrm{d}(\tau_1,\tau_2)\underbrace{\mathscr{G}_0(\tau-\tau_1)}_{\mathrm{I}}\underbrace{\mathscr{G}_0(\tau_1-0)}_{\mathrm{II}}\underbrace{\mathscr{D}_0(\tau_1-\tau_2)}_{\mathrm{III}}\underbrace{\mathscr{D}_0(0)}_{\mathrm{IV}} \tag{41.16}$$

and this gives for the Matsubara-components

$$\begin{aligned}\widetilde{\mathscr{G}}(\mathrm{i}\omega_n) &= \int_0^{\hbar\beta} \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\omega_n\tau}\, \widetilde{\mathscr{G}}(\tau) \\ &= \iiint_{[0,\hbar\beta]^3} \mathrm{d}(\tau,\tau_1,\tau_2)\, \mathrm{e}^{\mathrm{i}\omega_n\tau} \underset{\mathrm{I}}{\mathscr{G}_0}(\tau-\tau_1) \underset{\mathrm{II}}{\mathscr{G}_0}(\tau_1-0) \underset{\mathrm{III}}{\mathscr{D}_0}(\tau_1-\tau_2) \underset{\mathrm{IV}}{\mathscr{D}_0}(0) \\ &= \dots\end{aligned}$$

now we expand the statistical functions according to Lemma 1.11 and we obtain

$$\begin{aligned}\dots &= \frac{1}{(\hbar\beta)^4} \sum_{\substack{\omega_{n_1},\omega_{n_2}\in\Omega_{-1}\\ \omega_{n_3},\omega_{n_4}\in\Omega_{+1}}} \iiint_{[0,\hbar\beta]^3} \mathrm{d}(\tau,\tau_1,\tau_2) \underset{\mathrm{I}}{\mathscr{G}_0}(\mathrm{i}\omega_{n_1}) \underset{\mathrm{II}}{\mathscr{G}_0}(\mathrm{i}\omega_{n_2}) \underset{\mathrm{III}}{\mathscr{D}_0}(\mathrm{i}\omega_{n_3}) \underset{\mathrm{IV}}{\mathscr{D}_0}(\mathrm{i}\omega_{n_4})\, \mathrm{e}^{\mathrm{i}\left(\omega_n\tau-\omega_{n_1}(\tau-\tau_1)-\omega_{n_2}\tau_1-\omega_{n_3}(\tau_1-\tau_2)\right)} \\ &= \sum_{\substack{\omega_{n_1,n_2}\in\Omega_{-1}\\ \omega_{n_3,n_4}\in\Omega_{+1}}} \underset{\mathrm{I}}{\mathscr{G}_0}(\mathrm{i}\omega_{n_1}) \underset{\mathrm{II}}{\mathscr{G}_0}(\mathrm{i}\omega_{n_2}) \underset{\mathrm{III}}{\mathscr{D}_0}(\mathrm{i}\omega_{n_3}) \underset{\mathrm{IV}}{\mathscr{D}_0}(\mathrm{i}\omega_{n_4}) \frac{1}{(\hbar\beta)^4} \iiint_{[0,\hbar\beta]^3} \mathrm{d}(\tau,\tau_1,\tau_2) \mathrm{e}^{\mathrm{i}\left(\omega_n\tau-\omega_{n_1}(\tau-\tau_1)-\omega_{n_2}\tau_1-\omega_{n_3}(\tau_1-\tau_2)\right)} \\ &= \dots\end{aligned}$$

and we find for the integral-factor

$$\begin{aligned}\iiint_{[0,\hbar\beta]^3} \mathrm{d}(\tau,\tau_1,\tau_2) \mathrm{e}^{\mathrm{i}\left(\omega_n\tau-\omega_{n_1}(\tau-\tau_1)-\omega_{n_2}\tau_1-\omega_{n_3}(\tau_1-\tau_2)\right)} &= \int_0^{\hbar\beta} \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\tau\left(\omega_n-\omega_{n_1}\right)} \int_0^{\hbar\beta} \mathrm{d}\tau_1\, \mathrm{e}^{\mathrm{i}\tau_1\left(\omega_{n_1}-\omega_{n_2}-\omega_{n_3}\right)} \int_0^{\hbar\beta} \mathrm{d}\tau_2\, \mathrm{e}^{\mathrm{i}\tau_2\omega_{n_3}} \\ &= (\hbar\beta)^3 \delta_{\omega_n,\omega_{n_1}} \delta_{\omega_{n_1},\omega_{n_2}} \delta_{\omega_{n_3},0}\end{aligned}$$

TOBECONTINUED.

Part VII.

"Experimental" (Work in Progress): The High T_C Conundrum in Superconductivity

42. Experimental: Wannierizations

42.1. Wannierizations

Cf. `https://chatgpt.com/share/6a7cf205-a79c-83eb-8b26-ad5740690599?ogimg=plain`

Definition 42.1 We introduce the *Wannier*-functions associated with a unitary transformation-matrices $U_{mn}(\mathbf{k})$ as

$$w_{n\mathbf{R}}(\mathbf{r}) = \frac{1}{N_k} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}} \sum_{m} U^{(\mathbf{k})}_{mn} \psi_{m\mathbf{k}}(\mathbf{r}).$$

Remark 42.1.1 Notice that one finds due to the translational symmetry

$$w_{n\mathbf{R}}(\mathbf{r}) = w_{n\mathbf{0}}(\mathbf{r} - \mathbf{R}) \tag{42.1}$$

So every Wannier-function in another cell is just a translated copy of the *home-cell Wannier-function*.

Notation 42.2 Each of these Wannier-functions has an associated *Wannier-center* defined through

$$\boldsymbol{\tau}_n = \langle w_{n,\mathbf{0}} \mid \mathbf{r} \mid w_{n,\mathbf{0}} \rangle \tag{42.2}$$

with

$$\left\{ \boldsymbol{\tau}_1, \boldsymbol{\tau}_2, \boldsymbol{\tau}_3, \ldots \right\} \subset \mathrm{UC} \tag{42.3}$$

Corollary 42.3 We enumerate the Wannier-functions with their band- and lattice-index as $(n, \mathbf{R})$ and obtain for the Coulomb-matrix-element in second quantization

$$U_{n_1\mathbf{R}_1, n_2\mathbf{R}_2, n_3\mathbf{R}_3, n_4\mathbf{R}_4} = \iint d\mathbf{r}\, d\mathbf{r}'\, w^*_{n_1\mathbf{R}_1}(\mathbf{r}) w^*_{n_2\mathbf{R}_2}(\mathbf{r}') \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} w_{n_3\mathbf{R}_3}(\mathbf{r}') w_{n_4\mathbf{R}_4}(\mathbf{r}).$$

such that the whole Coulomb-interaction can be written as

$$\sum_{\substack{n_1,n_2,n_3,n_4 \in \{1,2,3,\ldots\} \\ \mathbf{R}_1,\mathbf{R}_2,\mathbf{R}_3,\mathbf{R}_4 \in \mathrm{L_f}}} U_{n_1\mathbf{R}_1, n_2\mathbf{R}_2, n_3\mathbf{R}_3, n_4\mathbf{R}_4} c^\dagger_{n_1\mathbf{R}_1} c^\dagger_{n_2\mathbf{R}_2} c_{n_4\mathbf{R}_4} c_{n_3\mathbf{R}_3} \tag{42.4}$$

Proof 42.3 Follows from the second quantization-procedure.

Lemma 42.4 One finds for the Coulomb matrix element

$$U_{n_1\mathbf{R}_1,n_2\mathbf{R}_2,n_3\mathbf{R}_3,n_4\mathbf{R}_4} = U_{n_1\mathbf{0},n_2(\mathbf{R}_2-\mathbf{R}_1),n_3(\mathbf{R}_3-\mathbf{R}_1),n_4(\mathbf{R}_4-\mathbf{R}_1)}. \tag{42.5}$$

Hence, the Coulomb matrix elements depend only on the relative positions of the Wannier functions.

Proof 42.4 The Wannier functions obey the translational property

$$w_{n\mathbf{R}}(\mathbf{r}) = w_{n\mathbf{0}}(\mathbf{r}-\mathbf{R}). \tag{42.6}$$

Starting from the Coulomb matrix element

$$U_{n_1\mathbf{R}_1,n_2\mathbf{R}_2,n_3\mathbf{R}_3,n_4\mathbf{R}_4} = \iint d\mathbf{r}\, d\mathbf{r}'\, w^*_{n_1\mathbf{R}_1}(\mathbf{r}) w^*_{n_2\mathbf{R}_2}(\mathbf{r}') \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} w_{n_3\mathbf{R}_3}(\mathbf{r}') w_{n_4\mathbf{R}_4}(\mathbf{r}), \tag{42.7}$$

we perform the change of variables

$$\mathbf{r} = \tilde{\mathbf{r}} + \mathbf{R}_1, \qquad \mathbf{r}' = \tilde{\mathbf{r}}' + \mathbf{R}_1. \tag{42.8}$$

Using translational invariance, the Wannier functions transform as

$$w_{n_i\mathbf{R}_i}(\tilde{\mathbf{r}} + \mathbf{R}_1) = w_{n_i,\mathbf{R}_i-\mathbf{R}_1}(\tilde{\mathbf{r}}), \tag{42.9}$$

and analogously for the functions depending on

$\tilde{\mathbf{r}}'$. Furthermore,

$$\left|(\tilde{\mathbf{r}} + \mathbf{R}_1) - (\tilde{\mathbf{r}}' + \mathbf{R}_1)\right| = |\tilde{\mathbf{r}} - \tilde{\mathbf{r}}'|. \tag{42.10}$$

The integration measure is unchanged, $d\mathbf{r}\, d\mathbf{r}' = d\tilde{\mathbf{r}}\, d\tilde{\mathbf{r}}'$.

Consequently,

$$U_{n_1\mathbf{R}_1,n_2\mathbf{R}_2,n_3\mathbf{R}_3,n_4\mathbf{R}_4} = U_{n_1\mathbf{0},n_2(\mathbf{R}_2-\mathbf{R}_1),n_3(\mathbf{R}_3-\mathbf{R}_1),n_4(\mathbf{R}_4-\mathbf{R}_1)}, \tag{42.11}$$

which proves the assertion.

Definition 42.5

We introduce the *pair densities*

$$\rho_{1,4}(\mathbf{r}) = w^*_{n_1\mathbf{R}_1}(\mathbf{r}) w_{n_4\mathbf{R}_4}(\mathbf{r}) \tag{42.12}$$

and

$$\rho_{2,3}(\mathbf{r}') = w^*_{n_2\mathbf{R}_2}(\mathbf{r}') w_{n_3\mathbf{R}_3}(\mathbf{r}'). \tag{42.13}$$

In terms of these pair densities, the Coulomb matrix element becomes

$$U_{1,2,3,4} = \iint \mathrm{d}^3\mathbf{r}\, \mathrm{d}^3\mathbf{r}'\, \rho_{1,4}(\mathbf{r}) \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \rho_{2,3}(\mathbf{r}'). \tag{42.14}$$

Theorem 42.6 The Coulomb matrix element can be rewritten in reciprocal space as

$$U_{1,2,3,4} = e^2 \int \frac{\mathrm{d}^3\mathbf{q}}{(2\pi)^3} \frac{4\pi}{q^2} \rho_{1,4}(-\mathbf{q}) \rho_{2,3}(\mathbf{q}), \tag{42.15}$$

where the Fourier transform of a pair density is defined by

$$\rho_{i,j}(\mathbf{q}) = \int \mathrm{d}^3\mathbf{r}\, e^{-i\mathbf{q}\cdot\mathbf{r}} \rho_{i,j}(\mathbf{r}). \tag{42.16}$$

Proof 42.6 We begin with the Fourier representation of the Coulomb kernel,

$$\frac{1}{|\mathbf{r} - \mathbf{r}'|} = \int \frac{\mathrm{d}^3\mathbf{q}}{(2\pi)^3} \frac{4\pi}{q^2} e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}. \tag{42.17}$$

Inserting this expression into the Coulomb matrix element gives

$$U_{1,2,3,4} = e^2 \iint \mathrm{d}^3\mathbf{r}\, \mathrm{d}^3\mathbf{r}'\, \rho_{1,4}(\mathbf{r}) \left[\int \frac{\mathrm{d}^3\mathbf{q}}{(2\pi)^3} \frac{4\pi}{q^2} e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \right] \rho_{2,3}(\mathbf{r}'). \tag{42.18}$$

Using

$$e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} = e^{i\mathbf{q}\cdot\mathbf{r}} e^{-i\mathbf{q}\cdot\mathbf{r}'}, \tag{42.19}$$

the integrations over $\mathbf{r}$ and $\mathbf{r}'$ separate, such that

$$U_{1,2,3,4} = e^2 \int \frac{\mathrm{d}^3\mathbf{q}}{(2\pi)^3} \frac{4\pi}{q^2} \left[\int \mathrm{d}^3\mathbf{r}\, \rho_{1,4}(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} \right] \left[\int \mathrm{d}^3\mathbf{r}'\, \rho_{2,3}(\mathbf{r}') e^{-i\mathbf{q}\cdot\mathbf{r}'} \right]. \tag{42.20}$$

By the definition of the Fourier-transformed pair densities,

$$\int \mathrm{d}^3\mathbf{r}\, \rho_{1,4}(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} = \rho_{1,4}(-\mathbf{q}), \tag{42.21}$$

and

$$\int \mathrm{d}^3\mathbf{r}'\, \rho_{2,3}(\mathbf{r}') e^{-i\mathbf{q}\cdot\mathbf{r}'} = \rho_{2,3}(\mathbf{q}). \tag{42.22}$$

Hence,

$$\boxed{U_{1,2,3,4} = e^2 \int \frac{\mathrm{d}^3\mathbf{q}}{(2\pi)^3} \frac{4\pi}{q^2} \rho_{1,4}(-\mathbf{q}) \rho_{2,3}(\mathbf{q})}. \tag{42.23}$$

43. Experimental: Electron-Phonon-Physics in the Wannier-Representation

Cf. https://chatgpt.com/share/6abdfeb7-f4e0-83eb-9acc-19cdfa0f132b?ogimg=plain

$$\mathcal{H} = \sum_{\sigma,\mathbf{R}\mathbf{R}',ij} t_{i\mathbf{R}j\mathbf{R}'}\, a^{\sigma\dagger}_{i\mathbf{R}} a^{\sigma}_{j\mathbf{R}'} + \frac{1}{2} \sum_{\sigma\rho,\mathbf{R}\mathbf{R}',ij} \left\{ U_{i\mathbf{R}j\mathbf{R}'}\, \hat{n}^{\sigma}_{i\mathbf{R}} \hat{n}^{\rho}_{j\mathbf{R}'} + J_{i\mathbf{R}j\mathbf{R}'} \left(a^{\sigma\dagger}_{i\mathbf{R}} a^{\rho\dagger}_{j\mathbf{R}'} a^{\rho}_{i\mathbf{R}} a^{\sigma}_{j\mathbf{R}'} + a^{\sigma\dagger}_{i\mathbf{R}} a^{\rho\dagger}_{i\mathbf{R}} a^{\rho}_{j\mathbf{R}'} a^{\sigma}_{j\mathbf{R}'} \right) \right\} \tag{43.1}$$

$$|\phi_{i\mathbf{k}}\rangle = \sum_{\alpha} U^{\mathbf{k}}_{\alpha i} \, |\psi_{\alpha\mathbf{k}}\rangle \tag{43.2}$$

$$U^{\mathrm{KS}}_{\alpha\beta\gamma\delta}(\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4) = \sum_{ijkl} U^{\mathbf{k}_1 *}_{\alpha i}\, U^{\mathbf{k}_2 *}_{\beta j}\, U_{ijkl}\, U^{\mathbf{k}_3}_{\gamma k}\, U^{\mathbf{k}_4}_{\delta l} \tag{43.3}$$

$$U^{\mathbf{k}}_{\alpha i} = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \langle \psi_{\alpha\mathbf{k}} | \phi_{i\mathbf{R}} \rangle \tag{43.4}$$

$$U^{\mathbf{R}}_{\alpha i} = \frac{1}{N_k} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}}\, U^{\mathbf{k}}_{\alpha i} \tag{43.5}$$

$$U^{\mathbf{k}}_{\alpha i} = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}}\, U^{\mathbf{R}}_{\alpha i} \tag{43.6}$$

$$H_{\text{int}} = \frac{1}{2} \sum_{ijkl} V_{ijkl}\, c^{\dagger}_{i\alpha} c^{\dagger}_{j\beta} c_{l\beta} c_{k\alpha} \tag{43.7}$$

$$\delta_{\alpha\delta}\delta_{\gamma\beta} = \tfrac{1}{2}\left(\delta_{\alpha\beta}\delta_{\gamma\delta} + \boldsymbol{\sigma}_{\alpha\beta}\cdot\boldsymbol{\sigma}_{\gamma\delta}\right) \tag{43.8}$$

$$H_{\text{int}} = \sum_{ijkl}\left[\tfrac{1}{2}V_{ijkl}\,\rho_{ik}\rho_{jl} \;-\; V_{ijkl}\left(\mathbf{S}_{il}\cdot\mathbf{S}_{jk} + \tfrac{1}{4}\rho_{il}\rho_{jk}\right)\right] \tag{43.9}$$

$$\rho_{ij} = c^{\dagger}_{i\alpha}c_{j\alpha}, \qquad \mathbf{S}_{ij} = \tfrac{1}{2}\, c^{\dagger}_{i\alpha}\boldsymbol{\sigma}_{\alpha\beta}c_{j\beta} \tag{43.10}$$

$$H_{\text{spin}} = -\sum_{a,b}\mathbf{S}_a\cdot M_{ab}\,\mathbf{S}_b, \qquad M_{(il),(jk)} = V_{ijkl} \tag{43.11}$$

$$e^{\int d\tau\, \mathbf{S}_a M_{ab}\mathbf{S}_b} = \int \mathscr{D}\boldsymbol{\phi}\, \exp\left[-\int d\tau\left(\tfrac{1}{4}\,\boldsymbol{\phi}_a(M^{-1})_{ab}\boldsymbol{\phi}_b - \boldsymbol{\phi}_a\cdot\mathbf{S}_a\right)\right] \tag{43.12}$$

$$\boldsymbol{\phi}_a\cdot\mathbf{S}_a = \tfrac{1}{2}\sum_{il}\boldsymbol{\phi}_{il}\cdot c^{\dagger}_{i\alpha}\boldsymbol{\sigma}_{\alpha\beta}c_{l\beta} \tag{43.13}$$

$$S_{\text{eff}}[\boldsymbol{\phi}] = \int d\tau\, \tfrac{1}{4}\,\boldsymbol{\phi}_a(M^{-1})_{ab}\boldsymbol{\phi}_b \;-\; \operatorname{Tr}\ln\left(-G_0^{-1} + \tfrac{1}{2}\,\boldsymbol{\phi}\cdot\boldsymbol{\sigma}\right) \tag{43.14}$$

44. Experimental: My Road to Reality - A Potential Solution for a Parameter-Free Superconductivity Prediction Pipeline

We orchestrate[1] the entire workflow with `https://kalhoefer.net/`

44.1. The Software Side of Life

We solve the problem by following the following steps (with more[2] steps in between to guarantee the executibility of the individual steps):

1. pw.x : We solve the Schrödinger-Bloch-Kohn-Sham-Equation for a single, spin-degenerate electron in a solid[3] (periodic potential) using Quantum Espresso.
2. ph.x : We use the obtained charge-density to compute via DFPT the phonon-spectrum.
3. ?.x : We compute the electron-phonon coupling-constants $g_{mn\nu}(\mathbf{k}, \mathbf{q})$ with quantum espresso along a k-path for a fixed $\mathbf{q}$-vector.
4. phono3py : We compute the phonon-phonon-coupling constants $\Phi_{\nu\nu'\nu''}(\mathbf{q}, \mathbf{q}', \mathbf{q}'')$ indirectly, by storing their real-space counter-parts on disk.
5. pw.x & wannier90.x : We compute the wavefunctions and the Wannier-functions on a given grid.
6. RESPACK : We compute the screened Coulomb-interaction matrix-elements (in real space).
7. epw.x : We compute the electron-phonon coupling-constants $g_{mn\nu}(\mathbf{k}, \mathbf{q})$ in *real space* and also their Debye-Waller counterparts $g^{\mathrm{DW}}_{mn\nu}(\mathbf{k}, \mathbf{q})$, using maximally localised Wannier-functions
8. grit.x : We solve generalized Eliashberg-equations from the field integral formalism that contains all the different interactions in their diagrammatic representation.

In particular: Matrix elements such as $V_{\mathrm{eff}}(k_1, k_2, k_3, k_4)$ can be computed on arbitrarily fine grids by Fourier-transforming their underlying real-space counterparts. The grid-size can be chosen at the very end of the calculation, which makes convergence-tracking very simple!

[1] Note: At the moment (2026-10) we are migrating the workflow from python-scripts to the online-platform for easier usage via the GUI.

[2] For example, we need the PDOS and the band-structure in order to make reasonable guesses about wannierization-parameters.

[3] Notice that we can tackle doped materials with the virtual crystal approximation.

44.2. Preparations: Phononic Partition-Function Expansion

We will evaluate the individual contributions in the expansion

$$Z_{\text{ph}}[j_{\text{ph}}=0,\bar{j}_{\text{ph}}=0] \approx Z_{\text{ph}}^{g^0,g^{\text{DW}^0},\Phi^0}\left(1 \quad + \quad \frac{Z_{\text{ph}}^{g^0,g^{\text{DW}^1},\Phi^0} \quad + \quad Z_{\text{ph}}^{g^2,g^{\text{DW}^0},\Phi^0} \quad + \quad Z_{\text{ph}}^{g^1,g^{\text{DW}^0},\Phi^1}}{Z_{\text{ph}}^{g^0,g^{\text{DW}^0},\Phi^0}}\right)_{[j_{\text{ph}}=0,\bar{j}_{\text{ph}}=0]} [\psi,\overline{\psi}] \tag{44.1}$$

44.2.1. The Functional Field Integral Description

Fact 44.1 Going over to the field-integral-description of the problem gives the action

$$S_{\text{ph, tot}}[\chi,\overline{\chi}] = \left(S_{\text{ph}} + S_{\text{ph-ph-int}}\right)[\phi,\overline{\phi}] + \left(S_{\text{el-ph-int}} + S_{\text{el-ph-int}}^{\text{DW}}\right)[\chi,\overline{\chi}] \tag{44.2}$$

with

- $S_{\text{ph}}[\phi,\overline{\phi}] = \sum\!\!\!\!\!\!\int\limits_{\substack{\mathbf{q}\in\text{Q}\\ \tau\in(0,\hbar\beta)\\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} \overline{\phi}_\nu(\tau,\mathbf{q})\left(\partial_\tau + \omega_\nu(\mathbf{q})\right)\phi_\nu(\tau,\mathbf{q})$
- $S_{\text{el-ph-int}}[\chi,\overline{\chi}] = \sum\!\!\!\!\!\!\int\limits_{\substack{\mathbf{k},\mathbf{q}\in\text{Q}\\ \tau\in(0,\hbar\beta)\\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}\\ m,n\in\{1,2,\ldots,\infty\}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\hbar\sqrt{N_p}}\left(\phi_\nu(\tau,\mathbf{q}) + \overline{\phi}_\nu(\tau,-\mathbf{q})\right)\overline{\psi}_{m\sigma}(\tau,\mathbf{k}+\mathbf{q})\psi_{n\sigma}(\tau,\mathbf{k})$
- $S_{\text{el-ph-int}}^{\text{DW}}[\chi,\overline{\chi}] = \sum\!\!\!\!\!\!\int\limits_{\substack{\mathbf{k},\mathbf{q},\mathbf{q}'\in\text{Q}\\ \tau\in(0,\hbar\beta)\\ \nu,\nu'\in\{1,2,\ldots,rd_{\mathbf{x}}\}\\ m,n\in\{1,2,\ldots,\infty\}}} \frac{g_{mn\nu\nu'}^{\text{DW}}(\mathbf{k},\mathbf{q},\mathbf{q}')}{\hbar N_p}\left(\phi_\nu(\tau,\mathbf{q}) + \overline{\phi}_\nu(\tau,-\mathbf{q})\right)\left(\phi_{\nu'}(\tau,\mathbf{q}') + \overline{\phi}_{\nu'}(\tau,-\mathbf{q}')\right)\overline{\psi}_{m\sigma}(\tau,\mathbf{k}+\mathbf{q}+\mathbf{q}')\psi_{n\sigma}(\tau,\mathbf{k})$
- $S_{\text{ph-ph-int}}[\phi,\overline{\phi}] = \sum\!\!\!\!\!\!\int\limits_{\substack{\mathbf{q},\mathbf{q}',\mathbf{q}''\in\text{Q}\\ \tau\in(0,\hbar\beta)\\ \nu,\nu',\nu''\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} \frac{\phi_{\nu\nu'\nu''}(\mathbf{q},\mathbf{q}',\mathbf{q}'')}{\hbar\sqrt{N_p}}\left(\phi_\nu(\tau,\mathbf{q}) + \overline{\phi}_\nu(\tau,-\mathbf{q})\right)\left(\phi_{\nu'}(\tau,\mathbf{q}') + \overline{\phi}_{\nu'}(\tau,-\mathbf{q}')\right)\left(\phi_{\nu''}(\tau,\mathbf{q}'') + \overline{\phi}_{\nu''}(\tau,-\mathbf{q}'')\right)$

We find the value of the individual terms in Equation (44.1) by considering the appropriate terms in

$$\frac{1}{Z_{\text{ph}}^{g^0,g^{\text{DW}^0},\Phi^0}}\int \mathscr{D}(\overline{\phi},\phi)\exp -S_{\text{ph, tot}}[\chi,\overline{\chi}] \tag{44.3}$$

44.2.2. The Debye-Waller-Contribution

We focus on the term

$$\left(\frac{Z_{\text{ph}}^{g^0,g^{\text{DW}^1},\Phi^0}}{Z_{\text{ph}}^{g^0,g^{\text{DW}^0},\Phi^0}}\right)[\psi,\overline{\psi}] \tag{44.4}$$

by writing down its explicit representation. This yields therefore

$$\begin{aligned}\left(\frac{Z_{\text{ph}}^{g^0,g^{\text{DW}^1},\Phi^0}}{Z_{\text{ph}}^{g^0,g^{\text{DW}^0},\Phi^0}}\right)[\psi,\overline{\psi}] &= -\oint\!\!\!\!\!\!\sum_{\substack{\mathbf{k},\mathbf{q},\mathbf{q}'\in\mathrm{Q}\\ \tau\in(0,\hbar\beta)\\ \nu,\nu'\in\{1,2,\ldots,rd_{\mathbf{x}}\}\\ m,n\in\{1,2,\ldots,\infty\}}} \frac{g^{\text{DW}}_{mn\nu\nu'}(\mathbf{k},\mathbf{q},\mathbf{q}')}{\hbar N_p}\left\langle\left(\phi_\nu(\tau,\mathbf{q})+\overline{\phi}_\nu(\tau,-\mathbf{q})\right)\left(\phi_{\nu'}(\tau,\mathbf{q}')+\overline{\phi}_{\nu'}(\tau,-\mathbf{q}')\right)\right\rangle_0 \overline{\psi}_{m\sigma}(\tau,\mathbf{k}+\mathbf{q}+\mathbf{q}')\psi_{n\sigma}(\tau,\mathbf{k})\\ &= \oint\!\!\!\!\!\!\sum_{\substack{\mathbf{k},\mathbf{q},\mathbf{q}'\in\mathrm{Q}\\ \tau\in(0,\hbar\beta)\\ \nu,\nu'\in\{1,2,\ldots,rd_{\mathbf{x}}\}\\ m,n\in\{1,2,\ldots,\infty\}}} \frac{g^{\text{DW}}_{mn\nu\nu'}(\mathbf{k},\mathbf{q},\mathbf{q}')}{N_p}\mathscr{D}_{\substack{0\\ \nu,\nu'\\ \mathbf{q},-\mathbf{q}'}}(\tau_\bullet=0)\overline{\psi}_{m\sigma}(\tau,\mathbf{k}+\mathbf{q}+\mathbf{q}')\psi_{n\sigma}(\tau,\mathbf{k})\\ &= \oint\!\!\!\!\!\!\sum_{\substack{\mathrm{i}\omega\in\mathrm{i}\Omega_{-1}\\ \mathbf{k},\mathbf{q},\mathbf{q}'\in\mathrm{Q}\\ \nu,\nu'\in\{1,2,\ldots,rd_{\mathbf{x}}\}\\ m,n\in\{1,2,\ldots,\infty\}}} \frac{g^{\text{DW}}_{mn\nu\nu'}(\mathbf{k},\mathbf{q},\mathbf{q}')}{N_p}\mathscr{D}_{\substack{0\\ \nu,\nu'\\ \mathbf{q},-\mathbf{q}'}}(\tau_\bullet=0)\overline{\psi}_{m\sigma}(\mathrm{i}\omega,\mathbf{k}+\mathbf{q}+\mathbf{q}')\psi_{n\sigma}(\mathrm{i}\omega,\mathbf{k})=\ldots\end{aligned} \tag{44.5}$$

notice that resolving the Kronecker-deltas yields

$$\left(\frac{Z_{\text{ph}}^{g^0,g^{\text{DW}^1},\Phi^0}}{Z_{\text{ph}}^{g^0,g^{\text{DW}^0},\Phi^0}}\right)[\psi,\overline{\psi}] = \ldots = \oint\!\!\!\!\!\!\sum_{\substack{\mathrm{i}\omega\in\mathrm{i}\Omega_{-1}\\ \mathbf{k},\mathbf{q}\in\mathrm{Q}\\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}\\ m,n\in\{1,2,\ldots,\infty\}}} \frac{g^{\text{DW}}_{mn\nu\nu}(\mathbf{k},\mathbf{q},-\mathbf{q})}{N_p}\mathscr{D}_{\substack{0\\ \nu,\mathbf{q}}}(\tau_\bullet=0)\overline{\psi}_{m\sigma}(\mathrm{i}\omega,\mathbf{k})\psi_{n\sigma}(\mathrm{i}\omega,\mathbf{k}) \tag{44.6}$$

44.2.3. The electron-phonon^3-Contribution

We focus on the term

$$\left(\frac{Z_{\text{ph}}^{g^1,g^{\text{DW}^0},\Phi^1}}{Z_{\text{ph}}^{g^0,g^{\text{DW}^0},\Phi^0}}\right)[\psi,\overline{\psi}] \tag{44.7}$$

by writing down its explicit representation. This yields therefore, after introducing $\mathcal{A}_\nu(\tau,\mathbf{q}) \equiv \phi_\nu(\tau,\mathbf{q})+\overline{\phi}_\nu(\tau,-\mathbf{q})$, the equation

$$\begin{aligned}\left(\frac{Z_{\text{ph}}^{g^1,g^{\text{DW}^0},\Phi^1}}{Z_{\text{ph}}^{g^0,g^{\text{DW}^0},\Phi^0}}\right)[\psi,\overline{\psi}] &= \left\langle \oint\!\!\!\!\!\!\sum_{\substack{\mathbf{k},\mathbf{q}\in\mathrm{Q}\\ \tau\in(0,\hbar\beta)\\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}\\ m,n\in\{1,2,\ldots,\infty\}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\hbar\sqrt{N_p}}\mathcal{A}_\nu(\tau,\mathbf{q})\overline{\psi}_{m\sigma}(\tau,\mathbf{k}+\mathbf{q})\psi_{n\sigma}(\tau,\mathbf{k}) \oint\!\!\!\!\!\!\sum_{\substack{\mathbf{q}',\mathbf{q}'',\mathbf{q}'''\in\mathrm{Q}\\ \tau'\in(0,\hbar\beta)\\ \nu',\nu'',\nu'''\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} \frac{\phi_{\nu'\nu''\nu'''}(\mathbf{q}',\mathbf{q}'',\mathbf{q}''')}{\hbar\sqrt{N_p}}\mathcal{A}_{\nu'}(\tau',\mathbf{q}')\mathcal{A}_{\nu''}(\tau',\mathbf{q}'')\mathcal{A}_{\nu'''}(\tau',\mathbf{q}''')\right\rangle_0\\ &= \oint\!\!\!\!\!\!\sum_{\substack{\mathbf{k},\mathbf{q},\mathbf{q}',\mathbf{q}'',\mathbf{q}'''\in\mathrm{Q}\\ \tau,\tau'\in(0,\hbar\beta)\\ \nu,\nu',\nu'',\nu'''\in\{1,2,\ldots,rd_{\mathbf{x}}\}\\ m,n\in\{1,2,\ldots,\infty\}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\hbar\sqrt{N_p}}\frac{\phi_{\nu'\nu''\nu'''}(\mathbf{q}',\mathbf{q}'',\mathbf{q}''')}{\hbar\sqrt{N_p}}\left\langle\mathcal{A}_\nu(\tau,\mathbf{q})\mathcal{A}_{\nu'}(\tau',\mathbf{q}')\mathcal{A}_{\nu''}(\tau',\mathbf{q}'')\mathcal{A}_{\nu'''}(\tau',\mathbf{q}''')\right\rangle_0 \overline{\psi}_{m\sigma}(\tau,\mathbf{k}+\mathbf{q})\psi_{n\sigma}(\tau,\mathbf{k})=\ldots\end{aligned} \tag{44.8}$$

Now we need to evaluate these expectation-values by applying the Wick-theorem:

$$\begin{aligned}\left\langle\mathcal{A}_\nu(\tau,\mathbf{q})\mathcal{A}_{\nu'}(\tau',\mathbf{q}')\mathcal{A}_{\nu''}(\tau',\mathbf{q}'')\mathcal{A}_{\nu'''}(\tau',\mathbf{q}''')\right\rangle_0 &\equiv \langle\mathcal{A}_1\mathcal{A}_2\mathcal{A}_3\mathcal{A}_4\rangle_0\\ &= \langle\mathcal{A}_1\mathcal{A}_2\rangle_0\langle\mathcal{A}_3\mathcal{A}_4\rangle_0+\langle\mathcal{A}_1\mathcal{A}_3\rangle_0\langle\mathcal{A}_2\mathcal{A}_4\rangle_0+\langle\mathcal{A}_1\mathcal{A}_4\rangle_0\langle\mathcal{A}_2\mathcal{A}_3\rangle_0\end{aligned} \tag{44.9}$$

The clue is now to observe that because of Equation (8.36) we only need to evaluate one of these terms, as the other ones give identical contributions... We therefore consider

$$\begin{aligned}\langle\mathcal{A}_1\mathcal{A}_2\rangle_0\langle\mathcal{A}_3\mathcal{A}_4\rangle_0 &\equiv \left\langle\mathcal{A}_\nu(\tau,\mathbf{q})\mathcal{A}_{\nu'}(\tau',\mathbf{q}')\right\rangle_0\left\langle\mathcal{A}_{\nu''}(\tau',\mathbf{q}'')\mathcal{A}_{\nu'''}(\tau',\mathbf{q}''')\right\rangle_0\\ &\equiv (-\hbar)^2\mathscr{D}_{\substack{0\\ \nu,\nu'\\ \mathbf{q},-\mathbf{q}'}}(\tau-\tau')\mathscr{D}_{\substack{0\\ \nu',\nu''\\ \mathbf{q}',-\mathbf{q}''}}(0)\\ &\equiv \hbar^2\delta_{\nu,\nu'}\delta_{\nu'',\nu'''}\delta_{\mathbf{q},-\mathbf{q}'}\delta_{\mathbf{q}'',-\mathbf{q}'''}\mathscr{D}_{\substack{0\\ \nu,\mathbf{q}}}(\tau-\tau')\mathscr{D}_{\substack{0\\ \nu''\mathbf{q}''}}(0)\end{aligned} \tag{44.10}$$

$$\begin{aligned}\left(\frac{Z_{\text{ph}}^{g^1,g^{\text{DW}^0},\Phi^1}}{Z_{\text{ph}}^{g^0,g^{\text{DW}^0},\Phi^0}}\right)[\psi,\overline{\psi}] &= \dots \\ &= \oint_{\substack{\mathbf{k},\mathbf{q},\mathbf{q}',\mathbf{q}'',\mathbf{q}'''\in \mathrm{Q} \\ \tau,\tau'\in(0,\hbar\beta) \\ \nu,\nu',\nu'',\nu'''\in\{1,2,\dots,rd_{\mathbf{x}}\} \\ m,n\in\{1,2,\dots,\infty\}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\hbar\sqrt{N_p}}\frac{\phi_{\nu'\nu''\nu'''}(\mathbf{q}',\mathbf{q}'',\mathbf{q}''')}{\hbar\sqrt{N_p}}\hbar^2\delta_{\nu,\nu'}\delta_{\nu'',\nu'''}\delta_{\mathbf{q},-\mathbf{q}'}\delta_{\mathbf{q}'',-\mathbf{q}'''}\mathscr{D}^{\ 0}_{\nu,\mathbf{q}}(\tau-\tau')\mathscr{D}^{\ 0}_{\nu''\mathbf{q}''}(0)\overline{\psi}_{m\sigma}(\tau,\mathbf{k}+\mathbf{q})\psi_{n\sigma}(\tau,\mathbf{k}) \\ &= \oint_{\substack{\mathbf{k},\mathbf{q},\mathbf{q}''\in \mathrm{Q} \\ \tau,\tau'\in(0,\hbar\beta) \\ \nu,\nu''\in\{1,2,\dots,rd_{\mathbf{x}}\} \\ m,n\in\{1,2,\dots,\infty\}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\sqrt{N_p}}\frac{\phi_{\nu\nu''\nu''}(-\mathbf{q},\mathbf{q}'',-\mathbf{q}'')}{\sqrt{N_p}}\mathscr{D}^{\ 0}_{\nu,\mathbf{q}}(\tau-\tau')\mathscr{D}^{\ 0}_{\nu''\mathbf{q}''}(\tau_\bullet=0)\overline{\psi}_{m\sigma}(\tau,\mathbf{k}+\mathbf{q})\psi_{n\sigma}(\tau,\mathbf{k})\end{aligned} \tag{44.11}$$

Lemma 44.2 Switching to Matsubara-space yields

$$\left(\frac{Z_{\text{ph}}^{g^1,g^{\text{DW}^0},\Phi^1}}{Z_{\text{ph}}^{g^0,g^{\text{DW}^0},\Phi^0}}\right)[\psi,\overline{\psi}] = \dots = \oint_{\substack{\mathrm{i}\omega_m\in\mathrm{i}\Omega_{-1} \\ \mathbf{k},\mathbf{q},\mathbf{q}''\in\mathrm{Q} \\ \nu,\nu''\in\{1,2,\dots,rd_{\mathbf{x}}\} \\ m,n\in\{1,2,\dots,\infty\}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\sqrt{N_p}}\frac{\phi_{\nu\nu''\nu''}(-\mathbf{q},\mathbf{q}'',-\mathbf{q}'')}{\sqrt{N_p}}\mathscr{D}^{\ 0}_{\nu,\mathbf{q}}(\mathrm{i}\omega_\bullet=0)\mathscr{D}^{\ 0}_{\nu''\mathbf{q}''}(\tau_\bullet=0)\overline{\psi}_{m\sigma}(\mathrm{i}\omega_m,\mathbf{k}+\mathbf{q})\psi_{n\sigma}(\mathrm{i}\omega_m,\mathbf{k}) \tag{44.12}$$

Proof 44.2 We compute straightforwardly

$$\begin{aligned}\int \mathrm{d}(\tau,\tau')\mathscr{D}_{0,\nu,\mathbf{q}}(\tau-\tau')\overline{\psi}_{m,\sigma,\mathbf{k}+\mathbf{q}}(\tau)\psi_{n,\sigma,\mathbf{k}}(\tau) &= \frac{1}{(\hbar\beta)^2}\sum_{\substack{\omega_n\in\Omega_{+1} \\ \omega_m,\omega_{m'}\in\Omega_{-1}}}\mathscr{D}_{0,\nu,\mathbf{q}}(\mathrm{i}\omega_n)\int \mathrm{d}(\tau,\tau')\mathrm{e}^{-\mathrm{i}\omega_n(\tau-\tau')}\overline{\psi}_{m,\sigma,\mathbf{k}+\mathbf{q}}(\mathrm{i}\omega_m)\psi_{n,\sigma,\mathbf{k}}(\mathrm{i}\omega'_m)\mathrm{e}^{\mathrm{i}\omega_m\tau-\mathrm{i}\omega'_m\tau} \\ &= \sum_{\substack{\omega_n\in\Omega_{+1} \\ \omega_m,\omega_{m'}\in\Omega_{-1}}}\mathscr{D}_{0,\nu,\mathbf{q}}(\mathrm{i}\omega_n)\overline{\psi}_{m,\sigma,\mathbf{k}+\mathbf{q}}(\mathrm{i}\omega_m)\psi_{n,\sigma,\mathbf{k}}(\mathrm{i}\omega_{m'})\frac{1}{\hbar\beta}\int \mathrm{d}\tau\mathrm{e}^{\mathrm{i}\tau\left(-\omega_n+\omega_m-\omega_{m'}\right)}\frac{1}{\hbar\beta}\int \mathrm{d}\tau'\mathrm{e}^{\mathrm{i}\tau'\omega_n} \\ &= \sum_{\substack{\omega_n\in\Omega_{+1} \\ \omega_m,\omega_{m'}\in\Omega_{-1}}}\mathscr{D}_{0,\nu,\mathbf{q}}(\mathrm{i}\omega_n)\overline{\psi}_{m,\sigma,\mathbf{k}+\mathbf{q}}(\mathrm{i}\omega_m)\psi_{n,\sigma,\mathbf{k}}(\mathrm{i}\omega_{m'})\delta_{\omega_m,\omega_{m'}}\delta_{\omega_n,0} \\ &= \sum_{\substack{\omega_n\in\Omega_{+1} \\ \omega_m,\omega_{m'}\in\Omega_{-1}}}\mathscr{D}_{0,\nu,\mathbf{q}}(\mathrm{i}\omega_\bullet=0)\overline{\psi}_{m,\sigma,\mathbf{k}+\mathbf{q}}(\mathrm{i}\omega_m)\psi_{n,\sigma,\mathbf{k}}(\mathrm{i}\omega_m)\end{aligned} \tag{44.13}$$

44.3. The Mathematical Side of Life

We consider the model from Definition 8.43. Then we follow the following steps.

1. We write down the underlying field theory (and hence partition-function Z) of the problem and equip it with external sources.
2. We integrate out the phononic degrees of freedom by computing their contribution

$$\begin{aligned}Z[j,\bar{j}] &= \int \mathscr{D}(\overline{\psi},\psi)\mathrm{e}^{-\left(S_{0,\text{el}}+S_{\text{Coulomb}}\right)[\psi,\overline{\psi}]+j_{\text{el}}^\dagger\psi+\psi^\dagger j_{\text{el}}}\int \mathscr{D}(\overline{\phi},\phi)\mathrm{e}^{-\left[\left(S_{0,\text{ph}}+S_{\text{ph-ph-int}}\right)[\phi,\overline{\phi}]+S^{++}_{\text{el-ph-int}}[\chi,\overline{\chi}]\right]+j_{\text{ph}}^\dagger\phi+\phi^\dagger j_{\text{ph}}} \\ &= \int \mathscr{D}(\overline{\psi},\psi)\mathrm{e}^{-\left(S_{0,\text{el}}+S_{\text{Coulomb}}\right)[\psi,\overline{\psi}]+j_{\text{el}}^\dagger\psi+\psi^\dagger j_{\text{el}}}Z_{\text{ph}}[j_{\text{ph}},\bar{j}_{\text{ph}}] \\ &= \dots\end{aligned} \tag{44.14}$$

3. We acknowledge, that by straight-forward computation, we will obtain a series-expansion as

$$Z_{\mathrm{ph}}[j_{\mathrm{ph}}, \bar{j}_{\mathrm{ph}}] = \left(\sum_{n_1, n_2, n_3 \in \mathbb{N}} Z^{g^{n_1}, g^{\mathrm{DW}^{n_2}} \Phi^{n_3}}_{\substack{\mathrm{ph} \\ [j_{\mathrm{ph}}, \bar{j}_{\mathrm{ph}}]}} \right) [\psi, \overline{\psi}] \tag{44.15}$$

with

$$Z^{g^{n_1}, g^{\mathrm{DW}^{n_2}} \Phi^{n_3}}_{\mathrm{ph}} = \mathcal{O}\left(g^{n_1}, g^{\mathrm{DW}^{n_2}} \Phi^{n_3} \right) \tag{44.16}$$

and

$$\log Z^{g^0, g^{\mathrm{DW}^0}, \Phi^0}_{\substack{\mathrm{ph} \\ [j_{\mathrm{ph}} = \bar{j}_{\mathrm{ph}} = 0]}} [\psi = \overline{\psi} = 0] \tag{44.17}$$

fulfilling Lemma 24.12.

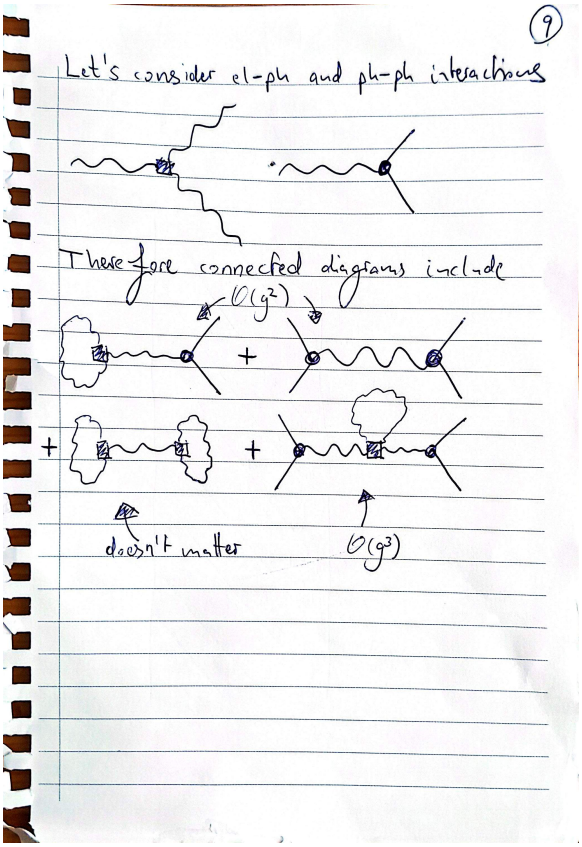


Figure 44.1.: Identifying the lowest order diagrams with notation that is inconsistent with the text above (TBFixed).

4. We keep the lowest order contributions that matter for the electronic part of the system, i.e. we approximate

$$\begin{aligned} Z_{\text{ph}}[j_{\text{ph}}=0,\bar{j}_{\text{ph}}=0] &\approx \left(Z_{\text{ph}}^{g^0,g^{\text{DW}^0},\Phi^0} + Z_{\text{ph}}^{g^0,g^{\text{DW}^1},\Phi^0} + Z_{\text{ph}}^{g^2,g^{\text{DW}^0},\Phi^0} + Z_{\text{ph}}^{g^1,g^{\text{DW}^0},\Phi^1} \right)_{[j_{\text{ph}}=0,\bar{j}_{\text{ph}}=0]} [\psi,\overline{\psi}] \\ &\approx Z_{\text{ph}}^{g^0,g^{\text{DW}^0},\Phi^0} \left(1 + \frac{Z_{\text{ph}}^{g^0,g^{\text{DW}^1},\Phi^0} + Z_{\text{ph}}^{g^2,g^{\text{DW}^0},\Phi^0} + Z_{\text{ph}}^{g^1,g^{\text{DW}^0},\Phi^1}}{Z_{\text{ph}}^{g^0,g^{\text{DW}^0},\Phi^0}} \right)_{[j_{\text{ph}}=0,\bar{j}_{\text{ph}}=0]} [\psi,\overline{\psi}] \end{aligned} \tag{44.18}$$

5. Using now $\log(1+x) = x + \mathcal{O}(x^2)$ we obtain hence

$$\begin{aligned} \log Z_{\substack{\text{ph} \\ [j_{\text{ph}}=0,\bar{j}_{\text{ph}}=0]}} [\psi,\overline{\psi}] &\approx \left(\log Z_{\text{ph}}^{g^0,\Phi^0} + \log\left(1 + \frac{Z_{\text{ph}}^{g^0,g^{\text{DW}^1},\Phi^0} + Z_{\text{ph}}^{g^2,g^{\text{DW}^0},\Phi^0} + Z_{\text{ph}}^{g^1,g^{\text{DW}^0},\Phi^1}}{Z_{\text{ph}}^{g^0,g^{\text{DW}^0},\Phi^0}} \right) \right)_{[j_{\text{ph}}=0,\bar{j}_{\text{ph}}=0]} [\psi,\overline{\psi}] \\ &\approx \left(\log Z_{\text{ph}}^{g^0,\Phi^0} + \frac{Z_{\text{ph}}^{g^0,g^{\text{DW}^1},\Phi^0} + Z_{\text{ph}}^{g^2,g^{\text{DW}^0},\Phi^0} + Z_{\text{ph}}^{g^1,g^{\text{DW}^0},\Phi^1}}{Z_{\text{ph}}^{g^0,g^{\text{DW}^0},\Phi^0}} \right)_{[j_{\text{ph}}=0,\bar{j}_{\text{ph}}=0]} [\psi,\overline{\psi}] \end{aligned} \tag{44.19}$$

6. This gives us thous

$$\begin{aligned} Z[j,\bar{j}] &\approx \int \mathscr{D}(\overline{\psi},\psi)\, \mathrm{e}^{-\left(S_{0,\text{el}}+S_{\text{Coulomb}}\right)[\psi,\overline{\psi}]+j_{\text{el}}^\dagger\psi+\psi^\dagger j_{\text{el}}} \exp\left[\left(\log Z_{\text{ph}}^{g^0,\Phi^0} + \frac{Z_{\text{ph}}^{g^0,g^{\text{DW}^1},\Phi^0} + Z_{\text{ph}}^{g^2,g^{\text{DW}^0},\Phi^0} + Z_{\text{ph}}^{g^1,g^{\text{DW}^0},\Phi^1}}{Z_{\text{ph}}^{g^0,g^{\text{DW}^0},\Phi^0}} [\psi,\overline{\psi}] \right) \right] \\ &\equiv \int \mathscr{D}(\overline{\psi},\psi) \exp\left[-\left(S_{0,\text{el}} + S_{\text{eff-int}}\right)[\psi,\overline{\psi}] + j_{\text{el}}^\dagger\psi + \psi^\dagger j_{\text{el}} + \left(\frac{Z_{\text{ph}}^{g^0,g^{\text{DW}^1},\Phi^0} + Z_{\text{ph}}^{g^1,g^{\text{DW}^0},\Phi^1}}{Z_{\text{ph}}^{g^0,g^{\text{DW}^0},\Phi^0}} \right) [\psi,\overline{\psi}] \right] \\ &\equiv \int \mathscr{D}(\overline{\psi},\psi) \exp\left[-\left(S_{0,\text{el}} + S_{\text{eff-int}}\right)[\psi,\overline{\psi}] + j_{\text{el}}^\dagger\psi + \psi^\dagger j_{\text{el}} - \left(V^{\text{DW}} + V^{\text{el-ph}^3} \right)[\psi,\overline{\psi}] \right] \end{aligned} \tag{44.20}$$

whereas in the last step, we neglected the constant term, and we introduced

$$S_{\text{eff-int}} = S_{\text{Coulomb}} - \frac{Z_{\text{ph}}^{g^2,g^{\text{DW}^0},\Phi^0}}{Z_{\text{ph}}^{g^0,g^{\text{DW}^0},\Phi^0}} \tag{44.21}$$

7. Now we introduce auxiliary fields to decouple our interaction term

$$V_{\substack{\text{eff} \\ n_1,n_2,n_3,n_4 \\ \sigma_1,\sigma_2,\sigma_3,\sigma_4}} (k_1,k_2,k_3,k_4) = W_{\substack{\text{Screened} \\ \text{Coulomb} \\ n_1,n_2,n_3,n_4 \\ \sigma_1,\sigma_2,\sigma_3,\sigma_4}} (k_1,k_2,k_3,k_4) + V_{\substack{\text{Phonons} \\ n_1,n_2,n_3,n_4 \\ \sigma_1,\sigma_2,\sigma_3,\sigma_4}} (k_1,k_2,k_3,k_4) \tag{44.22}$$

and apply a mean-field theory in analogy to the mean-field theory chapter on Eliashberg-theory:

Approximation 44.3 We approximate the interactions by focusing on the ET-↓↑-contributions and neglecting the other terms as

$$S_{\text{el-el-int}}[\psi,\overline{\psi}] = S^{\text{ET}}_{\downarrow\uparrow}[\psi,\overline{\psi}] + S_{\Delta V}[\psi,\overline{\psi}] \approx S^{\text{ET}}_{\downarrow\uparrow}[\psi,\overline{\psi}]$$

with the Eliashberg contribution

$$S^{\text{ET}}_{\downarrow\uparrow}[\psi,\overline{\psi}] = \sum_{\substack{k,k'\in \mathrm{i}\Omega_{-1}\times\mathrm{Q} \\ m,n\in\{1,2,3\dots\}}} \overline{\psi}_{m\uparrow}(k)\overline{\psi}_{m\downarrow}(-k)V^{\text{ET}}_{\substack{\downarrow\uparrow \\ m,n}}(k,k')\psi_{n\downarrow}(-k')\psi_{n\uparrow}(k')$$

and the vertex as above.

Notation 44.4 We condense the notation even further, by introducing the multi-index

$$A \equiv (k,m,\downarrow,\uparrow)\in\Pi, \quad B\equiv(k',n;\downarrow,\uparrow)\in\Pi \quad \text{with} \quad \Pi \equiv \mathrm{i}\Omega_{-1}\times\mathrm{Q}\times\{1,2,3,\dots\}\times\{\downarrow\}\times\{\uparrow\} \tag{44.23}$$

and density-like terms

$$\overline{\rho}(A)\equiv\overline{\psi}_{m\uparrow}(k)\overline{\psi}_{m\downarrow}(-k), \qquad \rho(B)\equiv\psi_{n\downarrow}(-k')\psi_{n\uparrow}(k') \tag{44.24}$$

with $\rho(A)=\psi_{m\downarrow}(-k)\psi_{m\uparrow}(k)$.

Remark 44.4.1 Notice that with this, we can rewrite the Eliashberg-interaction term as a bilinear

$$S^{\text{ET}}_{\downarrow\uparrow}[\psi,\overline{\psi}] = \sum_{A,B\in\Pi}\overline{\rho}(A)V^{\text{ET}}_{\downarrow\uparrow}(A,B)\rho(B) \tag{44.25}$$

44.3.1. Hubbard-Stratanovich-Transformation

We now exchange the quartic interaction for a quadratic-part through the Cooper-channel. We therefore have to find the inverse of $V^{\text{ET}}_{\downarrow\uparrow}$.

Hypothesis 44.5 We assume, the existence of another generalised matrix $\left(V^{\text{ET}}_{\downarrow\uparrow}\right)^{-1}\equiv\Lambda^{\text{ET}}_{\downarrow\uparrow}$ such that the inverse relation holds

$$\left(V^{\text{ET}}_{\downarrow\uparrow}\cdot\Lambda^{\text{ET}}_{\downarrow\uparrow}\right)(A,A') = \sum_{B}V^{\text{ET}}_{\downarrow\uparrow}(A,B)\Lambda^{\text{ET}}_{\downarrow\uparrow}(B,A') = \delta(A,A'). \tag{44.26}$$

Remark 44.5.1 For the moment, we will not bother with the concrete shape of this inverse matrix. We simply assume its existence and give it a name to perform further mathematical operations.

Lemma 44.6 Performing a Hubbard-Stratanovich-transformation of the Eliashberg-interaction term through the Cooper-channel yields

$$\begin{aligned}\exp\, -S^{\mathrm{ET}}_{\downarrow\uparrow}[\psi,\overline{\psi}] &= \exp\, -\sum_{A,B\in\Pi^2}\overline{\rho}(A)V^{\mathrm{ET}}_{\downarrow\uparrow}(A,B)\rho(B)\\ &= \int \mathscr{D}(\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow})\exp+\left[\sum_{A,B\in\Pi^2}\overline{\delta}(A)\Lambda^{\mathrm{ET}}_{\downarrow\uparrow}(A,B)\delta(B)-\sum_{A\in\Pi}\left(\overline{\delta}(A)\rho(A)+\overline{\rho}(A)\delta(A)\right)\right]\\ &= \int \mathscr{D}(\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow})\exp-\Big[S_{\mathrm{aux.}}[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]+S_{\mathrm{int}}[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow},\psi,\overline{\psi}]\Big].\end{aligned}$$

Proof 44.6 Shifting variables according to

$$\delta(A)\mapsto\delta(A)+\sum_{B\in\Pi}V^{\mathrm{ET}}_{\downarrow\uparrow}(A,B)\rho(B),\qquad \overline{\delta}(A)\mapsto\overline{\delta}(A)+\sum_{B\in\Pi}\overline{\rho}(B)V^{\mathrm{ET}}_{\downarrow\uparrow}(B,A)\tag{44.27}$$

proves the Lemma.

Fact 44.7 The full action, in absense of external sources, now reads

$$S_{\mathrm{tot}}[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow},\psi,\overline{\psi}]=S_{\mathrm{el}}[\psi,\overline{\psi}]+S_{\mathrm{aux}}[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]+S_{\mathrm{int}}[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow},\psi,\overline{\psi}]\tag{44.28}$$

with

- $S_{\mathrm{el}}[\psi,\overline{\psi}]\equiv\sum_{\substack{\sigma\in\{\downarrow,\uparrow\}\\ k\in\mathrm{i}\Omega_{-1}\times\mathbb{Q}\\ m\in\{1,2,3,\dots\}}}\overline{\psi}_{m\sigma}(k)\left(-\frac{1}{\hbar}\mathscr{G}^{-\mathrm{F}}_{0\,m,\sigma}(k)\right)\psi_{m\sigma}(k)$
- $S_{\mathrm{aux}}[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]=-\sum_{A,B\in\Pi^2}\overline{\delta}(A)\Lambda^{\mathrm{ET}}_{\downarrow\uparrow}(A,B)\delta(B)$
- $S_{\mathrm{int}}[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow},\psi,\overline{\psi}]=\sum_{\substack{k\in\mathrm{i}\Omega_{-1}\times\mathbb{Q}\\ m\in\{1,2,3,\dots\}}}\overline{\delta}_{m\downarrow\uparrow}(k)\psi_{m\downarrow}(-k)\psi_{m\uparrow}(k)+\overline{\psi}_{m\uparrow}(k)\overline{\psi}_{m\downarrow}(-k)\delta_{m\downarrow\uparrow}(k)$

Definition 44.8 We now introduce Nambu-spinors as

$$\eta^{\dagger}_{m}(k)=\begin{pmatrix}\overline{\psi}_{m,\uparrow}(k) & \psi_{m,\downarrow}(-k)\end{pmatrix},\qquad \eta_{m'}(k')=\begin{pmatrix}\psi_{m'\uparrow}(k')\\ \overline{\psi}_{m'\downarrow}(-k')\end{pmatrix}\tag{44.29}$$

Remark 44.8.1 Notice that this allows us to rewrite the electronic contributions as

$$
\begin{aligned}
S_{\mathrm{el}}[\psi,\overline{\psi}] + S_{\mathrm{int}}[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow},\psi,\overline{\psi}] &= \sum_{\substack{k\in \mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ m\in\{1,2,\dots\}}} \begin{pmatrix} \overline{\psi}_{m,\uparrow}(k) \\ \psi_{m,\downarrow}(-k) \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} -\frac{1}{\hbar}\mathscr{G}_{0\ m\uparrow}^{-\mathrm{F}}(k) & \delta_{m\downarrow\uparrow}(k) \\ \overline{\delta}_{m\downarrow\uparrow}(k) & +\frac{1}{\hbar}\mathscr{G}_{0\ m\downarrow}^{-\mathrm{F}}(-k) \end{pmatrix} \begin{pmatrix} \psi_{m\uparrow}(k) \\ \overline{\psi}_{m\downarrow}(-k) \end{pmatrix} \\
&= \sum_{\substack{k\in \mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ m\in\{1,2,\dots\}}} \overline{\eta}_m^{\mathrm{T}}(k) \left[-\frac{1}{\hbar}\mathscr{G}^{-1}{}_{\substack{0m\\ [\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}(k) \right] \eta_m(k)
\end{aligned}
$$

Notice that we have added the index 0 in the substack of indices of the Green-function: The *full* Green-function of the system is the one that includes the interaction terms from Equation (44.20). To this end, we write

$$
S_{\mathrm{el}}[\psi,\overline{\psi}] + S_{\mathrm{int}}[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow},\psi,\overline{\psi}] + \left(V^{\mathrm{DW}} + V^{\text{el-ph}^3}\right)[\psi,\overline{\psi}] = \sum_{\substack{k\in \mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ m\in\{1,2,\dots\}}} \eta_n^{\dagger}(k) \left[-\frac{1}{\hbar}\mathscr{G}^{-1}{}_{\substack{nn'\\ [\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}(k,k') \right] \eta_{n'}(k')
$$

with

$$
\begin{aligned}
V^{\mathrm{DW}}[\psi,\overline{\psi}] = -\left(\frac{Z_{\mathrm{ph}}^{g^0,g^{\mathrm{DW}1},\Phi^0}}{Z_{\mathrm{ph}}^{g^0,g^{\mathrm{DW}0},\Phi^0}}\right)[\psi,\overline{\psi}] &= -\sum_{\substack{\mathrm{i}\omega\in\mathrm{i}\Omega_{-1}\\ \mathbf{k},\mathbf{q}\in\mathrm{Q}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ m,n\in\{1,2,\dots,\infty\}\\ \sigma\in\{\downarrow,\uparrow\}}} \frac{g^{\mathrm{DW}}_{mn\nu\nu}(\mathbf{k},\mathbf{q},-\mathbf{q})}{N_p} \mathscr{D}_{\nu,\mathbf{q}}{}_{0}(\tau_\bullet=0)\overline{\psi}_{m\sigma}(\mathrm{i}\omega,\mathbf{k})\psi_{n\sigma}(\mathrm{i}\omega,\mathbf{k}) \\
&= \sum_{\substack{k\in \mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ m,n\in\{1,2,\dots,\infty\}\\ \sigma\in\{\downarrow,\uparrow\}}} \overline{\psi}_{m\sigma}(k) \left(-\sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}}} \frac{g^{\mathrm{DW}}_{mn\nu\nu}(\mathbf{k},\mathbf{q},-\mathbf{q})}{N_p} \mathscr{D}_{\nu,\mathbf{q}}{}_{0}(\tau_\bullet=0) \right) \psi_{n\sigma}(k)
\end{aligned}
\tag{44.30}
$$

and

$$
\begin{aligned}
V^{\text{el-ph}^3}[\psi,\overline{\psi}] &= -\left(\frac{Z_{\text{ph}}^{g^1,g^{\text{DW}0},\Phi^1}}{Z_{\text{ph}}^{g^0,g^{\text{DW}0},\Phi^0}}\right)[\psi,\overline{\psi}] \\
&= \dots \\
&= -\sum_{\substack{\mathrm{i}\omega_m\in\mathrm{i}\Omega_{-1}\\ \mathbf{k},\mathbf{q},\mathbf{q}''\in\mathrm{Q}\\ \nu,\nu''\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ m,n\in\{1,2,\dots,\infty\}\\ \sigma\in\{\downarrow,\uparrow\}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\sqrt{N_p}}\frac{\phi_{\nu\nu''\nu''}(-\mathbf{q},\mathbf{q}'',-\mathbf{q}'')}{\sqrt{N_p}}\mathscr{D}_{\substack{0\\ \nu,\mathbf{q}}}(\mathrm{i}\omega_\bullet=0)\mathscr{D}_{\substack{0\\ \nu''\mathbf{q}''}}(\tau_\bullet=0)\overline{\psi}_{m\sigma}(\mathrm{i}\omega_m,\mathbf{k}+\mathbf{q})\psi_{n\sigma}(\mathrm{i}\omega_m,\mathbf{k}) \\
&= -\sum_{\substack{\mathrm{i}\omega_m\in\mathrm{i}\Omega_{-1}\\ \mathbf{k},\widetilde{\mathbf{k}},\mathbf{q}''\in\mathrm{Q}\\ \nu,\nu''\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ m,n\in\{1,2,\dots,\infty\}\\ \sigma\in\{\downarrow,\uparrow\}}} \frac{g_{mn\nu}(\mathbf{k},\widetilde{\mathbf{k}}-\mathbf{k})}{\sqrt{N_p}}\frac{\phi_{\nu\nu''\nu''}(\mathbf{k}-\widetilde{\mathbf{k}},\mathbf{q}'',-\mathbf{q}'')}{\sqrt{N_p}}\mathscr{D}_{\substack{0\\ \nu,\widetilde{\mathbf{k}}-\mathbf{k}}}(\mathrm{i}\omega_\bullet=0)\mathscr{D}_{\substack{0\\ \nu''\mathbf{q}''}}(\tau_\bullet=0)\overline{\psi}_{m\sigma}(\mathrm{i}\omega_m,\widetilde{\mathbf{k}})\psi_{n\sigma}(\mathrm{i}\omega_m,\mathbf{k}) \\
&= -\sum_{\substack{\mathrm{i}\omega_m\in\mathrm{i}\Omega_{-1}\\ \mathbf{k},\widetilde{\mathbf{k}}\in\mathrm{Q}\\ m,n\in\{1,2,\dots,\infty\}\\ \sigma\in\{\downarrow,\uparrow\}}} \overline{\psi}_{m\sigma}(\mathrm{i}\omega_m,\widetilde{\mathbf{k}})\left(\sum_{\substack{\mathbf{q}''\in\mathrm{Q}\\ \nu,\nu''\in\{1,2,\dots,rd_{\mathbf{x}}\}}} \frac{g_{mn\nu}(\mathbf{k},\widetilde{\mathbf{k}}-\mathbf{k})}{\sqrt{N_p}}\frac{\phi_{\nu\nu''\nu''}(\mathbf{k}-\widetilde{\mathbf{k}},\mathbf{q}'',-\mathbf{q}'')}{\sqrt{N_p}}\mathscr{D}_{\substack{0\\ \nu,\widetilde{\mathbf{k}}-\mathbf{k}}}(\mathrm{i}\omega_\bullet=0)\mathscr{D}_{\substack{0\\ \nu''\mathbf{q}''}}(\tau_\bullet=0)\right)\psi_{n\sigma}(\mathrm{i}\omega_m,\mathbf{k})
\end{aligned}
\tag{44.31}
$$

We therefore introduce

$$
\begin{aligned}
V[\psi,\overline{\psi}] &= \sum_{\substack{k,k'\in\mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ m,m'\in\{1,2,\dots,\infty\}\\ \sigma\in\{\downarrow,\uparrow\}}} \overline{\psi}_{m\sigma}(k)\widetilde{V}_{m,m'}(k,k')\psi_{m'\sigma}(k') \\
&= \sum_{\substack{k,k'\in\mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ m,m'\in\{1,2,\dots,\infty\}}} \left[\overline{\psi}_{m\uparrow}(k)\widetilde{V}_{m,m'}(k,k')\psi_{m'\uparrow}(k') - \psi_{m'\downarrow}(k')\widetilde{V}_{m,m'}(k,k')\overline{\psi}_{m\downarrow}(k)\right] \\
&= \sum_{\substack{k,k'\in\mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ m,m'\in\{1,2,\dots,\infty\}}} \left[\overline{\psi}_{m\uparrow}(k)\widetilde{V}_{m,m'}(k,k')\psi_{m'\uparrow}(k') - \psi_{m\downarrow}(-k)\widetilde{V}_{m',m}(-k',-k)\overline{\psi}_{m'\downarrow}(-k')\right] \\
&= \sum_{\substack{k,k'\in\mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ m,m'\in\{1,2,\dots,\infty\}}} \eta_m^\dagger(k)\begin{pmatrix}\widetilde{V}_{m,m'}(k,k') & 0\\ 0 & -\widetilde{V}_{m',m}(-k',-k)\end{pmatrix}\eta_{m'}(k')
\end{aligned}
\tag{44.32}
$$

and obtain

$$
\begin{aligned}
-\frac{1}{\hbar}\mathscr{G}^{-1}_{\substack{[\delta_{\downarrow\uparrow},\bar{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}} &\equiv -\frac{1}{\hbar}\mathscr{G}^{-1}_{\substack{0\\ [\delta_{\downarrow\uparrow},\bar{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}} + \frac{1}{\hbar}\left(\widetilde{V}^{\text{DW}}+\widetilde{V}^{\text{el-ph}^3}\right) \\
&= -\frac{1}{\hbar}\mathscr{G}^{-1}_{\substack{0\\ [\delta_{\downarrow\uparrow},\bar{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}\left[1-\mathscr{G}_{\substack{0\\ [\delta_{\downarrow\uparrow},\bar{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}\left(\widetilde{V}^{\text{DW}}+\widetilde{V}^{\text{el-ph}^3}\right)\right]
\end{aligned}
\tag{44.33}
$$

We will take care of the computation of $\mathscr{G}$ later. For now, we will be complacent with this formal expression.

Lemma 44.9 Integrating out the fermions gives us an effective bosonic theory

$$S_{\text{tot}}[\delta_{\downarrow\uparrow}, \overline{\delta}_{\downarrow\uparrow}] \quad = \quad S_{\text{aux.}}[\delta_{\downarrow\uparrow}, \overline{\delta}_{\downarrow\uparrow}] \quad - \quad \text{Tr Log} - \frac{1}{\hbar} \underset{\text{Gorkov}}{\mathscr{G}^{-1}_{[\delta_{\downarrow\uparrow}, \overline{\delta}_{\downarrow\uparrow}]}} \tag{44.34}$$

Proof 44.9 By using standard-identities about Gauss-Berezin-integrals and using the standard-identity Tr Log • = Log Det • gives us the desired identity.

44.3.2. Spontaneous Symmetry Breaking and Gap-Equations

We now break the U(1) symmetry by applying a saddle-point approximation and keeping only one contribution, analogous to section 30.2.5.

Lemma 44.10 We note the identity

$$\frac{\partial}{\partial \delta(\bullet)} \text{Tr Log} - \frac{1}{\hbar} \underset{\text{Gorkov}}{\mathscr{G}^{-1}_{[\delta_{\downarrow\uparrow}, \overline{\delta}_{\downarrow\uparrow}]}} = + \text{Tr} \underset{\text{Gorkov}}{\mathscr{G}_{[\delta_{\downarrow\uparrow}, \overline{\delta}_{\downarrow\uparrow}]}} \frac{\partial}{\partial \delta(\bullet)} \underset{\text{Gorkov}}{\mathscr{G}^{-1}_{[\delta_{\downarrow\uparrow}, \overline{\delta}_{\downarrow\uparrow}]}} \tag{44.35}$$

Proof 44.10 With Altlands prescription: We define $f(x) = \text{Log}\left(-\frac{1}{\hbar}x\right)$, such that we obtain $f'(x) = \frac{1}{x}$. This yields for a x-dependent matrix $A \equiv A(x)$ the identity

$$\partial_x \text{Tr } f(A) = \text{Tr}\left(A^{-1}\partial_x A\right). \tag{44.36}$$

The main "difficulty" compared to ordinary Eliashberg-theory as we have introduced it earlier lies now in the computation of the *full* Green-function, that is also influenced by the Debye-Waller and electron-phonon^3 terms in Equation (44.20). To this end, we will utilize the von Neumann series from Corollary 15.12. To this end, we invert Equation (44.33)

$$\begin{aligned} -\hbar \underset{\text{Gorkov}}{\mathscr{G}_{[\delta_{\downarrow\uparrow}, \overline{\delta}_{\downarrow\uparrow}]}} &= -\hbar \Big[1 - \underset{\text{Gorkov}}{\mathscr{G}^{0}_{[\delta_{\downarrow\uparrow}, \overline{\delta}_{\downarrow\uparrow}]}} \left(\widetilde{V}^{\text{DW}} + \widetilde{V}^{\text{el-ph}^3} \right) \Big]^{-1} \underset{\text{Gorkov}}{\mathscr{G}^{0}_{[\delta_{\downarrow\uparrow}, \overline{\delta}_{\downarrow\uparrow}]}} \\ &= -\hbar \sum_{n=0}^{\infty} \Big[\underset{\text{Gorkov}}{\mathscr{G}^{0}_{[\delta_{\downarrow\uparrow}, \overline{\delta}_{\downarrow\uparrow}]}} \left(\widetilde{V}^{\text{DW}} + \widetilde{V}^{\text{el-ph}^3} \right) \Big]^{n} \underset{\text{Gorkov}}{\mathscr{G}^{0}_{[\delta_{\downarrow\uparrow}, \overline{\delta}_{\downarrow\uparrow}]}} \end{aligned} \tag{44.37}$$

which can be simplified to

$$\underset{\text{Gorkov}}{\mathscr{G}_{[\delta_{\downarrow\uparrow}, \overline{\delta}_{\downarrow\uparrow}]}} = \sum_{n=0}^{\infty} \Big[\underset{\text{Gorkov}}{\mathscr{G}^{0}_{[\delta_{\downarrow\uparrow}, \overline{\delta}_{\downarrow\uparrow}]}} \left(\widetilde{V}^{\text{DW}} + \widetilde{V}^{\text{el-ph}^3} \right) \Big]^{n} \underset{\text{Gorkov}}{\mathscr{G}^{0}_{[\delta_{\downarrow\uparrow}, \overline{\delta}_{\downarrow\uparrow}]}} \tag{44.38}$$

Corollary 44.11 The stationary points of the action are determined by the set of coupled equations

$$\overline{\delta}_{n\downarrow\uparrow}(k') = -\sum_{\substack{k\in \mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ m\in\{1,2,3,\dots\}}} \mathrm{Tr}\left(\underset{\text{Gorkov}}{\mathscr{G}_{[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]}} \frac{\partial}{\partial\delta_{m\downarrow\uparrow}(k)} \underset{\text{Gorkov}}{\mathscr{G}^{-1}_{[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]}} \right) \underset{\text{ET}}{V_{m,n}}(k,k')$$

Proof 44.11 See Appendix, Proofs, page 632.

Lemma 44.12 One has the identities

$$\frac{\partial}{\partial\delta_{m\downarrow\uparrow}(k)} \underset{\text{Gorkov}}{\mathscr{G}^{-1}_{0,m\,[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]}} = \begin{pmatrix} 0 & -\hbar \\ 0 & 0 \end{pmatrix} \tag{44.39}$$

and

$$\underset{\text{Gorkov}}{\mathscr{G}_{[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]}} = \sum_{n=0}^{\infty} \Big[\underset{\text{Gorkov}}{\mathscr{G}_{0\,[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]}} \left(\widetilde{V}^{\mathrm{DW}} + \widetilde{V}^{\text{el-ph}^3} \right) \Big]^n \underset{\text{Gorkov}}{\mathscr{G}_{0\,[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]}} \tag{44.40}$$

Proof 44.12 See Appendix, Proofs, page 632.

Theorem 44.13 To first order in $\widetilde{V} \equiv \widetilde{V}^{\mathrm{DW}} + \widetilde{V}^{\text{el-ph}^3}$ and for $\epsilon_m(-\mathbf{k}) = \epsilon_m(\mathbf{k})$, the gap equations become

$$\begin{aligned}\overline{\delta}_{n\downarrow\uparrow}(k') = -\sum_{\substack{k\in \mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ m\in\{1,2,3,\dots\}}} \frac{\overline{\delta}_{m\downarrow\uparrow}(k)}{\pi_m(k)} \Bigg\{ 1 - \frac{1}{\hbar\pi_m(k)} \Big[\mathrm{i}\omega_k \left(\widetilde{V}_{m,m}(k,k) - \widetilde{V}_{m,m}(-k,-k) \right) \\ + \frac{\epsilon_m(\mathbf{k}) - \mu}{\hbar} \left(\widetilde{V}_{m,m}(k,k) + \widetilde{V}_{m,m}(-k,-k) \right) \Big] \Bigg\} \underset{\text{ET}}{V_{m,n}}(k,k')\end{aligned}$$

with $\pi_m(k) = \omega_k^2 + (\epsilon_m(\mathbf{k}) - \mu)^2/\hbar^2 + |\delta_{m\downarrow\uparrow}(k)|^2$. The first term reproduces the gap equation of Theorem 26.70, the second term is the correction due to the Debye-Waller and electron-phonon^3 interactions.

Proof 44.13 We compute straight forwardly

$$\overline{\delta}_n(k') = -\sum_{\substack{k\in \mathrm{i}\Omega\times\mathrm{Q}\\ m\in\{1,2,\dots\}}} \mathrm{Tr}\left(\mathscr{G} \cdot \frac{\partial}{\partial\delta_m(k)} \mathscr{G}^{-1} \right) V_{m,n}(k,k') \tag{44.41}$$

To this end, we compute

$$\begin{aligned}\mathrm{Tr}\left(\mathscr{G}\cdot\frac{\partial}{\partial\delta_m(k)}\mathscr{G}^{-1}\right) &= \mathrm{Tr}\sum_{\tilde{n}=0}^{\infty}\left(\left[\mathscr{G}_0\widetilde{V}\right]^{\tilde{n}}\mathscr{G}_0\cdot\frac{\partial}{\partial\delta_m(k)}\mathscr{G}^{-1}\right)\\ &= \sum_{\tilde{n}=0}^{\infty}\mathrm{Tr}\left(\left[\mathscr{G}_0\widetilde{V}\right]^{\tilde{n}}\mathscr{G}_0\cdot\frac{\partial}{\partial\delta_m(k)}\mathscr{G}^{-1}\right)\\ &= \mathrm{Tr}\left(\mathscr{G}_0\cdot\frac{\partial}{\partial\delta_m(k)}\mathscr{G}^{-1}\right)+\mathrm{Tr}\left(\mathscr{G}_0\widetilde{V}\mathscr{G}_0\cdot\frac{\partial}{\partial\delta_m(k)}\mathscr{G}^{-1}\right)+\mathcal{O}\left(\widetilde{V}^2\right)\end{aligned} \tag{44.42}$$

The first term gives the contribution that we already found in the previous chapter. For the second term we obtain with the cyclicity of the trace and using the identity[4]

$$\partial_x K^{-1} = -K^{-1}\left(\partial_x K\right)K^{-1} \tag{44.43}$$

the equation becomes

$$\begin{aligned}\mathrm{Tr}\left(\mathscr{G}_0\widetilde{V}\mathscr{G}_0\cdot\frac{\partial}{\partial\delta_m(k)}\mathscr{G}^{-1}\right) &\approx \mathrm{Tr}\left(\left[\mathscr{G}_0\cdot\left(\frac{\partial}{\partial\delta_m(k)}\mathscr{G}_0^{-1}\right)\mathscr{G}_0\right]\widetilde{V}\right)\\ &= -\mathrm{Tr}\left[\left(\frac{\partial}{\partial\delta_m(k)}\mathscr{G}_0\right)\widetilde{V}\right]\end{aligned} \tag{44.44}$$

For the zeroth order term we find with the identity for $\partial\mathscr{G}^{-1}/\partial\delta$ from above

$$\mathrm{Tr}\left(\underset{\substack{[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}{\mathscr{G}_{0,m}}(k)\begin{pmatrix}0 & -\hbar\\ 0 & 0\end{pmatrix}\right) = \frac{\overline{\delta}_{m\downarrow\uparrow}(k)}{\pi_m(k)}, \tag{44.45}$$

while the first order term is given by Corollary 44.15 below. Collecting both contributions, the gap equations become

$$\begin{aligned}\overline{\delta}_n(k') &= -\sum_{\substack{k\in\mathrm{i}\Omega\times\mathrm{Q}\\ m\in\{1,2,\dots\}}}\left[\mathrm{Tr}\left(\mathscr{G}_0\cdot\frac{\partial}{\partial\delta_m(k)}\mathscr{G}^{-1}\right)-\mathrm{Tr}\left[\left(\frac{\partial}{\partial\delta_m(k)}\mathscr{G}_0\right)\widetilde{V}\right]\right]V_{m,n}(k,k')\\ &= -\sum_{\substack{k\in\mathrm{i}\Omega\times\mathrm{Q}\\ m\in\{1,2,\dots\}}}\frac{\overline{\delta}_m(k)}{\pi_m(k)}\Bigg\{1-\frac{1}{\hbar\pi_m(k)}\Big[\mathrm{i}\omega_k\left(\widetilde{V}_{m,m}(k,k)-\widetilde{V}_{m,m}(-k,-k)\right)\\ &\qquad\qquad+\frac{\epsilon_m(\mathbf{k})-\mu}{\hbar}\left(\widetilde{V}_{m,m}(k,k)+\widetilde{V}_{m,m}(-k,-k)\right)\Big]\Bigg\}V_{m,n}(k,k'),\end{aligned} \tag{44.46}$$

where we have used $\epsilon_m(-\mathbf{k})=\epsilon_m(\mathbf{k})$ in the last step.

Lemma 44.14 For $\epsilon_m(-\mathbf{k})=\epsilon_m(\mathbf{k})$ and the non-interacting Gorkov-Green-function

[4] Cf. `https://math.stackexchange.com/questions/1471825/derivative-of-the-inverse-of-a-matrix`

$$\underset{\substack{[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}{\mathscr{G}^{0,m}}(k) = -\frac{1}{\hbar}\frac{\begin{pmatrix} +\mathrm{i}\omega_k + (\epsilon_m(-\mathbf{k})-\mu)/\hbar & +\delta_{m\downarrow\uparrow}(k) \\ +\overline{\delta}_{m\downarrow\uparrow}(k) & +\mathrm{i}\omega_k - (\epsilon_m(\mathbf{k})-\mu)/\hbar \end{pmatrix}}{+\omega_k^2 + \frac{\left(\epsilon_m(\mathbf{k})-\mu\right)^2}{\hbar^2} + |\delta_{m\downarrow\uparrow}(k)|^2} \tag{44.47}$$

one has the identity

$$\frac{\partial}{\partial\delta_{m\downarrow\uparrow}(k)}\underset{\substack{[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}{\mathscr{G}^{0,m}}(k) = \frac{1}{\hbar\pi_m^2(k)}\begin{pmatrix} \overline{\delta}_{m\downarrow\uparrow}(k)\left[\mathrm{i}\omega_k + (\epsilon_m(-\mathbf{k})-\mu)/\hbar\right] & -\omega_k^2 - \frac{\left(\epsilon_m(\mathbf{k})-\mu\right)^2}{\hbar^2} \\ \overline{\delta}_{m\downarrow\uparrow}^2(k) & \overline{\delta}_{m\downarrow\uparrow}(k)\left[\mathrm{i}\omega_k - (\epsilon_m(\mathbf{k})-\mu)/\hbar\right] \end{pmatrix} \tag{44.48}$$

with

$$\pi_m(k) \equiv \omega_k^2 + \frac{\left(\epsilon_m(\mathbf{k})-\mu\right)^2}{\hbar^2} + |\delta_{m\downarrow\uparrow}(k)|^2, \tag{44.49}$$

where the derivative is taken with respect to $\delta_{m\downarrow\uparrow}(k)$ while holding $\overline{\delta}_{m\downarrow\uparrow}(k)$ fixed.

Proof 44.14 For brevity, we write $\delta \equiv \delta_{m\downarrow\uparrow}(k)$, $\overline{\delta} \equiv \overline{\delta}_{m\downarrow\uparrow}(k)$, $\pi \equiv \pi_m(k)$ and

$$a \equiv \mathrm{i}\omega_k + (\epsilon_m(-\mathbf{k})-\mu)/\hbar, \qquad d \equiv \mathrm{i}\omega_k - (\epsilon_m(\mathbf{k})-\mu)/\hbar, \tag{44.50}$$

such that

$$\underset{\substack{[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}{\mathscr{G}^{0,m}}(k) = -\frac{1}{\hbar\pi}\begin{pmatrix} a & \delta \\ \overline{\delta} & d \end{pmatrix}. \tag{44.51}$$

Treating δ and $\overline{\delta}$ as independent variables, we find

$$\frac{\partial}{\partial\delta}\begin{pmatrix} a & \delta \\ \overline{\delta} & d \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad \frac{\partial\pi}{\partial\delta} = \overline{\delta}. \tag{44.52}$$

The quotient rule then gives

$$\frac{\partial}{\partial\delta}\underset{\substack{[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}{\mathscr{G}^{0,m}}(k) = -\frac{1}{\hbar}\left[\frac{1}{\pi}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} - \frac{\overline{\delta}}{\pi^2}\begin{pmatrix} a & \delta \\ \overline{\delta} & d \end{pmatrix}\right] = \frac{1}{\hbar\pi^2}\begin{pmatrix} a\overline{\delta} & \delta\overline{\delta} - \pi \\ \overline{\delta}^2 & d\overline{\delta} \end{pmatrix}, \tag{44.53}$$

and with $\delta\overline{\delta} - \pi = -\omega_k^2 - (\epsilon_m(\mathbf{k})-\mu)^2/\hbar^2$ the claim follows.

Corollary 44.15 Let $\epsilon_m(-\mathbf{k}) = \epsilon_m(\mathbf{k})$, which holds e.g. for time-reversal symmetric systems with negligible spin-orbit coupling, or for inversion-symmetric crystals. The first-order contribution of $\widetilde{V} \equiv \widetilde{V}^{\mathrm{DW}} + \widetilde{V}^{\text{el-ph}^3}$ to the trace in the gap equation is

$$
\begin{aligned}
-\operatorname{Tr}\left[\left(\frac{\partial}{\partial\delta_{m\downarrow\uparrow}(k)}\mathscr{G}^{\ 0}_{\substack{[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}\right)\widetilde{V}\right] = -\frac{\overline{\delta}_{m\downarrow\uparrow}(k)}{\hbar\pi_m^2(k)}\Big[&\mathrm{i}\omega_k\left(\widetilde{V}_{m,m}(k,k)-\widetilde{V}_{m,m}(-k,-k)\right)\\
&+\frac{\epsilon_m(\mathbf{k})-\mu}{\hbar}\left(\widetilde{V}_{m,m}(k,k)+\widetilde{V}_{m,m}(-k,-k)\right)\Big].
\end{aligned}
\tag{44.54}
$$

Proof 44.15 Since $\widetilde{V}$ does not depend on $\delta_{\downarrow\uparrow}$, the derivative of the full and the non-interacting inverse Gorkov-Green-function coincide, such that the derivative in the trace acts only on $\mathscr{G}^{\ 0}_{\substack{[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}$. The latter is diagonal in (m,k), hence its derivative with respect to $\delta_{m\downarrow\uparrow}(k)$ is non-vanishing only in the $(m,k),(m,k)$ block. With the Nambu-form of $\widetilde{V}$, i.e.

$$
\widetilde{V}_{(m,k),(m',k')} = \begin{pmatrix} \widetilde{V}_{m,m'}(k,k') & 0 \\ 0 & -\widetilde{V}_{m',m}(-k',-k) \end{pmatrix},
\tag{44.55}
$$

the trace reduces to the trace over Nambu-space of the product of Lemma 44.14 with this block for $m'=m$, $k'=k$. Only the diagonal entries contribute, i.e.

$$
\begin{aligned}
-\operatorname{Tr}\left[\left(\frac{\partial}{\partial\delta_{m\downarrow\uparrow}(k)}\mathscr{G}^{\ 0}_{\substack{[\delta_{\downarrow\uparrow},\overline{\delta}_{\downarrow\uparrow}]\\ \text{Gorkov}}}\right)\widetilde{V}\right] = -\frac{\overline{\delta}_{m\downarrow\uparrow}(k)}{\hbar\pi_m^2(k)}\Big[&\left(\mathrm{i}\omega_k+(\epsilon_m(\mathbf{k})-\mu)/\hbar\right)\widetilde{V}_{m,m}(k,k)\\
&-\left(\mathrm{i}\omega_k-(\epsilon_m(\mathbf{k})-\mu)/\hbar\right)\widetilde{V}_{m,m}(-k,-k)\Big],
\end{aligned}
\tag{44.56}
$$

where we have used $\epsilon_m(-\mathbf{k})=\epsilon_m(\mathbf{k})$ in the upper-left entry of Lemma 44.14. Sorting by $\mathrm{i}\omega_k$ and $\epsilon_m(\mathbf{k})-\mu$ yields the claim.

Theorem 44.16 For time-reversal symmetric systems with negligible spin-orbit coupling, the gap equations including the Debye-Waller and electron-phonon[3] contributions become to first order in $\widetilde{V}$

$$
\overline{\delta}_{n\downarrow\uparrow}(k') = +\sum_{\substack{k\in\mathrm{i}\Omega_{-1}\times\mathrm{Q}\\ \nu\in\{1,\dots,rd\}\\ m\in\{1,2,3,\dots\}}} \frac{\overline{\delta}_{m\downarrow\uparrow}(k)}{\omega_k^2+\frac{\left(\widetilde{\epsilon}_m(\mathbf{k})-\mu\right)^2}{\hbar^2}+|\delta_{m\downarrow\uparrow}(k)|^2}\,\frac{2\omega_\nu(\mathbf{k}-\mathbf{k}')}{\omega_{k-k'}^2+\omega_\nu^2(\mathbf{k}-\mathbf{k}')}\,\frac{|g_{mn\nu}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{\hbar^3\beta N_p}
$$

with the renormalized band-energies

$$
\widetilde{\epsilon}_m(\mathbf{k}) = \epsilon_m(\mathbf{k}) + \widetilde{V}^{\mathrm{DW}}_{m,m}(\mathbf{k}) + \widetilde{V}^{\text{el-ph}^3}_{m,m}(\mathbf{k}),
\tag{44.57}
$$

where

$$\begin{aligned}\widetilde{V}^{\mathrm{DW}}_{m,m}(\mathbf{k}) &= -\sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}}} \frac{g^{\mathrm{DW}}_{mm\nu\nu}(\mathbf{k},\mathbf{q},-\mathbf{q})}{N_p}\,\mathscr{D}^{\,0}_{\nu,\mathbf{q}}(\tau_\bullet=0),\\ \widetilde{V}^{\text{el-ph}^3}_{m,m}(\mathbf{k}) &= -\sum_{\substack{\mathbf{q}''\in\mathrm{Q}\\ \nu,\nu''\in\{1,2,\dots,rd_{\mathbf{x}}\}}} \frac{g_{mm\nu}(\mathbf{k},\mathbf{0})}{\sqrt{N_p}}\,\frac{\phi_{\nu\nu''\nu''}(\mathbf{0},\mathbf{q}'',-\mathbf{q}'')}{\sqrt{N_p}}\,\mathscr{D}^{\,0}_{\nu,\mathbf{0}}(\mathrm{i}\omega_\bullet=0)\,\mathscr{D}^{\,0}_{\nu''\mathbf{q}''}(\tau_\bullet=0)\end{aligned} \tag{44.58}$$

are the band-diagonal elements $\widetilde{V}_{m,m}(k,k)$ of the Debye-Waller and electron-phonon^3 kernels.

Proof 44.16

We abbreviate $\xi_m(\mathbf{k}) \equiv \epsilon_m(\mathbf{k}) - \mu$ and $\widetilde{V}_m(\mathbf{k}) \equiv \widetilde{V}^{\mathrm{DW}}_{m,m}(\mathbf{k}) + \widetilde{V}^{\text{el-ph}^3}_{m,m}(\mathbf{k})$, and suppress arguments where unambiguous.

Step 1 (Symmetries). Both kernels are static, i.e. independent of $\mathrm{i}\omega_k$, such that $\widetilde{V}_{m,m}(k,k) = \widetilde{V}_m(\mathbf{k})$ and $\widetilde{V}_{m,m}(-k,-k) = \widetilde{V}_m(-\mathbf{k})$. Hermiticity of the interaction, $\widetilde{V}_{m,m'}(k,k')^* = \widetilde{V}_{m',m}(k',k)$, implies $\widetilde{V}_m(\mathbf{k}) \in \mathbb{R}$, and time-reversal symmetry implies $\widetilde{V}_m(-\mathbf{k}) = \widetilde{V}_m(\mathbf{k})^*$. Together,

$$\widetilde{V}_{m,m}(-k,-k) = \widetilde{V}_{m,m}(k,k) = \widetilde{V}_m(\mathbf{k}). \tag{44.59}$$

Step 2 (Bracket). Inserting this into the bracket of Theorem 44.13 gives

$$\mathrm{i}\omega_k\left(\widetilde{V}_{m,m}(k,k) - \widetilde{V}_{m,m}(-k,-k)\right) = 0, \qquad \frac{\xi_m}{\hbar}\left(\widetilde{V}_{m,m}(k,k) + \widetilde{V}_{m,m}(-k,-k)\right) = \frac{2\xi_m\widetilde{V}_m}{\hbar}, \tag{44.60}$$

such that

$$\frac{1}{\pi_m}\left\{1 - \frac{1}{\hbar\pi_m}\cdot\frac{2\xi_m\widetilde{V}_m}{\hbar}\right\} = \frac{1}{\pi_m} - \frac{2\xi_m\widetilde{V}_m}{\hbar^2\pi_m^2}. \tag{$*$}$$

Step 3 (Renormalized denominator). We define

$$\widetilde{D}_m(k) \equiv \omega_k^2 + \frac{\left(\xi_m + \widetilde{V}_m\right)^2}{\hbar^2} + |\delta_{m\downarrow\uparrow}(k)|^2. \tag{44.61}$$

With $(\xi_m + \widetilde{V}_m)^2 = \xi_m^2 + 2\xi_m\widetilde{V}_m + \widetilde{V}_m^2$ this is

$$\widetilde{D}_m = \pi_m + a + b, \qquad a \equiv \frac{2\xi_m\widetilde{V}_m}{\hbar^2}, \qquad b \equiv \frac{\widetilde{V}_m^2}{\hbar^2}. \tag{44.62}$$

Step 4 (Comparison). Bringing the difference of $1/\widetilde{D}_m$ and $(*)$ to a common denominator yields

$$\begin{aligned}\frac{1}{\widetilde{D}_m} - \left(\frac{1}{\pi_m} - \frac{a}{\pi_m^2}\right) &= \frac{\pi_m^2 - \pi_m(\pi_m + a + b) + a(\pi_m + a + b)}{\pi_m^2 \widetilde{D}_m} \\ &= \frac{a^2 + ab - b\pi_m}{\pi_m^2 \widetilde{D}_m} \\ &= \frac{\widetilde{V}_m^2}{\hbar^4} \frac{3\xi_m^2 + 2\xi_m \widetilde{V}_m - \hbar^2\left(\omega_k^2 + |\delta_{m\downarrow\uparrow}(k)|^2\right)}{\pi_m^2 \widetilde{D}_m}.\end{aligned} \tag{44.63}$$

The right-hand side is proportional to $\widetilde{V}_m^2$, hence

$$\frac{1}{\pi_m}\left\{1 - \frac{2\xi_m \widetilde{V}_m}{\hbar^2 \pi_m}\right\} = \frac{1}{\widetilde{D}_m} + \mathcal{O}\left(\widetilde{V}^2\right). \tag{44.64}$$

Step 5 (Vertex). Up to $\mathcal{O}(\widetilde{V}^2)$, Theorem 44.13 therefore reads

$$\overline{\delta}_{n\downarrow\uparrow}(k') = -\sum_{\substack{k \in \mathrm{i}\Omega_{-1}\times\mathrm{Q} \\ m \in \{1,2,\dots\}}} \frac{\overline{\delta}_{m\downarrow\uparrow}(k)}{\widetilde{D}_m(k)} V^{\mathrm{ET}}_{m,n}(k,k'). \tag{44.65}$$

With Equation (26.182),

$$-V^{\mathrm{ET}}_{m,n}(k,k') = +\sum_{\nu \in \{1,\dots,rd\}} \frac{2\omega_\nu(\mathbf{k}-\mathbf{k}')}{\omega_{k-k'}^2 + \omega_\nu^2(\mathbf{k}-\mathbf{k}')} \frac{|g_{mn\nu}(\mathbf{k}',\mathbf{k}-\mathbf{k}')|^2}{\hbar^3 \beta N_p}, \tag{44.66}$$

and $\xi_m(\mathbf{k}) + \widetilde{V}_m(\mathbf{k}) = \widetilde{\epsilon}_m(\mathbf{k}) - \mu$, the claim follows.

Remark 44.16.1 *[CP5] New remark.* The resummed form is in fact better than first order. Both kernels are static and conserve crystal momentum, hence $\widetilde{V}$ is block-diagonal in k. Neglecting the interband elements $\widetilde{V}_{m,m'}$, $m \neq m'$, which enter only at $\mathcal{O}(\widetilde{V}^2)$, Equation (44.33) shows that $-\frac{1}{\hbar}\mathscr{G}^{-1}$ follows from $-\frac{1}{\hbar}\mathscr{G}_0^{-1}$ by $\epsilon_m(\pm\mathbf{k}) \to \widetilde{\epsilon}_m(\pm\mathbf{k})$. The computation on page 634 then applies verbatim and gives $\mathrm{Tr}(\mathscr{G}\,\partial\mathscr{G}^{-1}/\partial\delta_{m\downarrow\uparrow}(k)) = \overline{\delta}_{m\downarrow\uparrow}(k)/\widetilde{D}_m(k)$ exactly. Conversely, the linearized form of Theorem 44.13 requires $|\widetilde{V}_m(\mathbf{k})| \ll \hbar\sqrt{\omega_k^2 + |\delta_{m\downarrow\uparrow}(k)|^2}$, the maximum of $2|\xi_m\widetilde{V}_m|/(\hbar^2\pi_m)$ over ξ_m. This fails near the Fermi surface at low temperatures as soon as $|\widetilde{V}_m| \gtrsim \pi k_B T$.

Remark 44.16.2 To first order, the Debye-Waller and electron-phonon^3 interactions therefore do not alter the structure of the gap equations, but only shift the band-energies $\epsilon_m(\mathbf{k}) \to \widetilde{\epsilon}_m(\mathbf{k})$ by a static, temperature dependent self-energy. Notice that $\widetilde{V}^{\text{el-ph}^3}_{m,m}(\mathbf{k})$ only involves phonons at the Γ-point, where for acoustic branches $\omega_\nu(\mathbf{0}) = 0$, such that $\mathscr{D}_{\nu,\mathbf{0}}(\mathrm{i}\omega_\bullet = 0)$ diverges while $g_{mm\nu}(\mathbf{k},\mathbf{0}) \to 0$. These contributions have to be understood as the limit $\mathbf{q} \to \mathbf{0}$.

45. Experimental: Other Useful Identities from ChatGPT related to HST

Remark 45.0.1 [Multi-band generalization] The channel formulas above implicitly assume a single-band model with spin as the only internal quantum number. In general one replaces σ by a multi-index $\alpha = (n, \sigma)$ (band and spin), or $\alpha = (o, \sigma)$ in an orbital basis, and the interaction becomes a four-index tensor:

$$S_{\text{int}} = \frac{1}{2} \sum_{k,k',q} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta}(k, k', q)\, \overline{\psi}_{k+q,\alpha}\, \overline{\psi}_{k'-q,\beta}\, \psi_{k',\gamma}\, \psi_{k,\delta}.$$

The bilinears then carry two internal indices each.

Direct channel (sign +):

$$P_k^{\alpha\delta}(q) = \overline{\psi}_{k+q,\alpha}\psi_{k,\delta}, \qquad \overline{P}_k^{\alpha\delta}(q) = \overline{\psi}_{k,\delta}\psi_{k+q,\alpha},$$
$$S_{\text{int}} = \frac{1}{2} \sum_{q} \sum_{k,k'} \overline{P}_{k'-q}^{\gamma\beta}(q)\, V_{\alpha\beta\gamma\delta}(k, k', q)\, P_k^{\alpha\delta}(q).$$

Cooper channel (sign +, with $Q = k + k'$):

$$P_k^{\gamma\delta}(Q) = \psi_{Q-k,\gamma}\psi_{k,\delta}, \qquad \overline{P}_k^{\gamma\delta}(Q) = \overline{\psi}_{k,\delta}\overline{\psi}_{Q-k,\gamma},$$
$$S_{\text{int}} = \frac{1}{2} \sum_{Q} \sum_{p,k} \overline{P}_p^{\beta\alpha}(Q)\, V_{\alpha\beta\gamma\delta}(k, Q-k, p-k)\, P_k^{\gamma\delta}(Q).$$

Note that $P_k^{\gamma\delta} = -P_{Q-k}^{\delta\gamma}$. One must either restrict to independent components or impose positive definiteness only on the antisymmetric subspace.

Exchange channel (sign −, with $Q = k + q - k'$):

$$P_{k'}^{\alpha\gamma}(Q) = \overline{\psi}_{k'+Q,\alpha}\psi_{k',\gamma}, \qquad \overline{P}_{k'}^{\alpha\gamma}(Q) = \overline{\psi}_{k',\gamma}\psi_{k'+Q,\alpha},$$
$$S_{\text{int}} = -\frac{1}{2} \sum_{Q} \sum_{k,k'} \overline{P}_{k-Q}^{\delta\beta}(Q)\, V_{\alpha\beta\gamma\delta}(k, k', Q+k'-k)\, P_{k'}^{\alpha\gamma}(Q).$$

In every channel the matrix index is $i = (k, \text{two internal indices})$ at fixed transfer momentum. Moreover:

1. Direct and exchange use the same particle–hole bilinear. They differ only in which fields are grouped together, so with general band indices the distinction between them is a matter of convention.
2. The single-band formulas from before follow from these by keeping one band and dropping the form factors. That is the usual intraband approximation.

46. Experimental: On the missing terms in Eliashberg-Theory from the Functional Field Integral Formalism

We write for the missing terms (starting from Equation (TBReferenced))

$$\begin{aligned} S^{\mathrm{NET}}_{\sigma\sigma}[\psi,\overline{\psi}] &= \sum_{\substack{\sigma,q,k\\ m,n}} \overline{\psi}_{m\sigma}(q)\psi_{m\sigma}(q)V^{\mathrm{NET}}_{\substack{\sigma\sigma\\ mn}}(q-k,k)\psi_{n\sigma}(-k)\overline{\psi}_{n\sigma}(-k) \\ &= \sum_{\substack{\sigma,q,k\\ m,n}} \overline{\psi}_{m\sigma}(q)\psi_{m\sigma}(q)\widetilde{V}_{\substack{\sigma\sigma\\ mn}}(q,k)\psi_{n\sigma}(k)\overline{\psi}_{n\sigma}(k) \end{aligned} \tag{46.1}$$

whereas we introduced

$$\begin{aligned} V^{\mathrm{NET}}_{\substack{\sigma\sigma\\ mn}}(q-k,k) = \widetilde{V}_{\substack{\sigma\sigma\\ mn}}(q,k) &= -\frac{1}{\hbar\beta N_p}\sum_{\nu}\frac{\omega_\nu(-\mathbf{k}+\mathbf{q})}{\omega^2_{-q+k}+\omega^2_\nu(-\mathbf{k}+\mathbf{q})}\frac{|g_{mn\nu}(\mathbf{k},-\mathbf{k}+\mathbf{q})|^2}{\hbar^2} \\ \overset{?}{=} \widetilde{V}_{\substack{\sigma\sigma\\ nm}}(k,q) &= -\frac{1}{\hbar\beta N_p}\sum_{\nu}\frac{\omega_\nu(-\mathbf{q}+\mathbf{k})}{\omega^2_{-q+k}+\omega^2_\nu(-\mathbf{q}+\mathbf{k})}\frac{|g_{nm\nu}(\mathbf{q},-\mathbf{q}+\mathbf{k})|^2}{\hbar^2} \end{aligned} \tag{46.2}$$

whereas in the last line we verified the symmetry of the vertex-function. Therefore Theorem 18.13 applies now with its second equation and

$$\rho_{n\sigma}(k) = \psi_{n\sigma}(k)\overline{\psi}_{n\sigma}(k) \tag{46.3}$$

which gives

$$\exp -S^{\mathrm{NET}}_{\substack{\sigma\sigma\\ m,n}} = \exp\left(\frac{1}{2}\sum_{\substack{m,n\\ q,k}}\varphi^{\mathrm{T}}_{m\sigma}(q)\left(-2\widetilde{V}_{\substack{\sigma\sigma\\ mn}}(q,k)\right)^{-1}\varphi_{n\sigma(k)} \quad + \quad \varphi^{\mathrm{T}}\rho\right) \tag{46.4}$$

Notice now that we obtain, by expanding the expressions,

$$\varphi^{\mathrm{T}}\rho \equiv \sum_{n\sigma k}\varphi_{n\sigma}(k)\psi_{n\sigma}(k)\overline{\psi}_{n\sigma}(k) \tag{46.5}$$

47. Experimental: More Notes on Superconductors

47.1. Material Candidates for the Application of the Theory

Stoichiometric Superconductors

Material	Space Group (No.)	T_C [K]	Pressure	Presumed Mechanism
Conventional (phonon-mediated)				
Al	$Fm\bar{3}m$ (225)	1.18	ambient	Electron-phonon
β-Sn	$I4_1/amd$ (141)	3.72	ambient	Electron-phonon
α-Hg	$R\bar{3}m$ (166)	4.15	ambient	Electron-phonon
V	$Im\bar{3}m$ (229)	5.4	ambient	Electron-phonon
YbC_6	$P6_3/mmc$ (194)	6.5	ambient	Electron-phonon
Pb	$Fm\bar{3}m$ (225)	7.2	ambient	Electron-phonon
Tc	$P6_3/mmc$ (194)	7.4 – 11.2	ambient	Electron-phonon
Nb	$Im\bar{3}m$ (229)	9.25	ambient	Electron-phonon
ZrN	$Fm\bar{3}m$ (225)	8.1 – 10	ambient	Electron-phonon
TaC	$Fm\bar{3}m$ (225)	9.7 – 10.2	ambient	Electron-phonon
CaC_6	$R\bar{3}m$ (166)	11.5	ambient	Electron-phonon
NbN	$Fm\bar{3}m$ (225)	16	ambient	Electron-phonon
V_3Si	$Pm\bar{3}n$ (223)	17	ambient	Electron-phonon
Nb_3Al	$Pm\bar{3}n$ (223)	18	ambient	Electron-phonon
Nb_3Sn	$Pm\bar{3}n$ (223)	18.3	ambient	Electron-phonon
Nb_3Ga	$Pm\bar{3}n$ (223)	20.3	ambient	Electron-phonon
Nb_3Ge	$Pm\bar{3}n$ (223)	23.2	ambient	Electron-phonon
MgB_2	$P6/mmm$ (191)	39	ambient	Electron-phonon
Cuprates				
$YBa_2Cu_4O_8$	$Ammm$ (65)	80	ambient	Spin fluctuations (debated)
$YBa_2Cu_3O_7$ ($\delta = 0$)	$Pmmm$ (47)	≈ 89	ambient	Spin fluctuations (debated)
Iron-based				
FeSe	$P4/nmm$ (129)	8	ambient	Spin/orbital fluct. (debated)
LiFeAs	$P4/nmm$ (129)	18	ambient	Spin/orbital fluct. (debated)
$KCa_2Fe_4As_4F_2$	$I4/mmm$ (139)	33	ambient	Spin fluctuations ($s_\pm$)
$CaKFe_4As_4$	$P4/mmm$ (123)	35	ambient	Spin fluctuations ($s_\pm$)
$RbEuFe_4As_4$	$P4/mmm$ (123)	36	ambient	Spin fluctuations ($s_\pm$)
Nickelates				
$La_3Ni_2O_7$	$Amam$ (63)	≈ 80	≈ 14 GPa	Unknown (spin fluct.?)

Table 47.1.: Stoichiometric superconductors in the sense of Definition 47.1, i.e. superconducting without doping, with all sites fully occupied. The cuprates, iron-based superconductors and nickelates are unconventional (high-temperature) superconductors. Shaded rows (green and orange): ambient pressure, $T_C \gtrsim 30$ K. Orange rows: no crystal structure entry found in the ICSD or the Materials Project. See the Remark below for notes on individual entries.

Remark 47.0.1 Notes on individual entries of Table 47.1:

- $YBa_2Cu_3O_7$ is the fully oxygenated ($\delta = 0$), slightly overdoped end member of $YBa_2Cu_3O_{7-\delta}$ (Table 47.2); the maximal $T_C \approx 92 - 93$ K is reached at $\delta \approx 0.07$.
- For FeSe, the superconducting phase is $Fe_{1.01}Se$.
- $La_3Ni_2O_7$ superconducts only under pressure. The ambient-pressure structure is *Amam* (63), the superconducting high-pressure structure *Fmmm* (69).
- The transition-metal nitrides and carbides (ZrN, NbN, TaC) and the A15-compounds (V_3Si, Nb_3X) have homogeneity ranges. The quoted T_C refer to (nearly) stoichiometric samples and decrease with the deviation from stoichiometry.

Non-Stoichiometric (Doped) Superconductors

Material	Space Group (No.)	T_C [K]	Pressure	Presumed Mechanism
Cuprates				
$Nd_{2-x}Ce_xCuO_4$	$I4/mmm$ (139)	24	ambient	Spin fluctuations (debated)
$Sr_{0.9}La_{0.1}CuO_2$	$P4/mmm$ (123)	43	ambient	Spin fluctuations (debated)
$YBa_2Cu_3O_{7-\delta}$	$Pmmm$ (47)	92	ambient	Spin fluctuations (debated)
$HgBa_2CuO_{4+\delta}$	$P4/mmm$ (123)	94 – 97	ambient	Spin fluctuations (debated)
$HgBa_2Ca_2Cu_3O_{8+\delta}$	$P4/mmm$ (123)	134 (164)	ambient (30 GPa)	Spin fluctuations (debated)
Iron-based				
$LaFeAsO_{1-x}F_x$	$P4/nmm$ (129)	26	ambient	Spin fluctuations ($s_\pm$)
$Ba_{1-x}K_xFe_2As_2$	$I4/mmm$ (139)	38	ambient	Spin fluctuations ($s_\pm$)
$SmFeAsO_{1-x}F_x$	$P4/nmm$ (129)	55	ambient	Spin fluctuations ($s_\pm$)
Nickelates				
$Nd_{0.8}Sr_{0.2}NiO_2$	$P4/mmm$ (123)	9 – 15	ambient	Unknown (spin fluct.?)

Table 47.2.: Non-stoichiometric superconductors in the sense of Definition 47.1, i.e. superconducting only after substitution (doping x or fixed fractions) or with vacancies / interstitials (δ). All of them are unconventional (high-temperature) superconductors.

Definition 47.1 Consider an infinite crystal C_∞ as in Definition 3.7, i.e. an infinite Bravais-lattice L_∞ with lattice vectors $\bigcup_{j=1}^{d_x} \{\mathbf{a}_j\}$, unit-cell UC and atomic basis-vectors $\{\boldsymbol{R}_1, \dots, \boldsymbol{R}_r\} \subset$ UC, with crystal points $\boldsymbol{R}_{\mathbf{n}\kappa} = \mathbf{R}_\mathbf{n} + \boldsymbol{R}_\kappa$. In contrast to Definition 3.7, we interpret the $\boldsymbol{R}_{\mathbf{n}\kappa}$ here only as the *sites* at which an atom *can* sit (in the average structure, see below), and call $\kappa \in \{1, \dots, r\}$ the *site index*; sites that are never occupied are not included in the basis. Let $E_1, \dots, E_k$ be the chemical elements present, and let UC contain $N_{\text{fu}} \in \mathbb{N}$ *formula units*. For every site κ and element E_ℓ, $\ell \in \{1, \dots, k\}$, define the *site occupation*

$$o_{\kappa\ell} \in [0, 1], \qquad 0 < \sum_{\ell=1}^{k} o_{\kappa\ell} \leq 1, \tag{47.1}$$

i.e. the probability that the site $\boldsymbol{R}_{\mathbf{n}\kappa}$ is occupied by E_ℓ, equivalently the average over all $\mathbf{R}_\mathbf{n} \in \mathrm{L_f}$ of a finite crystal $\mathrm{C_f}$ (Remark 3.19.1) in the thermodynamic limit $N_p \to \infty$. Then $1 - \sum_\ell o_{\kappa\ell}$ is the vacancy probability of the site κ. The chemical formula $(E_1)_{\nu_1}(E_2)_{\nu_2}\cdots(E_k)_{\nu_k}$ has the indices

$$\nu_\ell = \frac{1}{N_{\mathrm{fu}}}\sum_{\kappa=1}^{r} o_{\kappa\ell}\,, \qquad \text{equivalently} \qquad \frac{\nu_\ell}{\nu_{\ell'}} = \lim_{N_p\to\infty}\frac{N_{a,\ell}}{N_{a,\ell'}}, \tag{47.2}$$

with $N_{a,\ell}$ the number of E_ℓ-atoms in the finite crystal $\mathrm{C_f}$ of N_p unit-cells, $\sum_\ell N_{a,\ell} \le rN_p = N_a$. The ν_ℓ do not depend on the (non-unique) decomposition „Crystal = Lattice + Basis“: enlarging UC by an integer factor m multiplies both r and N_{fu} by m.

1. The compound is called *stoichiometric* if every site is fully occupied by exactly one element, i.e. if for every κ there is exactly one $\ell(\kappa)$ with $o_{\kappa\ell} = \delta_{\ell,\ell(\kappa)}$. Then C_∞ is a crystal in the strict sense of Definition 3.7, i.e. every basis-vector $\boldsymbol{R}_\kappa$ carries a definite atom (with mass M_κ and charge Z_κe, as assumed in Chapter „Quantum Mechanics of Crystals“), the crystal is strictly L_∞-periodic, and $\sum_\ell N_{a,\ell} = N_a = rN_p$. With r_ℓ the number of basis-vectors carrying E_ℓ ($\sum_\ell r_\ell = r$) one has $\nu_\ell = r_\ell/N_{\mathrm{fu}} \in \mathbb{N}$ for $N_{\mathrm{fu}} = \gcd(r_1,\dots,r_k)$, i.e. the composition is fixed by the crystal structure. Examples: MgB_2 ($r=3$, $r_{\mathrm{Mg}}=1$, $r_{\mathrm{B}}=2$, $N_{\mathrm{fu}}=1$), Nb_3Sn ($r=8$, $r_{\mathrm{Nb}}=6$, $r_{\mathrm{Sn}}=2$, $N_{\mathrm{fu}}=2$), LiFeAs, FeSe. If a phase exists *only* at this composition, it is called a *line compound* (or *daltonide*).
2. The compound is called *non-stoichiometric* (or a *berthollide*) if $o_{\kappa\ell} \in (0,1)$ for some κ,ℓ. Then the ν_ℓ are in general not integers, and a single realization of the material is *not* a crystal in the sense of Definition 3.7: the assumptions „no disorder, no vacancies“ of Chapter „Quantum Mechanics of Crystals“ are violated, translation symmetry under L_∞ holds only for the configurational average, and the quoted space group is that of the *average structure*.

For non-stoichiometric compounds the following conventions for the indices are used:

1. *Fixed fraction* (e.g. $Sr_{0.9}La_{0.1}CuO_2$): a specific sample with *substitutional disorder*. Two (or more) elements share a site κ, here with $o_{\kappa,\mathrm{Sr}} = 0.9$, $o_{\kappa,\mathrm{La}} = 0.1$ and $o_{\kappa,\mathrm{Sr}} + o_{\kappa,\mathrm{La}} = 1$ ($N_{\mathrm{fu}} = 1$); the total number of atoms per formula unit is unchanged.
2. *Variable* x (e.g. $La_{2-x}Sr_xCuO_4$): a one-parameter family of *solid solutions*

$$x \mapsto \mathrm{La}_{2-x}\mathrm{Sr}_x\mathrm{CuO}_4, \qquad x \in [0, x_{\max}], \tag{47.3}$$

   obtained by substitution on shared sites: in the primitive unit-cell ($N_{\mathrm{fu}} = 1$) the two equivalent La-sites κ have $o_{\kappa,\mathrm{Sr}} = x/2$, $o_{\kappa,\mathrm{La}} = 1 - x/2$, so that $\nu_{\mathrm{La}} + \nu_{\mathrm{Sr}} = 2$ for all x. The parameter x is chosen in the synthesis and is called the *doping*. If the substituting element has a different valence, x fixes the carrier concentration; e.g. $La^{3+} \to Sr^{2+}$ adds $p = x$ holes per formula unit (per CuO_2-plane).
3. *Deviation* δ (e.g. $YBa_2Cu_3O_{7-\delta}$, $HgBa_2CuO_{4+\delta}$): a deviation from an ideal stoichiometric reference crystal (with basis $\{\boldsymbol{R}_1,\dots,\boldsymbol{R}_{r^{(0)}}\}$, occupations $o^{(0)}_{\kappa\ell} \in \{0,1\}$ and composition $\nu^{(0)}_\ell \in \mathbb{N}$) by *vacancies* ($-\delta$, $\delta > 0$: partially empty reference sites, $\sum_\ell o_{\kappa\ell} < 1$ for some $\kappa \le r^{(0)}$) or *interstitials* ($+\delta$: partially occupied additional sites $\boldsymbol{R}_\kappa$, $\kappa > r^{(0)}$, that are empty in the reference crystal). In contrast to x, the number of atoms per formula unit changes, $\sum_\ell \nu_\ell = \sum_\ell \nu^{(0)}_\ell \mp \delta$. Usually $0 \le \delta \ll 1$ (for YBCO, $\delta \in [0,1]$), and δ is set only indirectly, e.g. by annealing in oxygen, rather than fixed in the synthesis.

A superconductor that superconducts at a stoichiometric composition, i.e. without doping, is called a *stoichiometric superconductor*.

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