Phononic Influence on Spin and how to measure it in degenerate Energy-Levels ESR-Experiments

Uppsala University
Department of Physics and Astronomy, Materials Theory



Sebastian Kalhöfer

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1 Traditional ESR from a Non-Interacting Model

Notation 1.1 Consider a single particle[1] with charge q_e subject to the Hamiltonian[2]

$$H_0 \equiv -\boldsymbol{\mu} \cdot \boldsymbol{B} \equiv -\gamma_e \boldsymbol{S} \cdot \boldsymbol{B} \equiv g_{\mathrm{e}} \frac{-q_{\mathrm{e}}}{2m_{\mathrm{e}}} \boldsymbol{S} \cdot \boldsymbol{B} \equiv g_{\mathrm{e}} \frac{-q_{\mathrm{e}}}{2m_{\mathrm{e}}} \frac{\hbar}{2} \boldsymbol{\sigma} \cdot \boldsymbol{B} \equiv g_{\mathrm{e}} \frac{|e|}{2m_{\mathrm{e}}} \frac{\hbar}{2} \boldsymbol{\sigma} \cdot \boldsymbol{B} \tag{1.1}$$

with single-particle Hilbert-space $\mathcal{H} \equiv \mathbb{C}^2$.

Remark 1.1.1 Notice that this implies the following prefactor conventions and abbreviations:

$$\bullet\ q_{\mathrm{e}} \equiv -|e| < 0, \tag{1.2}$$

$$\bullet\ \boldsymbol{\mu} = +g_e \frac{q_e}{2m_e} \boldsymbol{S} = \gamma_e \boldsymbol{S}, \tag{1.3}$$

$$\bullet\ \gamma_e = +g_e \frac{q_e}{2m_e} = -g_e \frac{|e|}{2m_e} < 0, \tag{1.4}$$

$$\bullet\ \mu_{\mathrm{B}} = +\frac{|e|\hbar}{2m_e} > 0, \tag{1.5}$$

$$\bullet\ 0 < g_e \approx 2.002 = \text{"}g\text{-factor of a free electron"}. \tag{1.6}$$

Notation 1.2 Without loss of generality, we consider the magnetic field to be aligned in the z-direction

$$\boldsymbol{B} \equiv |B| \boldsymbol{e}_z \equiv B \boldsymbol{e}_z. \tag{1.7}$$

Lemma 1.3 For $\boldsymbol{B} = B\boldsymbol{e}_z$, eigenstates of the Hamiltonian are given by the usual unit-vectors

$$|\uparrow\rangle \equiv \boldsymbol{e}_x \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad |\downarrow\rangle \equiv \boldsymbol{e}_y \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{1.8}$$

with eigenenergies

[1] For example the electron with charge $q_e = -|e|$.

[2] Notice that this is the Hamiltonian that naturally appears in the Pauli-equation as Zeeman-contribution.

$$E_{\uparrow,0} \equiv +g_{\mathrm{e}}\frac{|e|}{2m_{\mathrm{e}}}\frac{\hbar}{2}B \equiv +g_{\mathrm{e}}\mu_{\mathrm{B}}\frac{B}{2} \equiv +\epsilon_z > 0 \quad \text{and} \quad E_{\downarrow,0} \equiv -g_{\mathrm{e}}\frac{|e|}{2m_{\mathrm{e}}}\frac{\hbar}{2}B = -g_{\mathrm{e}}\mu_{\mathrm{B}}\frac{B}{2} \equiv -\epsilon_z < 0 \tag{1.9}$$

Proof 1.3 Follows immediately from the diagonality of the third Pauli-matrix.

Using now the phenomenological fact, that electrons can be excited to higher energy-levels, when they absorb photons of a suitable frequency, we can excite the system (assuming it to be in the ground-state $|\downarrow\rangle$) by radiating electromagnetic waves on it with frequency ν fulfilling the equation

$$h\nu = \Delta E \equiv E_{\uparrow,0} - E_{\downarrow,0} = +g_{\mathrm{e}}\frac{|e|}{2m_{\mathrm{e}}}\hbar B. \tag{1.10}$$

Fixing the frequency ν to some typical value, and assuming $|e|, m_{\mathrm{e}}, \hbar$ to be known, and having an experimental setting to vary the magnetic field B and simultaneously detecting a possible energy-loss for the case of an excitation (see, for example, [Rieger] for details), one can determine the g-factor of the electron by using the equation above.

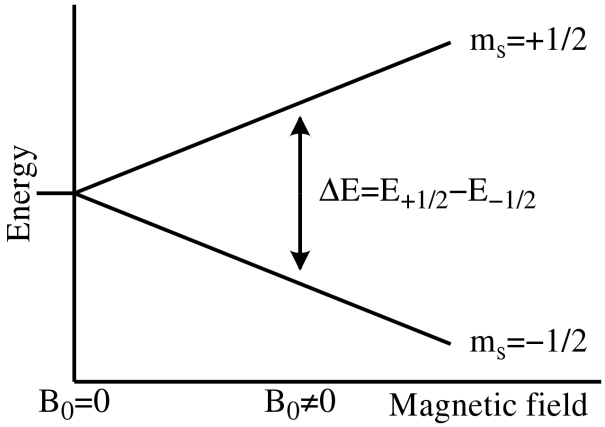


Figure 1.1: The image illustrates how one excites a spin-state with a photon of suitable energy.

2 ESR from an Interacting Model

2.1 Part 1: Electronic Part in Second Quantization

Notation 2.1 We assume to have the ordered single-particle basis of a single-particle Hilbert-space with two degenerate spin-states

$$\mathcal{H} = \text{span}_{\mathbb{C}} \{|1,\uparrow\rangle, |1,\downarrow\rangle, |2,\uparrow\rangle, |2,\downarrow\rangle\} \equiv \text{span}_{\mathbb{C}} \mathbb{B}, \tag{2.1}$$

such that the spin-operator (in SI-units) acts on these states as

$$\begin{aligned} S_z|j,\uparrow\rangle &= +\frac{\hbar}{2}|j,\uparrow\rangle, \\ S_z|j,\downarrow\rangle &= -\frac{\hbar}{2}|j,\downarrow\rangle, \end{aligned} \tag{2.2}$$

for $j = 1, 2$, as in the literature [].

Remark 2.1.1 Notice that this implies that the states are eigenstates of the Hamiltonian in Equation (1.1) as

$$\begin{aligned} H_0|j,\uparrow\rangle &= +\epsilon_z|j,\uparrow\rangle, \\ H_0|j,\downarrow\rangle &= -\epsilon_z|j,\downarrow\rangle, \end{aligned} \tag{2.3}$$

Remark 2.1.2 Notice that the single-particle Hilbert-space is 4-dimensional, i.e.

$$\dim_{\mathbb{C}} \mathcal{H} = \dim_{\mathbb{C}} \text{span}_{\mathbb{C}} \{|1,\uparrow\rangle, |1,\downarrow\rangle, |2,\uparrow\rangle, |2,\downarrow\rangle\} = 4 \tag{2.4}$$

Fact 2.2 Going over to the second quantized version yields for the spin-operator and the Hamiltonian the identities

$$S_z^{2Q} = \sum_{|\alpha\rangle\in\mathbb{B}} \langle\alpha|S_z|\alpha\rangle c_\alpha^\dagger c_\alpha = \frac{\hbar}{2}\left(n_{1,\uparrow} + n_{2,\uparrow} - (n_{1,\downarrow} + n_{2,\downarrow})\right), \tag{2.5}$$

$$H_0^{2Q} = \sum_{|\alpha\rangle\in\mathbb{B}} \langle\alpha|H_0|\alpha\rangle c_\alpha^\dagger c_\alpha = \epsilon_z\left(n_{1,\uparrow} + n_{2,\uparrow} - (n_{1,\downarrow} + n_{2,\downarrow})\right) = \mathbf{c}^\dagger\, \boldsymbol{\epsilon}\, \mathbf{c} \equiv \begin{pmatrix} c_{1,\uparrow} \\ c_{1,\downarrow} \\ c_{2,\uparrow} \\ c_{2,\downarrow} \end{pmatrix}^\dagger \begin{pmatrix} \epsilon_z & 0 & 0 & 0 \\ 0 & -\epsilon_z & 0 & 0 \\ 0 & 0 & \epsilon_z & 0 \\ 0 & 0 & 0 & -\epsilon_z \end{pmatrix} \begin{pmatrix} c_{1,\uparrow} \\ c_{1,\downarrow} \\ c_{2,\uparrow} \\ c_{2,\downarrow}, \end{pmatrix}$$

with the occupation-number operators $n_{j,\sigma} \equiv c^{\dagger}_{j,\sigma} c_{j,\sigma}$ for $(j,\sigma) \in \{1,2\} \times \{\uparrow,\downarrow\}$.

Remark 2.2.1 Most often, one drops the upper index and simply writes $H_0^{2Q} \equiv H_0$. One also oftentimes simply refers to the matrix ϵ as Hamiltonian $\epsilon \equiv H_0$.

Corollary 2.3 We obtain for the Green-function of the non-interacting electronic system

$$\mathscr{G}_0(\mathrm{i}\omega_n) = \frac{1}{\hbar} \frac{1}{\mathrm{i}\omega_n - \left(H_0 - \mu\right)/\hbar} = \begin{pmatrix} \frac{1}{\hbar\left(\mathrm{i}\omega_n - \omega_+\right)} & 0 & 0 & 0 \\ 0 & \frac{1}{\hbar\left(\mathrm{i}\omega_n - \omega_-\right)} & 0 & 0 \\ 0 & 0 & \frac{1}{\hbar\left(\mathrm{i}\omega_n - \omega_+\right)} & 0 \\ 0 & 0 & 0 & \frac{1}{\hbar\left(\mathrm{i}\omega_n - \omega_-\right)} \end{pmatrix} \tag{2.6}$$

with

$$\omega_\xi \equiv \frac{\xi \epsilon_z - \mu}{\hbar} \qquad \text{for } \xi \in \{-,+\}.$$

Proof 2.3 See [Flensberg, Negele Orland, Altland, Coleman].

2.2 Part 2: Introducing Phonons

We now introduce interactions with a single phonon-mode.

Notation 2.4 The Hamiltonian of the phonon-mode is

$$H_{\mathrm{Ph}} = \hbar\omega b^{\dagger} b. \tag{2.7}$$

and the interaction-Hamiltonian shall be obeying time-reversal symmetry

$$\begin{aligned} H_{\mathrm{int}} &\equiv \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}^{\dagger} \begin{pmatrix} 0 & V \\ V^{\dagger} & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \left(b + b^{\dagger}\right) \\ &\equiv \sum_{\substack{j,j' \in \{1,2\} \\ \sigma,\sigma' \in \{\uparrow,\downarrow\}}} W^{\sigma,\sigma'}_{j,j'} c^{\dagger}_{j,\sigma} c_{j',\sigma'} \left(b + b^{\dagger}\right) \end{aligned}$$

We denote the expansion of the interaction-matrix w.r.t. the Pauli-matrices as

$$\mathrm{V} \equiv v_0 \sigma^0 + \mathbf{v} \cdot \boldsymbol{\sigma}.$$

Lemma 2.5 Assuming we know the self-energy $\Sigma(\mathrm{i}\omega_n) \equiv \Sigma$, then it follows for the electronic Green-function

$$\mathscr{G}(\mathrm{i}\omega_n) = \frac{1}{\hbar} \frac{1}{\mathrm{i}\omega_n - \left(H_0 + \Sigma(\mathrm{i}\omega_n) - \mu\right)/\hbar} \tag{2.8}$$

Proof 2.5 See [Flensberg, Negele Orland, Altland, Coleman].

Remark 2.5.1 Notice that the entire system that we consider can now be written as

$$H_{\mathrm{Tot}} \approx H_{\mathrm{El}} + H_{\mathrm{Ph}} + H_{\mathrm{Int}}$$

with

- $H_{\mathrm{El}} = \mathbf{c}^\dagger \,\mathrm{diag}(+\epsilon_z, -\epsilon_z, +\epsilon_z, -\epsilon_z)\mathbf{c}$,
- $H_{\mathrm{Ph}} = \hbar\omega b^\dagger b$,
- $H_{\mathrm{Int}} = \sum_{\substack{j,j'\in\{1,2\} \\ \sigma,\sigma'\in\{\uparrow,\downarrow\}}} W_{j,j'}^{\sigma,\sigma'} c_{j,\sigma}^\dagger c_{j',\sigma'} \left(b + b^\dagger\right)$

2.3 Part 3: Key Formulae

Definition 2.6 We use the definition of the lesser and greater Green-function [][]

$$G^<_{\alpha,\alpha'}(t) = +\frac{\mathrm{i}}{\hbar} \left\langle c^\dagger_{\alpha'}(0) c_\alpha(t) \right\rangle \tag{2.9}$$

$$G^>_{\alpha,\alpha'}(t) = -\frac{\mathrm{i}}{\hbar} \left\langle c_\alpha(t) c^\dagger_{\alpha'}(0) \right\rangle \tag{2.10}$$

whereas $\langle \cdots \rangle$ denote the thermal expectation-value and we are using the grand canonical Heisenberg time-evolution-operators [].

Theorem 2.7 The [F]luctation-[D]issipation-[T]heorem states

$$G^<_{\alpha\alpha'}(\omega) = -2\mathrm{i}\, \mathrm{n}_F(\omega)\, \mathrm{Im} \lim_{\eta\to 0} G^{\mathrm{ret}}_{\alpha\alpha'}(\omega + \mathrm{i}\eta) \tag{2.11}$$

$$G^>_{\alpha\alpha'}(\omega) = 2\mathrm{i} \left(1 - \mathrm{n}_F(\omega)\right) \mathrm{Im} \lim_{\eta\to 0} G^{\mathrm{ret}}_{\alpha\alpha'}(\omega + \mathrm{i}\eta). \tag{2.12}$$

with Fermi-function

$$\mathrm{n}_F(\omega) = \frac{1}{\mathrm{e}^{\hbar\beta\omega} + 1} \tag{2.13}$$

Proof 2.7 See [][] for the proof in case of an electron gas.

Theorem 2.8 One can reexpress the average particle number through Green-functions as

$$\langle N_{\text{tot}} \rangle = \frac{-1}{\pi} \lim_{\eta \to 0} \int \mathrm{d}E \, \mathrm{F}_\beta(E) \, \mathrm{Im} \, \mathrm{Tr} \, G^{\text{ret}}_{\alpha,\alpha}(E + \mathrm{i}\eta) \tag{2.14}$$

Proof 2.8 Analog to the proof for the magnetization below.

Remark 2.8.1 The value of μ has to be determined, by (numerically) solving an equation dictating the average particle number.

Theorem 2.9 One obtains for the magnetization along the z-axis the formula

$$M_z = \langle \mu_z^{2\text{Q}} \rangle = g_e \frac{|e|}{2m_e} \frac{\hbar}{2\pi} \lim_{\tilde{\eta} \to 0} \oint\!\!\!\!\!\!\sum_{E,j} n_F(E) \, \mathrm{Im} \left[\left(G^{\text{ret}}_{\substack{j,j \\ \uparrow,\uparrow}} - G^{\text{ret}}_{\substack{j,j \\ \downarrow,\downarrow}} \right) (E + \mathrm{i}\tilde{\eta}) \right] \tag{2.15}$$

Remark 2.9.1 Notice that this equation yields the correct unit for the magnetic moment

$$\begin{aligned}
[M_z] &= \frac{[e]}{[m_e]}[\hbar][1] && (2.16)\\
&= \frac{\text{Coulomb}}{\text{kilogram}} \times \text{kilogram} \times \frac{\text{meter}^2}{\text{seconds}^2} \times \text{seconds} && (2.17)\\
&= \frac{\text{Coulomb}}{\text{seconds}} \times \text{meter}^2 && (2.18)\\
&= \text{Ampere} \times \text{meter}^2 && (2.19)
\end{aligned}$$

Proof 2.9 We can re-express the expectation-value of the spin-operator through the retarded Green-function[1] as

[1] Recall that the retarded Green can be obtained from the Matsubara-Green-function

$$\mathcal{G}(\mathrm{i}\omega_n) = \left(\mathrm{i}\hbar\omega_n - (\boldsymbol{\epsilon} + \boldsymbol{\Sigma}(\mathrm{i}\omega_n) - \mu) \right)^{-1} \tag{2.20}$$

by analytic continuation, with non-interacting contribution $\boldsymbol{\epsilon} = \mathrm{diag}(\epsilon_z, -\epsilon_z, \epsilon_z, -\epsilon_z)$ and self energy $\boldsymbol{\Sigma}^{(2)}(\mathrm{i}\omega_n) = \boldsymbol{\Sigma}^{\text{H}} + \boldsymbol{\Sigma}^{\text{F}}(\mathrm{i}\omega_n)$ as in the manuscript in the text above and below Equation (8), and in Equations (9)-(13).

$$\langle S_z^{2Q}\rangle = \frac{\hbar}{2}\left\langle n_{1,\uparrow} + n_{2,\uparrow} - \left(n_{1,\downarrow} + n_{2,\downarrow}\right)\right\rangle \tag{2.21}$$

$$= \frac{\hbar}{2}\frac{\hbar}{\mathrm{i}}\left[G^{<}_{\substack{1,1\\\uparrow,\uparrow}}(t=0) + G^{<}_{\substack{2,2\\\uparrow,\uparrow}}(t=0) - \left(G^{<}_{\substack{1,1\\\downarrow,\downarrow}}(t=0) + G^{<}_{\substack{2,2\\\downarrow,\downarrow}}(t=0)\right)\right] \tag{2.22}$$

$$= \frac{\hbar^2}{2\mathrm{i}}\sum_{j=1,2}\int\frac{\mathrm{d}\omega}{2\pi}\left(G^{<}_{\substack{j,j\\\uparrow,\uparrow}} - G^{<}_{\substack{j,j\\\downarrow,\downarrow}}\right)(\omega) \tag{2.23}$$

$$\overset{\text{FDT}}{=} \frac{\hbar^2}{4\pi\mathrm{i}}\cdot(-2\mathrm{i})\lim_{\eta\to 0}\sum_{j=1,2}\int_{-\infty}^{+\infty}\mathrm{d}\omega\, n_F(\omega)\,\mathrm{Im}\left[\left(G^{\mathrm{ret}}_{\substack{j,j\\\uparrow,\uparrow}} - G^{\mathrm{ret}}_{\substack{j,j\\\downarrow,\downarrow}}\right)(\omega+\mathrm{i}\eta)\right] \tag{2.24}$$

$$\equiv \frac{-\hbar}{2\pi}\lim_{\tilde{\eta}\to 0}\oint\!\!\!\!\!\!\sum_{E,j} n_F(E)\,\mathrm{Im}\left[\left(G^{\mathrm{ret}}_{\substack{j,j\\\uparrow,\uparrow}} - G^{\mathrm{ret}}_{\substack{j,j\\\downarrow,\downarrow}}\right)(E+\mathrm{i}\tilde{\eta})\right] \tag{2.25}$$

Since the spin-operator S_z is proportional to the operator for the magnetic moment (see Appendix, response to the second reviewer, Equation (TBReferenced)) with proportionality constant $\gamma_e\hbar$ as

$$\gamma_e \mathbf{S} = \boldsymbol{\mu} \tag{2.26}$$

we can compute the magnetization $\mathbf{M}$ of the system as expectation-value, e.g. (focusing on the z-component) by using the expression for the gyromagnetic ratio

$$M_z = \langle\mu_z^{2Q}\rangle = g_e\frac{|e|}{2m_e}\frac{\hbar}{2\pi}\lim_{\tilde{\eta}\to 0}\oint\!\!\!\!\!\!\sum_{E,j} n_F(E)\,\mathrm{Im}\left[\left(G^{\mathrm{ret}}_{\substack{j,j\\\uparrow,\uparrow}} - G^{\mathrm{ret}}_{\substack{j,j\\\downarrow,\downarrow}}\right)(E+\mathrm{i}\tilde{\eta})\right] \tag{2.27}$$

Theorem 2.10 Further "sanity-checks" can be introduced, by demanding that the CAR are fulfilled

$$\delta_{\alpha,\alpha'} = \left\langle\{c_\alpha,\, c^\dagger_{\alpha'}\}\right\rangle = -\frac{1}{\pi}\lim_{\eta\to 0}\int\mathrm{d}E\ \mathrm{Im}\, G^{\mathrm{ret}}_{\alpha,\alpha'}(E+\mathrm{i}\eta)$$

which leads, together with Equation (2.4) to the normalization-condition

$$4 = -\frac{1}{\pi}\lim_{\eta\to 0}\int\mathrm{d}E\ \mathrm{Im}\,\mathrm{Tr}\, G^{\mathrm{ret}}(E+\mathrm{i}\eta) \tag{2.28}$$

Proof 2.10 Follows from the fluctation-dissipation-theorem.

Fact 2.11 The electronic density of states $\rho(\omega)$ is given as

$$\rho(\omega) = -\frac{\hbar}{\pi}\sum_\alpha \mathrm{Im}\lim_{\eta\to 0} G^{\mathrm{ret}}_{\alpha,\alpha}(\omega+\mathrm{i}\eta) \tag{2.29}$$

Note that this formula holds in the non-interacting *and* in the interacting case [Mahan].

2.4 Part 4: Derivation of the Self-Energy

Theorem 2.12 In a second-order-approximation in the interaction-strength, there are two contributions to the self-energy originating from the Hartree- and the Fock-diagrams, whereas the former turns out to be energy-independent:

$$\Sigma(\mathrm{i}\omega_n) = \sum_{j=0}^{\infty} \Sigma^{(j)}(\mathrm{i}\omega_n) \approx 0 + \Sigma^{(2)}(\mathrm{i}\omega_n) + 0 + \mathcal{O}(\mathrm{V}^4) \tag{2.30}$$

with

$$\Sigma^{(2)}(\mathrm{i}\omega_n) = \Sigma^{\mathrm{Hartree}} + \Sigma^{\mathrm{Fock}}(\mathrm{i}\omega_n) \tag{2.31}$$

and self-energies as

$$\Sigma^{\mathrm{Hartree}}_{\xi,\xi'}(\mathrm{i}\omega_n) = W_{\xi\xi'}\mathscr{D}_0(0)\,\mathrm{Tr}\,(WC) \tag{2.32}$$

for the Hartree-contribution with a diagonal matrix C defined as

1. $\zeta = \zeta' \in \{(1,\uparrow),(2,\uparrow)\}$: $C_{\zeta'\zeta} = \mathrm{F}_{\hbar\beta}(\omega_+)$
2. $\zeta = \zeta' \in \{(1,\downarrow),(2,\downarrow)\}$: $C_{\zeta'\zeta} = \mathrm{F}_{\hbar\beta}(\omega_-)$

and

$$\Sigma^{\mathrm{Fock}}_{\xi,\zeta'}(\mathrm{i}\omega_n) \equiv -\Big[WM(\mathrm{i}\omega_n)W\Big]_{\xi,\zeta'}$$

1. $\xi' = \zeta \in \{(1,\uparrow),(2,\uparrow)\}$:

$$M_{\xi',\zeta}(\mathrm{i}\omega_n) = \frac{-1}{\hbar}\left[\frac{\mathrm{B}_{\hbar\beta}(\omega) + \mathrm{F}_{\hbar\beta}(\omega_+)}{\mathrm{i}\omega_n - \omega_+ + \omega} + \frac{\mathrm{B}_{\hbar\beta}(\omega) + 1 - \mathrm{F}_{\hbar\beta}(\omega_+)}{\mathrm{i}\omega_n - \omega_+ - \omega}\right]$$

2. $\xi' = \zeta \in \{(1,\downarrow),(2,\downarrow)\}$:

$$M_{\xi',\zeta}(\mathrm{i}\omega_n) = \frac{-1}{\hbar}\left[\frac{\mathrm{B}_{\hbar\beta}(\omega) + \mathrm{F}_{\hbar\beta}(\omega_-)}{\mathrm{i}\omega_n - \omega_- + \omega} + \frac{\mathrm{B}_{\hbar\beta}(\omega) + 1 - \mathrm{F}_{\hbar\beta}(\omega_-)}{\mathrm{i}\omega_n - \omega_- - \omega}\right]$$

Proof 2.12 of Theorem 2.12

Notice first, that going over to the field-integral-description of the problem gives the action

$$\begin{aligned} S[\chi,\overline{\chi}] = &\quad S_{\text{el}}[\psi,\overline{\psi}] &&+ \quad S_{\text{ph}}[\phi,\overline{\phi}] &&+ \quad S_{\text{el-ph-int}}[\chi,\overline{\chi}] \\ = &\oint\!\!\!\!\!\!\sum \overline{\psi}_{\alpha}(\tau)\Big[\Big(\partial_{\tau}-\frac{\mu}{\hbar}\Big)\delta_{\alpha,\alpha'}+\frac{h_{\alpha\alpha'}}{\hbar}\Big]\psi_{\alpha'}(\tau) + \int \overline{\phi}(\tau)\big[\partial_{\tau}+\omega\big]\phi(\tau) + S_{\text{el-ph-int}}[\chi,\overline{\chi}] \end{aligned}$$

with interaction-term

$$S_{\text{el-ph-int}}[\chi,\overline{\chi}] = \oint\!\!\!\!\!\!\sum \frac{W_{\xi\xi'}}{\hbar}\,\overline{\psi}_{\xi}(\tau)\psi_{\xi'}(\tau)\Big(\phi(\tau)+\overline{\phi}(\tau)\Big) \tag{2.33}$$

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

$$\mathscr{G}_{\alpha,\alpha'}(\mathrm{i}\omega_n) = \sum_{n=0}^{\infty}\Big[\big(\mathscr{G}_0\cdot\Sigma\big)^n(\mathrm{i}\omega_n)\cdot\mathscr{G}_0(\mathrm{i}\omega_n)\Big]_{\alpha,\alpha'} \tag{2.34}$$

$$\mathscr{G}_{\alpha,\alpha'}(\mathrm{i}\omega_n) = \int_0^{\hbar\beta}\mathrm{d}\tau\,\mathrm{e}^{\mathrm{i}\omega_n\tau}\,\mathscr{G}_{\alpha,\alpha'}(\tau) = \frac{-1}{\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau\,\mathrm{e}^{\mathrm{i}\omega_n\tau}\,\langle\psi_{\alpha}(\tau)\overline{\psi}_{\alpha'}(0)\rangle \tag{2.35}$$

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

$$\Sigma(\mathrm{i}\omega_n) = \sum_{j=0}^{\infty}\Sigma^{(j)}(\mathrm{i}\omega_n) \approx 0 + \Sigma^{(2)}(\mathrm{i}\omega_n) + 0 + \mathcal{O}(\mathrm{V}^4), \tag{2.36}$$

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

$$\mathscr{G}_{\alpha,\alpha'}(\mathrm{i}\omega_n) = \mathscr{G}_{\substack{0\\\alpha,\alpha'}}(\mathrm{i}\omega_n) + \big(\mathscr{G}_0\cdot\Sigma^{(2)}\cdot\mathscr{G}_0\big)_{\alpha,\alpha'}(\mathrm{i}\omega_n) \tag{2.37}$$

$$\mathscr{G}_{\alpha,\alpha'}(\mathrm{i}\omega_n) = \frac{-1}{\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau\,\mathrm{e}^{\mathrm{i}\omega_n\tau}\,\langle\psi_{\alpha}(\tau)\overline{\psi}_{\alpha'}(0)\rangle \tag{2.38}$$

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

$$\begin{aligned}\mathscr{G}_{\alpha,\alpha'}(\tau) &= \mathscr{G}^{(0)}_{\alpha,\alpha'}(\tau) + \mathscr{G}^{(1)}_{\alpha,\alpha'}(\tau) + \mathscr{G}^{(2)}_{\alpha,\alpha'}(\tau) + \dots \\ &= \mathscr{G}_{\substack{0\\ \alpha,\alpha'}}(\tau) + \quad 0 \quad + \mathscr{G}^{(2)}_{\alpha,\alpha'}(\tau) + \dots\end{aligned}$$

The second contribution reads

$$\mathscr{G}^{(2)}_{\alpha,\alpha'}(\tau) = \frac{1}{2!}\oint_{\substack{\tau_1,\tau_2\in[0,\hbar\beta]\\ \xi,\xi',\zeta,\zeta'\in\{1,2\}\times\{\uparrow,\downarrow\}}} \frac{-1}{\hbar}\frac{W_{\xi\xi'}W_{\zeta\zeta'}}{\hbar^2}\langle\psi_\alpha(\tau)\overline{\psi}_{\alpha'}(0)\left(\phi(\tau_1)+\overline{\phi}(\tau_1)\right)\overline{\psi}_\xi(\tau_1)\psi_{\xi'}(\tau_1)\left(\phi(\tau_2)+\overline{\phi}(\tau_2)\right)\overline{\psi}_\zeta(\tau_2)\psi_{\zeta'}(\tau_2)\rangle_0^{\mathrm{CD}} \tag{2.39}$$

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

$$\begin{aligned}&\frac{-1}{\hbar}\left\langle\psi_\alpha(\tau)\overline{\psi}_{\alpha'}(0)\left(\phi(\tau_1)+\overline{\phi}(\tau_1)\right)\overline{\psi}_\xi(\tau_1)\psi_{\xi'}(\tau_1)\left(\phi(\tau_2)+\overline{\phi}(\tau_2)\right)\overline{\psi}_\zeta(\tau_2)\psi_{\zeta'}(\tau_2)\right\rangle_0 \\ &= \frac{1}{\hbar}\left\langle\psi_\alpha(\tau)\psi_{\xi'}(\tau_1)\psi_{\zeta'}(\tau_2)\overline{\psi}_{\alpha'}(0)\overline{\psi}_\xi(\tau_1)\overline{\psi}_\zeta(\tau_2)\right\rangle_0\left\langle\left(\phi(\tau_1)+\overline{\phi}(\tau_1)\right)\left(\phi(\tau_2)+\overline{\phi}(\tau_2)\right)\right\rangle_0 \\ &= -\left\langle\psi_\alpha(\tau)\psi_{\xi'}(\tau_1)\psi_{\zeta'}(\tau_2)\overline{\psi}_{\alpha'}(0)\overline{\psi}_\xi(\tau_1)\overline{\psi}_\zeta(\tau_2)\right\rangle_0\mathscr{D}_0(\tau_1-\tau_2)\end{aligned}$$

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.

$$\begin{aligned}S_3 &= \left\{\pi_1,\pi_2,\pi_3,\pi_4,\pi_5,\pi_6\right\} \\ &= \left\{\begin{pmatrix}1&2&3\\1&2&3\end{pmatrix},\begin{pmatrix}1&2&3\\1&3&2\end{pmatrix},\begin{pmatrix}1&2&3\\2&1&3\end{pmatrix},\begin{pmatrix}1&2&3\\2&3&1\end{pmatrix},\begin{pmatrix}1&2&3\\3&1&2\end{pmatrix},\begin{pmatrix}1&2&3\\3&2&1\end{pmatrix}\right\}\end{aligned}$$

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

$$\begin{aligned}-\left\langle\psi_\alpha(\tau)\psi_{\xi'}(\tau_1)\psi_{\zeta'}(\tau_2)\overline{\psi}_{\alpha'}(0)\overline{\psi}_\xi(\tau_1)\overline{\psi}_\zeta(\tau_2)\right\rangle_0 &\equiv -\left\langle\psi(A_1)\psi(A_2)\psi(A_3)\overline{\psi}(B_1)\overline{\psi}(B_2)\overline{\psi}(B_3)\right\rangle_0 \\ &\equiv +\left\langle\psi(A_1)\psi(A_2)\psi(A_3)\overline{\psi}(B_3)\overline{\psi}(B_2)\overline{\psi}(B_1)\right\rangle_0 \\ &= +\sum_{\pi\in S_3}\mathrm{sgn}(\pi)\prod_{l=1}^{3}\left\langle\psi(A_l)\,\overline{\psi}(B_{\pi(l)})\right\rangle_0 \\ &= -\hbar^3\sum_{\pi\in S_3}\mathrm{sgn}(\pi)\prod_{l=1}^{3}\mathscr{G}_0(A_l,B_{\pi(l)})\end{aligned}$$

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

$$\begin{aligned} A_1 &\equiv (\alpha, \tau), \quad A_2 \equiv (\xi', \tau_1), \quad A_3 \equiv (\zeta', \tau_2) \\ B_1 &\equiv (\alpha', 0), \quad B_2 \equiv (\xi, \tau_1), \quad B_3 \equiv (\zeta, \tau_2) \end{aligned}$$

and therefore we obtain

$$\begin{aligned} B_{\pi_3(1)} \equiv B_2 \equiv (\xi, \tau_1), \quad B_{\pi_3(2)} \equiv B_1 \equiv (\alpha', 0), \quad B_{\pi_3(3)} \equiv B_3 \equiv (\zeta', \tau_2), \\ B_{\pi_4(1)} \equiv B_2 \equiv (\xi, \tau_1), \quad B_{\pi_4(2)} \equiv B_3 \equiv (\zeta, \tau_2), \quad B_{\pi_4(3)} \equiv B_1 \equiv (\alpha', 0). \end{aligned}$$

This gives now for the second-order-contribution

$$\begin{aligned} \mathscr{G}^{(2)}_{\alpha,\alpha'}(\tau) &= -\hbar \sum\!\!\!\!\!\!\int_{\substack{\tau_1,\tau_2 \in [0,\hbar\beta] \\ \xi,\xi',\zeta,\zeta' \in \{1,2\}\times\{\uparrow,\downarrow\}}} W_{\xi\xi'} W_{\zeta\zeta'}\, \mathscr{D}_0(\tau_1 - \tau_2) \sum_{\pi \in \{\pi_3,\pi_4\}} \operatorname{sgn}(\pi) \prod_{l=1}^{3} \mathscr{G}_0(A_l, B_{\pi(l)}) \\ &= \hbar \sum\!\!\!\!\!\!\int_{\substack{\tau_1,\tau_2 \in [0,\hbar\beta] \\ \xi,\xi',\zeta,\zeta' \in \{1,2\}\times\{\uparrow,\downarrow\}}} + W_{\xi\xi'} W_{\zeta\zeta'}\, \mathscr{G}_{0\,\alpha,\xi}(\tau - \tau_1)\, \mathscr{G}_{0\,\xi',\alpha'}(\tau_1 - 0)\, \mathscr{G}_{0\,\zeta',\zeta}(0)\, \mathscr{D}_0(\tau_1 - \tau_2) \\ &+ \hbar \sum\!\!\!\!\!\!\int_{\substack{\tau_1,\tau_2 \in [0,\hbar\beta] \\ \xi,\xi',\zeta,\zeta' \in \{1,2\}\times\{\uparrow,\downarrow\}}} - W_{\xi\xi'} W_{\zeta\zeta'}\, \mathscr{G}_{0\,\alpha,\xi}(\tau - \tau_1)\, \mathscr{G}_{0\,\xi',\zeta}(\tau_1 - \tau_2)\, \mathscr{G}_{0\,\zeta',\alpha'}(\tau_2 - 0)\, \mathscr{D}_0(\tau_1 - \tau_2) \\ &\equiv \mathscr{G}^{\text{Hartree}}_{\alpha,\alpha'}(\tau) \quad + \quad \mathscr{G}^{\text{Fock}}_{\alpha,\alpha'}(\tau) \end{aligned}$$

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 2.13 It holds

$$\mathscr{G}^{\text{Hartree}}_{\alpha,\alpha'}(\mathrm{i}\omega_n) = \sum_{\xi,\xi' \in \{1,2\}\times\{\uparrow,\downarrow\}} \mathscr{G}_{0\,\alpha,\xi}(\mathrm{i}\omega_n) \left(\frac{1}{\beta} \sum_{\substack{\omega_m \in \Omega_{-1} \\ \zeta,\zeta' \in \{1,2\}\times\{\uparrow,\downarrow\}}} + W_{\xi\xi'} W_{\zeta\zeta'} \mathscr{G}_{0\,\zeta',\zeta}(\mathrm{i}\omega_m)\, \mathscr{D}_0(0) \right) \mathscr{G}_{0\,\xi',\alpha'}(\mathrm{i}\omega_n) \tag{2.40}$$

Proof 2.13

We will now focus on the temporal components of the Hartree-contribution to the Green-function. For this we consider the function

$$\widetilde{\mathscr{G}}^{\text{Hartree}}(\tau) = \iint\limits_{[0,\hbar\beta]^2} \mathrm{d}(\tau_1,\tau_2)\, \mathscr{G}^{\,0}_{\alpha,\xi}(\tau-\tau_1)\mathscr{G}^{\,0}_{\xi',\alpha'}(\tau_1-0)\mathscr{G}^{\,0}_{\zeta',\zeta}(0)\mathscr{D}_0(\tau_1-\tau_2) \tag{2.41}$$

and this gives for the Matsubara-components

$$\begin{aligned}
\widetilde{\mathscr{G}}^{\text{Hartree}}(\mathrm{i}\omega_n) &= \int_0^{\hbar\beta} \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\omega_n\tau}\widetilde{\mathscr{G}}^{\text{Hartree}}(\tau) \\
&= \iiint\limits_{[0,\hbar\beta]^3} \mathrm{d}(\tau,\tau_1,\tau_2)\, \mathrm{e}^{\mathrm{i}\omega_n\tau}\mathscr{G}^{\,0}_{\alpha,\xi}(\tau-\tau_1)\mathscr{G}^{\,0}_{\xi',\alpha'}(\tau_1-0)\mathscr{G}^{\,0}_{\zeta',\zeta}(0)\mathscr{D}_0(\tau_1-\tau_2) \\
&= \dots
\end{aligned}$$

now we expand the statistical functions according to Lemma TBReferenced and we obtain

$$\begin{aligned}
\dots &= \frac{1}{(\hbar\beta)^4} \sum_{\substack{p_m\in\Omega_{+1}\\ \omega_{n_1},\omega_{n_2},\omega_{n_3}\in\Omega_{-1}}} \iiint\limits_{[0,\,\hbar\beta]^3} \mathrm{d}(\tau,\tau_1,\tau_2)\, \mathscr{G}^{\,0}_{\alpha,\xi}(\mathrm{i}\omega_{n_1})\mathscr{G}^{\,0}_{\xi',\alpha'}(\mathrm{i}\omega_{n_2})\mathscr{G}^{\,0}_{\zeta',\zeta}(\mathrm{i}\omega_{n_3})\,\mathscr{D}_0(\mathrm{i}p_m)\,\mathrm{e}^{\mathrm{i}\left(\omega_n\tau-\omega_{n_1}(\tau-\tau_1)-\omega_{n_2}\tau_1-p_m(\tau_1-\tau_2)\right)} \\
&= \sum_{\substack{p_m\in\Omega_{+1}\\ \omega_{n_1},\omega_{n_2},\omega_{n_3}\in\Omega_{-1}}} \mathscr{G}^{\,0}_{\alpha,\xi}(\mathrm{i}\omega_{n_1})\mathscr{G}^{\,0}_{\xi',\alpha'}(\mathrm{i}\omega_{n_2})\mathscr{G}^{\,0}_{\zeta',\zeta}(\mathrm{i}\omega_{n_3})\,\mathscr{D}_0(\mathrm{i}p_m)\frac{1}{(\hbar\beta)^4} \iiint\limits_{[0,\,\hbar\beta]^3} \mathrm{d}(\tau,\tau_1,\tau_2)\, \mathrm{e}^{\mathrm{i}\left(\tau(\omega_n-\omega_{n_1})+\tau_1(\omega_{n_1}-\omega_{n_2}-p_m)+\tau_2 p_m\right)} \\
&= \sum_{\substack{p_m\in\Omega_{+1}\\ \omega_{n_1},\omega_{n_2},\omega_{n_3}\in\Omega_{-1}}} \mathscr{G}^{\,0}_{\alpha,\xi}(\mathrm{i}\omega_{n_1})\mathscr{G}^{\,0}_{\xi',\alpha'}(\mathrm{i}\omega_{n_2})\mathscr{G}^{\,0}_{\zeta',\zeta}(\mathrm{i}\omega_{n_3})\,\mathscr{D}_0(\mathrm{i}p_m)\frac{1}{(\hbar\beta)}\delta_{\omega_n,\omega_{n_1}}\delta_{\omega_{n_1},\omega_{n_2}+p_m}\delta_{p_m,0} \\
&= \dots
\end{aligned}$$

We use the first, second and third delta-function in order to eliminate the summations over $\omega_{n_1}, \omega_{n_2}, p_m$ respectively. This yields then

$$\widetilde{\mathscr{G}}^{\text{Hartree}}(\mathrm{i}\omega_n) = \dots = \frac{1}{(\hbar\beta)} \sum_{\omega_{n_3}\in\Omega_{-1}} \mathscr{G}^{\,0}_{\alpha,\xi}(\mathrm{i}\omega_n)\mathscr{G}^{\,0}_{\xi',\alpha'}(\mathrm{i}\omega_n)\mathscr{G}^{\,0}_{\zeta',\zeta}(\mathrm{i}\omega_{n_3})\,\mathscr{D}_0(0)$$

or in short:

$$\begin{aligned}
&\widetilde{\mathscr{G}}^{\text{Hartree}}(\tau) = \iint\limits_{[0,\hbar\beta]^2} \mathrm{d}(\tau_1,\tau_2)\, \mathscr{G}^{\,0}_{\alpha,\xi}(\tau-\tau_1)\mathscr{G}^{\,0}_{\xi',\alpha'}(\tau_1-0)\mathscr{G}^{\,0}_{\zeta',\zeta}(0)\mathscr{D}_0(\tau_1-\tau_2) \\
\Rightarrow\quad &\widetilde{\mathscr{G}}^{\text{Hartree}}(\mathrm{i}\omega_n) = \frac{1}{(\hbar\beta)} \sum_{\omega_{n_3}\in\Omega_{-1}} \mathscr{G}^{\,0}_{\alpha,\xi}(\mathrm{i}\omega_n)\mathscr{G}^{\,0}_{\xi',\alpha'}(\mathrm{i}\omega_n)\mathscr{G}^{\,0}_{\zeta',\zeta}(\mathrm{i}\omega_{n_3})\,\mathscr{D}_0(0)
\end{aligned} \tag{2.42}$$

Using this identity for the Matsubara-component of a function proves the Lemma: We can compute the Fourier-Matsubara-component as

$$
\begin{aligned}
\mathscr{G}^{\text{Hartree}}_{\alpha,\alpha'}(\mathrm{i}\omega_n) &= \int_0^{\hbar\beta} \mathrm{d}\tau\, \mathscr{G}^{\text{Hartree}}_{\alpha,\alpha'}(\tau)\, \mathrm{e}^{\mathrm{i}\omega_n\tau} \\
&= \hbar \oint\!\!\!\!\!\!\sum_{\substack{\tau,\tau_1,\tau_2 \in [0,\hbar\beta] \\ \xi,\xi',\zeta,\zeta' \in \{1,2\}\times\{\uparrow,\downarrow\}}} + W_{\xi\xi'} W_{\zeta\zeta'}\, \mathscr{G}^{\,0}_{\alpha,\xi}(\tau-\tau_1)\, \mathscr{G}^{\,0}_{\xi',\alpha'}(\tau_1-0)\, \mathscr{G}^{\,0}_{\zeta',\zeta}(0)\, \mathscr{D}_0(\tau_1-\tau_2) \mathrm{e}^{\mathrm{i}\omega_n\tau} \\
&= \frac{1}{\beta} \sum_{\substack{\omega_{n_3} \in \Omega_{-1} \\ \xi,\xi',\zeta,\zeta' \in \{1,2\}\times\{\uparrow,\downarrow\}}} + W_{\xi\xi'} W_{\zeta\zeta'}\, \mathscr{G}^{\,0}_{\alpha,\xi}(\mathrm{i}\omega_n)\, \mathscr{G}^{\,0}_{\xi',\alpha'}(\mathrm{i}\omega_n)\, \mathscr{G}^{\,0}_{\zeta',\zeta}(\mathrm{i}\omega_{n_3})\, \mathscr{D}_0(0) \\
&= \sum_{\xi,\xi' \in \{1,2\}\times\{\uparrow,\downarrow\}} \mathscr{G}^{\,0}_{\alpha,\xi}(\mathrm{i}\omega_n) \left(\frac{1}{\beta} \sum_{\substack{\omega_{n_3} \in \Omega_{-1} \\ \zeta,\zeta' \in \{1,2\}\times\{\uparrow,\downarrow\}}} + W_{\xi\xi'} W_{\zeta\zeta'}\, \mathscr{G}^{\,0}_{\zeta',\zeta}(\mathrm{i}\omega_{n_3})\, \mathscr{D}_0(0) \right) \mathscr{G}^{\,0}_{\xi',\alpha'}(\mathrm{i}\omega_n)
\end{aligned}
$$

Fourier-Matsubara-Component of the Fock-Contribution

Lemma 2.14 It holds

$$
\mathscr{G}^{\text{Fock}}_{\alpha,\alpha'}(\mathrm{i}\omega_n) = \sum_{\xi,\zeta' \in \{1,2\}\times\{\uparrow,\downarrow\}} \mathscr{G}^{\,0}_{\alpha,\xi}(\mathrm{i}\omega_n) \left(\frac{1}{\beta} \sum_{\substack{\omega_m \in \Omega_{-1} \\ \xi',\zeta \in \{1,2\}\times\{\uparrow,\downarrow\}}} - W_{\xi\xi'} W_{\zeta\zeta'} \mathscr{G}^{\,0}_{\xi',\zeta}(\mathrm{i}\omega_m)\, \mathscr{D}_0(\mathrm{i}\omega_n - \mathrm{i}\omega_m) \right) \mathscr{G}^{\,0}_{\zeta',\alpha'}(\mathrm{i}\omega_n) \tag{2.43}
$$

Proof 2.14

We will now focus on the temporal components of the Fock-contribution to the Green-function. For this we consider the function

$$
\widetilde{\mathscr{G}}^{\text{Fock}}(\tau) = \iint_{[0,\hbar\beta]^2} \mathrm{d}(\tau_1,\tau_2)\, \mathscr{G}^{\,0}_{\alpha,\xi}(\tau-\tau_1) \mathscr{G}^{\,0}_{\xi',\zeta}(\tau_1-\tau_2) \mathscr{G}^{\,0}_{\zeta',\alpha'}(\tau_2) \mathscr{D}_0(\tau_1-\tau_2) \tag{2.44}
$$

and this gives for the Matsubara-components

$$
\begin{aligned}
\widetilde{\mathscr{G}}^{\text{Fock}}(\mathrm{i}\omega_n) &= \int_0^{\hbar\beta} \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\omega_n\tau} \widetilde{\mathscr{G}}^{\text{Fock}}(\tau) \\
&= \iiint_{[0,\hbar\beta]^3} \mathrm{d}(\tau,\tau_1,\tau_2)\, \mathrm{e}^{\mathrm{i}\omega_n\tau} \mathscr{G}^{\,0}_{\alpha,\xi}(\tau-\tau_1) \mathscr{G}^{\,0}_{\xi',\zeta}(\tau_1-\tau_2) \mathscr{G}^{\,0}_{\zeta',\alpha'}(\tau_2) \mathscr{D}_0(\tau_1-\tau_2) \\
&= \dots
\end{aligned}
$$

now we expand the statistical functions according to Lemma TBReferenced and we obtain

$$
\begin{aligned}
\dots &= \sum_{\substack{p_m \in \Omega_{+1} \\ \omega_{n'}, \omega_{n''}, \omega_{n'''} \in \Omega_{-1}}} \mathscr{G}^{\,0}_{\alpha,\xi}(\mathrm{i}\omega_{n'}) \mathscr{G}^{\,0}_{\xi',\zeta}(\mathrm{i}\omega_{n''}) \mathscr{G}^{\,0}_{\zeta',\alpha'}(\mathrm{i}\omega_{n'''}) \mathscr{D}_0(\mathrm{i}p_m) \frac{1}{(\hbar\beta)^4} \iiint\limits_{[0,\hbar\beta]^3} \mathrm{d}(\tau,\tau_1,\tau_2)\, \mathrm{e}^{\mathrm{i}\left(\omega_n\tau - \omega_{n'}(\tau-\tau_1) - \omega_{n''}(\tau_1-\tau_2) - \omega_{n'''}\tau_2 - p_m(\tau_1-\tau_2)\right)} \\
&= \sum_{\substack{p_m \in \Omega_{+1} \\ \omega_{n'}, \omega_{n''}, \omega_{n'''} \in \Omega_{-1}}} \mathscr{G}^{\,0}_{\alpha,\xi}(\mathrm{i}\omega_{n'}) \mathscr{G}^{\,0}_{\xi',\zeta}(\mathrm{i}\omega_{n''}) \mathscr{G}^{\,0}_{\zeta',\alpha'}(\mathrm{i}\omega_{n'''}) \mathscr{D}_0(\mathrm{i}p_m) \frac{1}{(\hbar\beta)^4} \iiint\limits_{[0,\hbar\beta]^3} \mathrm{d}(\tau,\tau_1,\tau_2)\, \mathrm{e}^{\mathrm{i}\left(\tau(\omega_n-\omega_{n'})+\tau_1(-p_m+\omega_{n'}-\omega_{n''})+\tau_2(p_m+\omega_{n''}-\omega_{n'''})\right)} \\
&= \sum_{\substack{p_m \in \Omega_{+1} \\ \omega_{n'}, \omega_{n''}, \omega_{n'''} \in \Omega_{-1}}} \mathscr{G}^{\,0}_{\alpha,\xi}(\mathrm{i}\omega_{n'}) \mathscr{G}^{\,0}_{\xi',\zeta}(\mathrm{i}\omega_{n''}) \mathscr{G}^{\,0}_{\zeta',\alpha'}(\mathrm{i}\omega_{n'''}) \mathscr{D}_0(\mathrm{i}p_m) \frac{1}{(\hbar\beta)} \delta_{\omega_n,\omega_{n'}} \delta_{p_m,\omega_{n'}-\omega_{n''}} \delta_{\omega_{n'''},p_m+\omega_{n''}} \\
&= \dots
\end{aligned}
\tag{2.45}
$$

Now notice that the Kronecker-deltas imply the relations

$$
\begin{aligned}
\omega_{n'} &= \omega_n \\
p_m &= \omega_{n'} - \omega_{n''} = \omega_n - \omega_{n''} \\
\omega_{n'''} &= p_m + \omega_{n''} = \omega_n
\end{aligned}
$$

which we will use to terminate the summations over $\omega_{n'}, p_m, \omega_{n'''}$.

This yields then

$$
\widetilde{\mathscr{G}}^{\mathrm{Fock}}(\mathrm{i}\omega_n) = \dots = \frac{1}{(\hbar\beta)} \sum_{\omega_{n''} \in \Omega_{-1}} \mathscr{G}^{\,0}_{\alpha,\xi}(\mathrm{i}\omega_n) \mathscr{G}^{\,0}_{\xi',\zeta}(\mathrm{i}\omega_{n''}) \mathscr{G}^{\,0}_{\zeta',\alpha'}(\mathrm{i}\omega_n) \mathscr{D}_0\left(\mathrm{i}(\omega_n - \omega_{n''})\right)
$$

Using this identity for the Matsubara-component of a function proves the Lemma: We can compute the Fourier-Matsubara-component as

$$
\begin{aligned}
\mathscr{G}^{\mathrm{Fock}}_{\alpha,\alpha'}(\mathrm{i}\omega_n) &= \int_0^{\hbar\beta} \mathrm{d}\tau\, \mathscr{G}^{\mathrm{Fock}}_{\alpha,\alpha'}(\tau)\, \mathrm{e}^{\mathrm{i}\omega_n\tau} \\
&= \hbar \sum\!\!\!\!\!\!\int_{\substack{\mathbf{q} \in \mathrm{Q} \\ \tau,\tau_1,\tau_2 \in [0,\hbar\beta] \\ \xi,\xi',\zeta,\zeta' \in \{1,2\}\times\{\uparrow,\downarrow\}}} -W_{\xi\xi'} W_{\zeta\zeta'} \mathscr{G}^{\,0}_{\alpha,\xi}(\tau-\tau_1) \mathscr{G}^{\,0}_{\xi',\zeta}(\tau_1-\tau_2) \mathscr{G}^{\,0}_{\zeta',\alpha'}(\tau_2-0) \mathscr{D}_0(\tau_1-\tau_2)\, \mathrm{e}^{\mathrm{i}\omega_n\tau} \\
&= \frac{1}{\beta} \sum_{\substack{\omega_{n''} \in \Omega_{-1} \\ \xi,\xi',\zeta,\zeta' \in \{1,2\}\times\{\uparrow,\downarrow\}}} -W_{\xi\xi'} W_{\zeta\zeta'} \mathscr{G}^{\,0}_{\alpha,\xi}(\mathrm{i}\omega_n) \mathscr{G}^{\,0}_{\xi',\zeta}(\mathrm{i}\omega_{n''}) \mathscr{G}^{\,0}_{\zeta',\alpha'}(\mathrm{i}\omega_n) \mathscr{D}_0\left(\mathrm{i}(\omega_n - \omega_{n''})\right) \\
&= \sum_{\xi,\zeta' \in \{1,2\}} \mathscr{G}^{\,0}_{\alpha,\xi}(\mathrm{i}\omega_n) \left(\frac{1}{\beta} \sum_{\substack{\omega_{n''} \in \Omega_{-1} \\ \xi',\zeta \in \{1,2\}\times\{\uparrow,\downarrow\}}} -W_{\xi\xi'} W_{\zeta\zeta'} \mathscr{G}^{\,0}_{\xi',\zeta}(\mathrm{i}\omega_{n''}) \mathscr{D}_0\left(\mathrm{i}(\omega_n - \omega_{n''})\right) \right) \mathscr{G}^{\,0}_{\zeta',\alpha'}(\mathrm{i}\omega_n)
\end{aligned}
$$

which proves the lemma.

Continuation of the Initial Proof

Continuing with the initial proof, we obtained in total

$$\begin{aligned}
\mathscr{G}^{(2)}_{\alpha,\alpha'}(\mathrm{i}\omega_n) &= \mathscr{G}^{\text{Hartree}}_{\alpha,\alpha'}(\mathrm{i}\omega_n) \quad + \quad \mathscr{G}^{\text{Fock}}_{\alpha,\alpha'}(\mathrm{i}\omega_n) \\
&\equiv \sum_{\xi,\xi' \in \{1,2\}\times\{\uparrow,\downarrow\}} \mathscr{G}^{\,0}_{\alpha,\xi}(\mathrm{i}\omega_n) \left(\frac{1}{\beta} \sum_{\substack{\omega_m \in \Omega_{-1} \\ \zeta,\zeta' \in \{1,2\}\times\{\uparrow,\downarrow\}}} + W_{\xi\xi'} W_{\zeta\zeta'} \mathscr{G}^{\,0}_{\zeta',\zeta}(\mathrm{i}\omega_m)\, \mathscr{D}_0(0) \right) \mathscr{G}^{\,0}_{\xi',\alpha'}(\mathrm{i}\omega_n) \\
&+ \sum_{\xi,\zeta' \in \{1,2\}\times\{\uparrow,\downarrow\}} \mathscr{G}^{\,0}_{\alpha,\xi}(\mathrm{i}\omega_n) \left(\frac{1}{\beta} \sum_{\substack{\omega_m \in \Omega_{-1} \\ \xi',\zeta \in \{1,2\}\times\{\uparrow,\downarrow\}}} - W_{\xi\xi'} W_{\zeta\zeta'} \mathscr{G}^{\,0}_{\xi',\zeta}(\mathrm{i}\omega_m)\, \mathscr{D}_0(\mathrm{i}\omega_n - \mathrm{i}\omega_m) \right) \mathscr{G}^{\,0}_{\zeta',\alpha'}(\mathrm{i}\omega_n) \\
&\equiv + \sum_{\xi,\xi' \in \{1,2\}\times\{\uparrow,\downarrow\}} \mathscr{G}^{\,0}_{\alpha,\xi}(\mathrm{i}\omega_n)\, \Sigma^{\text{Hartree}}_{\xi,\xi'}(\mathrm{i}\omega_n)\, \mathscr{G}^{\,0}_{\xi',\alpha'}(\mathrm{i}\omega_n) + \sum_{(\xi,\zeta') \in \{1,2\}^2} \mathscr{G}^{\,0}_{\alpha,\xi}(\mathrm{i}\omega_n)\, \Sigma^{\text{Fock}}_{\xi,\zeta'}(\mathrm{i}\omega_n)\, \mathscr{G}^{\,0}_{\zeta',\alpha'}(\mathrm{i}\omega_n) \\
&= \quad + \left(\mathscr{G}_0 \cdot \Sigma^{\text{Hartree}} \cdot \mathscr{G}_0 \right)_{\alpha,\alpha'}(\mathrm{i}\omega_n) \quad + \quad \left(\mathscr{G}_0 \cdot \Sigma^{\text{Fock}} \cdot \mathscr{G}_0 \right)_{\alpha,\alpha'}(\mathrm{i}\omega_n)
\end{aligned}$$

In the next step we will perform the Matsubara-summations and simplify the self-energy expressions.

The Hartree-Contribution

We focus on the first self-energy-contribution

$$\Sigma^{\text{Hartree}}_{\xi,\xi'}(\mathrm{i}\omega_n) = \frac{1}{\beta} \sum_{\substack{\omega_m \in \Omega_{-1} \\ \zeta,\zeta' \in \{1,2\}\times\{\uparrow,\downarrow\}}} + W_{\xi\xi'} W_{\zeta\zeta'}\, \mathscr{G}^{\,0}_{\zeta',\zeta}(\mathrm{i}\omega_m)\, \mathscr{D}_0(0) \equiv \sum_{\zeta,\zeta' \in \{1,2\}\times\{\uparrow,\downarrow\}} + W_{\xi\xi'} W_{\zeta\zeta'}\, \mathscr{D}_0(0) C_{\zeta'\zeta}$$

and evaluate the four different values of the Matsubara-sum

$$\frac{1}{\beta} \sum_{\omega_m \in \Omega_{-1}} \mathscr{G}^{\,0}_{\zeta',\zeta}(\mathrm{i}\omega_m) \equiv C_{\zeta'\zeta} \quad \text{for } \zeta, \zeta' \in \{1,2\} \times \{\uparrow,\downarrow\},$$

whereas only two of them will differ. This problem is tackled, by evaluating the two sums

1. $\zeta = \zeta' \in \{(1,\uparrow),(2,\uparrow)\}$:

   $$C_{\zeta'\zeta} = \frac{1}{\beta} \sum_{\omega_m \in \Omega_{-1}} \frac{1}{\hbar} \frac{1}{\mathrm{i}\omega_m - \omega_+} \equiv \frac{1}{\hbar\beta} \sum_{\omega_m \in \Omega_{-1}} h_\uparrow(\omega_m)$$

2. $\zeta = \zeta' \in \{(1,\downarrow),(2,\downarrow)\}$:

   $$C_{\zeta'\zeta} = \frac{1}{\beta} \sum_{\omega_m \in \Omega_{-1}} \frac{1}{\hbar} \frac{1}{\mathrm{i}\omega_m - \omega_-} \equiv \frac{1}{\hbar\beta} \sum_{\omega_m \in \Omega_{-1}} h_\downarrow(\omega_m)$$

For this, cf. also corollary "Corollary:Single-Pole-Summation" in the main document. In both cases we have to search for the poles of the functions $\mathbb{C} \ni z \mapsto h_\bullet(-\mathrm{i}z)$ which are $\omega_\pm$. Then it follows by the residual theorem with the auxiliary-function $z \mapsto g(z) = \dfrac{\hbar\beta}{\mathrm{e}^{\hbar\beta z} + 1}$

1. $\zeta = \zeta' \in \{(1,\uparrow),(2,\uparrow)\}$:

   $$C_{\zeta'\zeta} = \frac{1}{\beta} \sum_{\omega_m \in \Omega_{-1}} \frac{1}{\hbar} \frac{1}{\mathrm{i}\omega_m - \omega_+} \equiv \frac{1}{\hbar\beta} \sum_{\omega_m \in \Omega_{-1}} h_\uparrow(\omega_m) = \frac{1}{\hbar\beta} \operatorname{Res}\left(g(z)\, h_\uparrow(-\mathrm{i}z), z = \omega_+ \right) = \mathrm{F}_{\hbar\beta}(\omega_+)$$

2. $\zeta = \zeta' \in \{(1,\downarrow),(2,\downarrow)\}$:

$$C_{\zeta'\zeta} = \frac{1}{\beta}\sum_{\omega_m\in\Omega_{-1}} \frac{1}{\hbar}\frac{1}{\mathrm{i}\omega_m - \omega_-} \equiv \frac{1}{\hbar\beta}\sum_{\omega_m\in\Omega_{-1}} h_\downarrow(\omega_m) = \frac{1}{\hbar\beta}\,\mathrm{Res}\left(g(z)\,h_\downarrow(-\mathrm{i}z), z=\omega_-\right) = \mathrm{F}_{\hbar\beta}(\omega_-)$$

in this way we obtain

$$\begin{aligned}\Sigma^{\mathrm{Hartree}}_{\xi,\xi'}(\mathrm{i}\omega_n) &= \frac{1}{\beta}\sum_{\substack{\omega_m\in\Omega_{-1}\\ \zeta,\zeta'\in\{1,2\}\times\{\uparrow,\downarrow\}}} +W_{\xi\xi'}W_{\zeta\zeta'}\mathscr{G}_{\substack{0\\ \zeta',\zeta}}(\mathrm{i}\omega_m)\,\mathscr{D}_0(0)\\ &= \sum_{\zeta,\zeta'\in\{1,2\}\times\{\uparrow,\downarrow\}} +W_{\xi\xi'}W_{\zeta\zeta'}C_{\zeta',\zeta}\mathscr{D}_0(0)\\ &= W_{\xi\xi'}\mathscr{D}_0(0)\,\mathrm{Tr}\,(WC)\end{aligned} \tag{2.46}$$

The Fock-Contribution

$$\begin{aligned}\Sigma^{\mathrm{Fock}}_{\xi,\zeta'}(\mathrm{i}\omega_n) &= -\frac{1}{\beta}\sum_{\substack{\omega_m\in\Omega_{-1}\\ \xi',\zeta\in\{1,2\}\times\{\uparrow,\downarrow\}}} W_{\xi\xi'}W_{\zeta\zeta'}\mathscr{G}_{\substack{0\\ \xi',\zeta}}(\mathrm{i}\omega_m)\,\mathscr{D}_0(\mathrm{i}\omega_n - \mathrm{i}\omega_m)\\ &= -\sum_{\xi',\zeta\in\{1,2\}\times\{\uparrow,\downarrow\}} W_{\xi\xi'}\left(\frac{1}{\beta}\sum_{\omega_m\in\Omega_{-1}}\mathscr{G}_{\substack{0\\ \xi',\zeta}}(\mathrm{i}\omega_m)\,\mathscr{D}_{\substack{0\\ \mathbf{q},\mathbf{q}}}(\mathrm{i}\omega_n - \mathrm{i}\omega_m)\right)W_{\zeta\zeta'}\\ &= -\left[W\left(\frac{1}{\beta}\sum_{\omega_m\in\Omega_{-1}}\mathscr{G}_0(\mathrm{i}\omega_m)\,\mathscr{D}_0(\mathrm{i}\omega_n - \mathrm{i}\omega_m)\right)W\right]_{\xi,\zeta'}\\ &\equiv -\Big[WMW\Big]_{\xi,\zeta'}\end{aligned}$$

and evaluate the two different (four in total) different values of the Matsubara-sum

$$\frac{1}{\beta}\sum_{\omega_m\in\Omega_{-1}}\mathscr{G}_{\substack{0\\ \xi',\zeta}}(\mathrm{i}\omega_m)\,\mathscr{D}_0(\mathrm{i}\omega_n - \mathrm{i}\omega_m) \equiv M_{\xi',\zeta} \quad \text{for } \xi' = \zeta \in \{1,2\}\times\{\uparrow,\downarrow\},$$

by evaluating the sum

1. $\xi' = \zeta \in \{(1,\uparrow),(2,\uparrow)\}$:

$$M_{\xi',\zeta} = \frac{1}{\beta}\sum_{\omega_m\in\Omega_{-1}}\mathscr{G}_{\substack{0\\ \xi',\zeta}}(\mathrm{i}\omega_m)\,\mathscr{D}_0(\mathrm{i}\omega_n - \mathrm{i}\omega_m) = \frac{-2\omega}{\hbar^2\beta}\sum_{\omega_m\in\Omega_{-1}}\frac{1}{\mathrm{i}\omega_m - \omega_+}\frac{1}{\left(\omega_n - \omega_m\right)^2 + \omega^2} \equiv \sum_{\omega_m\in\Omega_{-1}} h_+(\omega_m)$$

2. $\xi' = \zeta \in \{(1,\downarrow),(2,\downarrow)\}$:

$$M_{\xi',\zeta} = \frac{1}{\beta}\sum_{\omega_m\in\Omega_{-1}}\mathscr{G}_{\substack{0\\ \xi',\zeta}}(\mathrm{i}\omega_m)\,\mathscr{D}_0(\mathrm{i}\omega_n - \mathrm{i}\omega_m) = \frac{-2\omega}{\hbar^2\beta}\sum_{\omega_m\in\Omega_{-1}}\frac{1}{\mathrm{i}\omega_m - \omega_-}\frac{1}{\left(\omega_n - \omega_m\right)^2 + \omega^2} \equiv \sum_{\omega_m\in\Omega_{-1}} h_-(\omega_m)$$

Evaluating the sums with the residue-theorem and rewriting the appearing terms with Fermi- and Bose-functions (cf. the corollary "Corollary:Triple-Pole-Summation" in the main document) yields

$$\sum_{\omega_m \in \Omega_{-1}} h_{\pm}(\omega_m) = \frac{-1}{\hbar}\left[\frac{\mathrm{B}_{\hbar\beta}(\omega) + \mathrm{F}_{\hbar\beta}(\omega_{\pm})}{\mathrm{i}\omega_n - \omega_{\pm} + \omega} + \frac{\mathrm{B}_{\hbar\beta}(\omega) + 1 - \mathrm{F}_{\hbar\beta}(\omega_{\pm})}{\mathrm{i}\omega_n - \omega_{\pm} - \omega}\right] \tag{2.47}$$

proving the before claimed identities for the self-energy.