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Heat Capacities in Crystals
(Reference Version)

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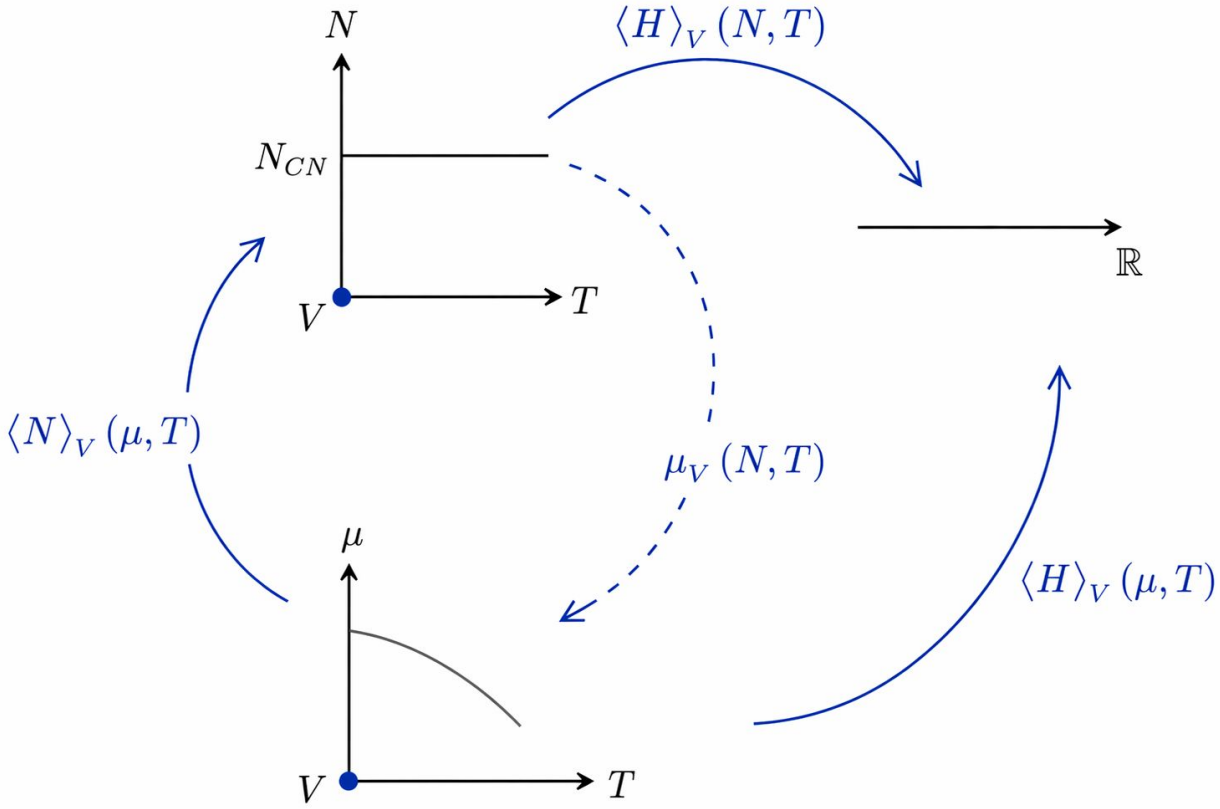
Quick Repetition on Thermodynamics:

Definition 9.31 We define the *heat capacity* of a system in the canonical ensemble as derivative

$$C_{V,N}(T) = T\left(\frac{\partial S}{\partial T}\right)_{V,N}(T) \tag{9.44}$$

Lemma 9.32 The following identities are immediate

$$\begin{aligned}
&\bullet \quad C_{V,N}(T) = \partial_T \langle H \rangle_{V,N}(T) \\
&\bullet \quad C_{V,N}(T) = -T\left(\partial_T^2 F\right)(N,T,V) \\
&\bullet \quad C_{V,N}(T) = k_{\mathrm{B}}\beta^2\left(\langle H^2\rangle_{N,V}(T) - \langle H\rangle_{N,V}^2(T)\right) = k_{\mathrm{B}}\beta^2\left\langle (H - \langle H\rangle)^2\right\rangle_{N,V,T} \geq 0
\end{aligned} \tag{9.45}$$


N
N_{CN}
V
T
$\langle H \rangle_V (N,T)$
$\mathbb{R}$
$\langle N \rangle_V (\mu,T)$
$\mu_V (N,T)$
μ
V
T
$\langle H \rangle_V (\mu,T)$

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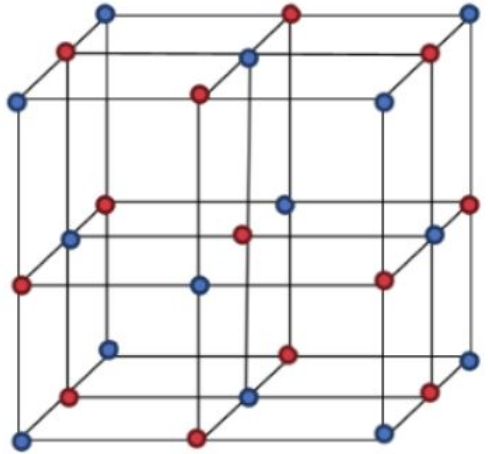
Corollary 9.38 Computing the specific heat capacity in the grand canonical ensemble one finds

$$\begin{aligned}
C_{N,V}(T) &= \partial_T \langle H\rangle(N,T,V) \\
&= \left(\partial_T \langle H\rangle\right)(\mu(T,V),T,V) + \left(\partial_\mu \langle H\rangle\right)(\mu(T,V),T,V)\cdot\left(\partial_T \mu\right)(N,V,T)
\end{aligned} \tag{9.53}$$

whereas the particle number N is kept constant.

Quick Repetition on Material-Theory:

- Crystal with …
  - volume V
  - number of cells N_p
  - r atoms in the unit-cell
  - temperature T



- Born-Oppenheimer-Approximation (...)

- Mean Field Approximation (...)

(“reliable” for “many” observables & materials)

Notation 20.19 Within usual approximations, we describe the union of two non-interacting gases

$$H = H_{\mathrm{el}} + H_{\mathrm{ph}} = \sum_{\substack{\mathbf{k}\in Q \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\dots,\infty\}}} \epsilon_{m\mathbf{k}\sigma} c^{\dagger}_{m\mathbf{k}\sigma} c_{m\mathbf{k}\sigma} + \sum_{\substack{\mathbf{q}\in Q \\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} \Omega_{\mathbf{q},\nu} b^{\dagger}_{\mathbf{q}\nu} b_{\mathbf{q}\nu} \tag{20.26}$$

$$\langle A\rangle \equiv \frac{\mathrm{Tr}_{\mathscr{H}}\, A\, \mathrm{e}^{-\beta\left(H_{\mathrm{el}}-\mu N_{\mathrm{el}}+H_{\mathrm{ph}}\right)}}{\mathrm{Tr}_{\mathscr{H}}\, \mathrm{e}^{-\beta\left(H_{\mathrm{el}}-\mu N_{\mathrm{el}}+H_{\mathrm{ph}}\right)}} \equiv \frac{\mathrm{Tr}_{\mathscr{H}}\, A\, \mathrm{e}^{-\beta\left(H_{\mathrm{el}}-\mu N_{\mathrm{el}}+H_{\mathrm{ph}}\right)}}{Z}. \qquad \mathscr{H} = \mathscr{H}_{\mathrm{F}} \otimes \mathscr{H}_{\mathrm{B}}$$

Fact 20.20 The expectation-value of the total internal energy can be computed as

$$\begin{aligned} \langle H\rangle_0 &= \langle H_{\mathrm{el}}\rangle_0 + \langle H_{\mathrm{ph}}\rangle_0 \\ &= \sum_{\substack{\mathbf{k}\in Q \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\dots,\infty\}}} \epsilon_{m\mathbf{k}\sigma}\, \mathrm{F}_{\beta}(\epsilon_{m\mathbf{k}\sigma}-\mu) + \sum_{\substack{\mathbf{q}\in Q \\ \nu\in\{1,\dots,rd_{\mathbf{x}}\}}} \Omega_{\nu}(\mathbf{q})\, \mathrm{B}_{\beta}(\Omega_{\nu}(\mathbf{q})) \end{aligned} \tag{20.27}$$

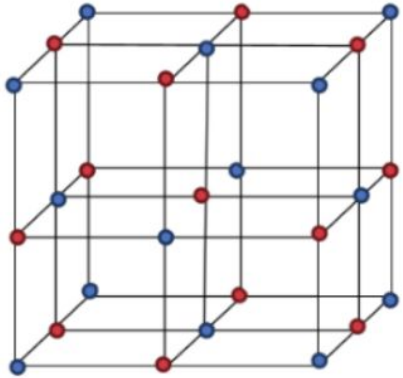
Sommerfeld-Approximation (1928 (?!)) + Low-Temperature Analysis of Ions:

$$C_{V,N,\mathrm{molar}}(T) = \frac{1}{n}\cdot C_{V,N}(T) \approx \gamma_m \cdot T + A\cdot T^3$$

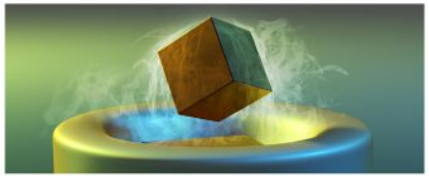
Quick repetition on Green-Functions

System („Cartoon“):

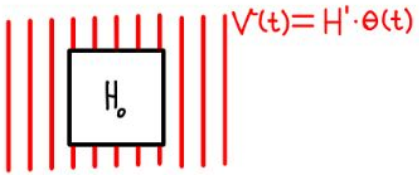
- **Any arbitrary Crystal:**



- **Superconductor**:



- **An arbitrary observable A of a System subjected to a „weak“ Perturbation H':**



Observable(s):

- **Electronic Density of States / Band-Structure:**

$$\rho_{n\mathbf{k}}(\omega) = -\frac{\hbar}{\pi}\,\mathrm{Im}\lim_{\epsilon\to 0} G^{\mathrm{ret}}_{\substack{n,n\\ \mathbf{k},\mathbf{k}}}(\omega + \mathrm{i}\epsilon) \qquad (10.12)$$

- **Magnetization[4]:**

$$\langle M\rangle \propto \sum_{\substack{\mathbf{k}\in\mathrm{Q}\\ n\in\{1,2,\dots\}\\ \omega\in(-\infty,+\infty)}} \int G^{<}_{\substack{n,n\\ \mathbf{k},\mathbf{k}\\ \uparrow,\uparrow}}(\omega) - G^{<}_{\substack{n,n\\ \mathbf{k},\mathbf{k}\\ \downarrow,\downarrow}}(\omega) \qquad (10.13)$$

- **Electronic / Phononic Heat Capacity:**

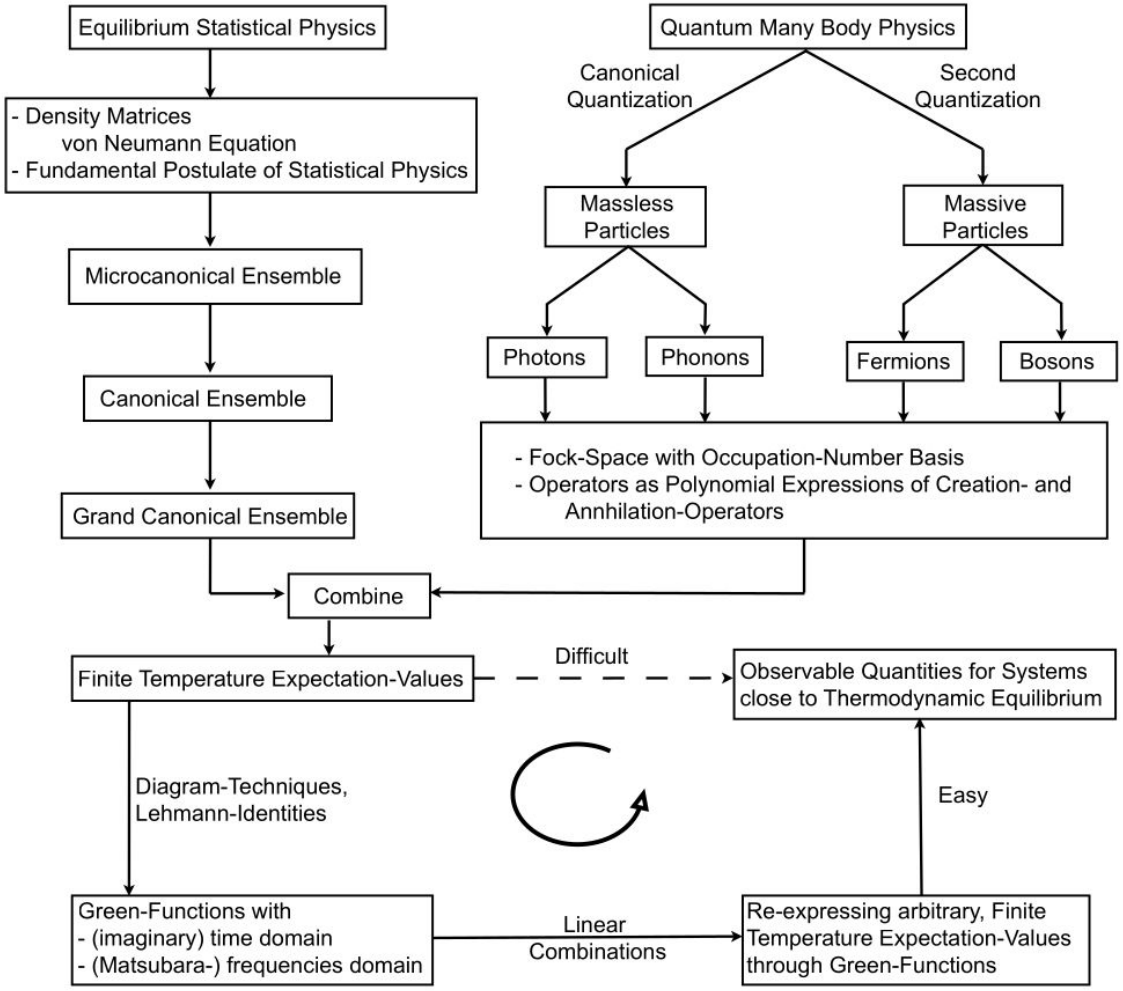
$$C_V(T) = \partial_T\langle H\rangle = \text{"sum of Green-functions"}^{5} \qquad (10.14)$$

- **Order Parameter[6] (in Eliashberg-Theory):**

$$\Delta_n(k) \propto \mathscr{G}^{\mathrm{Gorkov}}_{\substack{n\\ 1,2}}(k) \qquad (10.15)$$

- **Kubo-Formula:**

$$\langle A\rangle(t) = \langle A\rangle(t=-\infty) + \int \mathrm{d}t'\, G^{\mathrm{ret}}_{AH'}(t,t') + \mathcal{O}(H')^2$$


Equilibrium Statistical Physics
- Density Matrices
von Neumann Equation
- Fundamental Postulate of Statistical Physics
Microcanonical Ensemble
Canonical Ensemble
Grand Canonical Ensemble
Quantum Many Body Physics
Canonical Quantization
Second Quantization
Massless Particles
Massive Particles
Photons
Phonons
Fermions
Bosons
- Fock-Space with Occupation-Number Basis
- Operators as Polynomial Expressions of Creation- and Annhilation-Operators
Combine
Finite Temperature Expectation-Values
Difficult
Observable Quantities for Systems close to Thermodynamic Equilibrium
Diagram-Techniques, Lehmann-Identities
Easy
Green-Functions with
- (imaginary) time domain
- (Matsubara-) frequencies domain
Linear Combinations
Re-expressing arbitrary, Finite Temperature Expectation-Values through Green-Functions

Definition 7.26 We introduce the *statistical occupation-numbers* as set

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

Notation 8.1 When we speak about "Green-functions" (to be introduced later), we consider one of the following Hilbert-spaces:

$$(1)\quad \mathscr{H} \equiv \mathscr{H}_{m=0} = \mathrm{span}_{\mathbb{C}} \left\{ \prod_{j=1}^{\mathrm{d}} \frac{1}{\sqrt{n_j!}} \left(c_j^\dagger\right)^{n_j} |\,\mathrm{vac.}\,\rangle \equiv |n_1, n_2, \dots, n_{\mathrm{d}}\rangle \,\middle|\, n_1, n_2, \dots, n_{\mathrm{d}} \in \mathbb{N}_\zeta \right\} \quad \text{(massless particles)},$$

$$(2)\quad \mathscr{H} \equiv \mathscr{H}_{m>0} = \mathrm{span}_{\mathbb{C}} \left\{ \prod_{j=1}^{\mathrm{d}_M} \frac{1}{\sqrt{n_j!}} \left(c_j^\dagger\right)^{n_j} |\,\mathrm{vac.}\,\rangle \equiv |n_1, n_2, \dots, n_{\mathrm{d}_M}\rangle \,\middle|\, n_1, n_2, \dots, n_{\mathrm{d}_M} \in \mathbb{N}_\zeta \right\} \quad \text{(massive particles)},$$

$$(3)\quad \mathscr{H} = \mathscr{H}_{m>0} \otimes \mathscr{H}_{m=0} \quad \text{(massive-massless-mixtures)},$$

$$(4)\quad \mathscr{H} = \mathscr{H}_{m_1>0} \otimes \mathscr{H}_{m_2=0} \otimes \mathscr{H}_{m_3=0} \quad \text{(massive-massless-massless-mixtures)},$$

$$(5)\quad \mathscr{H} = \mathscr{H}_{m_1>0} \otimes \mathscr{H}_{m_2>0} \otimes \mathscr{H}_{m_3=0} \quad \text{(massive-massive-massless-mixtures)},$$

$$\vdots$$

Definition 8.3 We introduce the so-called *ensemble Hamiltonian* Ξ as

$$\Xi = \begin{cases} H & \text{for } \eta = 0 \text{ (massless particles)}, \\ H - \mu N & \text{for } \eta = 1 \text{ (massive particles)}, \\ H_{m>0} - \mu N_{m>0} + H_{m=0} + V_{\mathrm{int}} & \text{for massive-massless-mixtures}, \\ \quad \vdots & \end{cases} \tag{8.2}$$

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

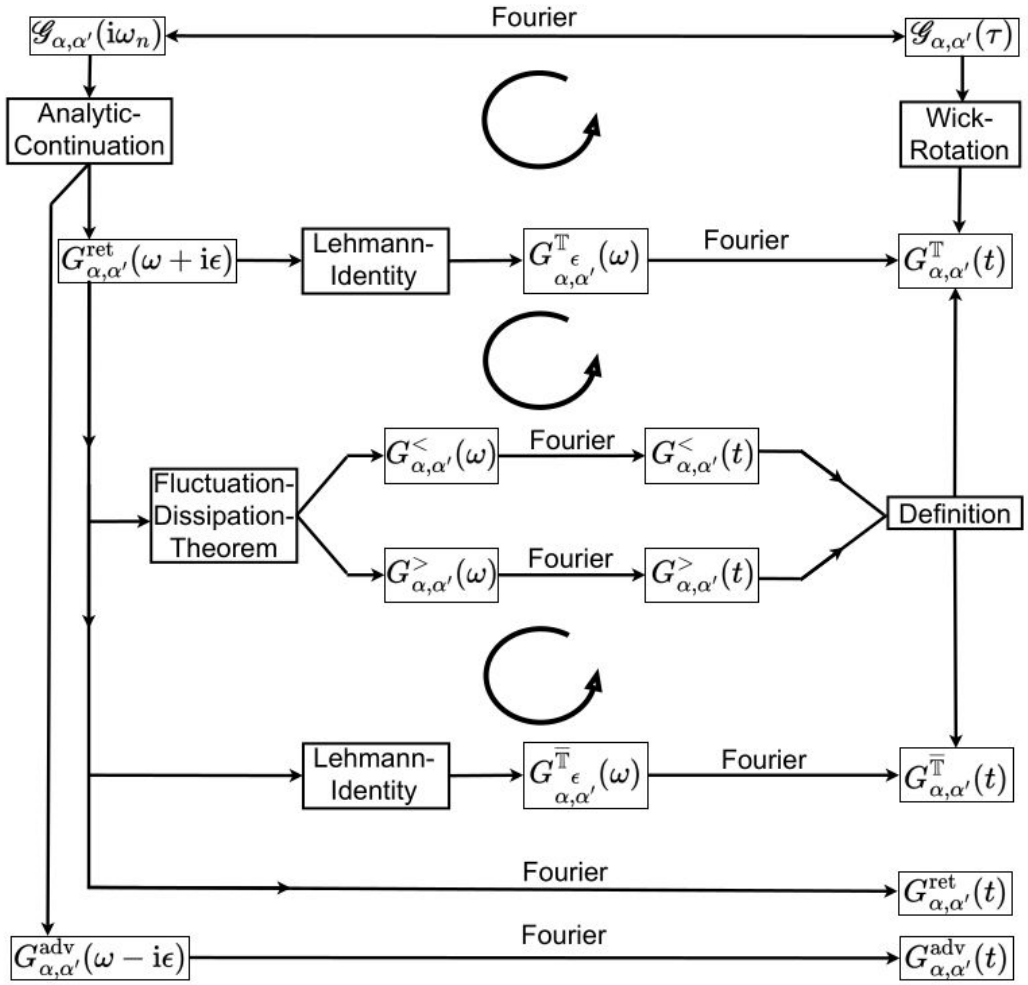
$$\left[c_\alpha, c^\dagger_{\alpha'}\right]_\zeta = \delta_{\alpha,\alpha'}, \qquad \mathrm{S}(c_\alpha) = \mathrm{S}(c^\dagger_{\alpha'}) = \zeta.$$

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*

$$\begin{aligned}
&\bullet\ G(A,A') \equiv G^{++}(A,A') \equiv G^{\mathrm{T}}(A,A') \equiv -\frac{\mathrm{i}}{\hbar}\left\langle \mathrm{T}_t\, c_\alpha(t) c^\dagger_{\alpha'}(t')\right\rangle,\\
&\bullet\qquad G^{+-}(A,A') \equiv G^{<}(A,A') \equiv -\frac{\mathrm{i}}{\hbar}\zeta\left\langle c^\dagger_{\alpha'}(t') c_\alpha(t)\right\rangle,\\
&\bullet\qquad G^{-+}(A,A') \equiv G^{>}(A,A') \equiv -\frac{\mathrm{i}}{\hbar}\left\langle c_\alpha(t) c^\dagger_{\alpha'}(t')\right\rangle,\\
&\bullet\qquad G^{--}(A,A') \equiv G^{\overline{\mathrm{T}}}(A,A') \equiv -\frac{\mathrm{i}}{\hbar}\left\langle \overline{\mathrm{T}}_t c_\alpha(t) c^\dagger_{\alpha'}(t')\right\rangle,\\
&\bullet\qquad G^{\mathrm{ret}}(A,A') = -\frac{\mathrm{i}}{\hbar}\theta(t-t')\left\langle \left[c_\alpha(t),\, c^\dagger_{\alpha'}(t')\right]_\zeta\right\rangle,\\
&\bullet\qquad G^{\mathrm{adv}}(A,A') = +\frac{\mathrm{i}}{\hbar}\theta(t'-t)\left\langle \left[c_\alpha(t),\, c^\dagger_{\alpha'}(t')\right]_\zeta\right\rangle.
\end{aligned}$$

with time-ordering-operator and ensemble-Heisenberg-time-evolution as usual.

Green's Chart



holds for

- **non-interacting systems**

AND for

- **interacting systems!**

Lemma 14.13 For a given chemical potential μ, we can compute the average number of particles as

$$\langle N \rangle = \frac{-1}{\pi} \lim_{\epsilon \to 0} \sum\!\!\!\!\!\!\int_{\substack{\alpha \in \mathscr{A} \\ E \in (-\infty, +\infty)}} \mathrm{n}_{\beta}^{\zeta}(E)\ \mathrm{Im}\ G_{\alpha,\alpha}^{\mathrm{ret}}(E + \mathrm{i}\epsilon)$$

Proof 26.45 of Lemma 14.13

We re-express the average particle number as lesser Green-functions and then use the fluctuation-dissipation-theorem

$$\begin{aligned} \langle N \rangle &= \sum_{\alpha \in \mathscr{A}} \langle c_{\alpha}^{\dagger} c_{\alpha} \rangle \\ &= -\zeta \frac{\hbar}{\mathrm{i}} \sum_{\alpha \in \mathscr{A}} G_{\alpha,\alpha}^{<}(t = 0) \\ &= -\zeta \frac{1}{2\pi \mathrm{i}} \sum\!\!\!\!\!\!\int_{\substack{\alpha \in \mathscr{A} \\ E \in (-\infty, +\infty)}} G_{\alpha,\alpha}^{<}(E) \\ &= \frac{-1}{\pi} \lim_{\eta \to 0} \sum\!\!\!\!\!\!\int_{\substack{\alpha \in \mathscr{A} \\ E \in (-\infty, +\infty)}} \mathrm{n}_{\beta}^{\zeta}(E)\ \mathrm{Im}\ G_{\alpha,\alpha}^{\mathrm{ret}}(E + \mathrm{i}\eta) \end{aligned} \tag{26.77}$$

Notation 21.1 We consider the interacting system that is described by the Hamiltonian from Definition 8.28 as

$$H = \sum_{\substack{\mathbf{k}\in Q \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\}}} \epsilon_{m\mathbf{k}\sigma} c^{\dagger}_{m\mathbf{k}\sigma} c_{m\mathbf{k}\sigma} + \sum_{\substack{\mathbf{q}\in Q \\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\}}} \hbar\omega_{\mathbf{q},\nu} b^{\dagger}_{\mathbf{q}\nu} b_{\mathbf{q}\nu} + \sum_{\substack{\mathbf{k},\mathbf{q}\in Q \\ \sigma\in\{\uparrow,\downarrow\} \\ \nu\in\{1,\ldots,rd_{\mathbf{x}}\} \\ m,n\in\{1,\ldots,\infty\}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\sqrt{N_p}} c^{\dagger}_{\mathbf{k}+\mathbf{q}m\sigma} c_{\mathbf{k}n\sigma} \left(b_{\mathbf{q}\nu} + b^{\dagger}_{-\mathbf{q}\nu} \right) \tag{21.1}$$

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Theorem 18.3 The electronic self-energy of this system reads can be approximated

$$\Sigma^{\mathrm{Fock}}_{\substack{\mathbf{k},\mathbf{k}'\\ m,m'\\ \mu,\mu'}}(\mathrm{i}\omega_n) = \delta_{\mathbf{k},\mathbf{k}'}\delta_{\mu,\mu'} \sum_{\substack{\mathbf{q}\in\mathrm{Q}\\ n\in\{1,2,\ldots\}\\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} \frac{g^{*}_{nm\nu}(\mathbf{k},\mathbf{q}) g_{nm'\nu'}(\mathbf{k},\mathbf{q})}{N_p} \left[\frac{\mathrm{B}_{\beta}(\Omega_{\nu}(\mathbf{q})) + \mathrm{F}_{\beta}(\xi_{\mathbf{q}+\mathbf{k}n\mu})}{\mathrm{i}\hbar\omega_n - \xi_{\mathbf{q}+\mathbf{k}n\mu} + \Omega_{\nu}(\mathbf{q})} + \frac{\mathrm{B}_{\beta}(\Omega_{\nu}(\mathbf{q})) + 1 - \mathrm{F}_{\beta}(\xi_{\mathbf{q}+\mathbf{k}n\mu})}{\mathrm{i}\hbar\omega_n - \xi_{\mathbf{q}+\mathbf{k}n\mu} - \Omega_{\nu}(\mathbf{q})} \right]$$

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$$\mathscr{G}_{\substack{m,m'\\ \sigma,\sigma'}}(\mathrm{i}\omega_n,\mathbf{k}) = \frac{\delta_{\sigma,\sigma'}}{\hbar} \left(\frac{1}{\mathrm{i}\omega_n - \left(H_{0,\sigma}(\mathbf{k}) + \Sigma_{\sigma}(\mathbf{k},\mathrm{i}\omega_n) - \mu \right)/\hbar} \right)_{m,m'}$$

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$$\langle N \rangle = \sum_{\substack{\mathbf{k}\in Q \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\}}} \langle n_{m\mathbf{k}\sigma} \rangle = \frac{-1}{\pi} \lim_{\delta\to 0} \oint \sum_{\substack{\mathbf{k}\in Q \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\} \\ E\in(-\infty,+\infty)}} \mathrm{F}_{\beta}(E)\, \mathrm{Im}\, G^{\mathrm{ret}}_{\substack{m,m \\ \sigma,\sigma \\ \mathbf{k},\mathbf{k}}}(E + \mathrm{i}\delta)$$

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$$\langle H_{\mathrm{el}} \rangle = \sum_{\substack{\mathbf{k}\in Q \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\}}} \epsilon_{m\mathbf{k}\sigma} \langle n_{m\mathbf{k}\sigma} \rangle = \frac{-1}{\pi} \lim_{\delta\to 0} \oint \sum_{\substack{\mathbf{k}\in Q \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\} \\ E\in(-\infty,+\infty)}} \epsilon_{m\mathbf{k}\sigma} \mathrm{F}_{\beta}(E) \operatorname{Im} G^{\mathrm{ret}}_{\substack{m,m \\ \sigma,\sigma}}(E+\mathrm{i}\delta,\mathbf{k})$$

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$$\langle N \rangle = \sum_{\substack{\mathbf{k}\in Q \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\}}} \langle n_{m\mathbf{k}\sigma} \rangle = \frac{-1}{\pi} \lim_{\delta\to 0} \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}\in Q \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\} \\ E\in(-\infty,+\infty)}} \mathrm{F}_{\beta}(E)\, \mathrm{Im}\, G^{\mathrm{ret}}_{\substack{m,m \\ \sigma,\sigma \\ \mathbf{k},\mathbf{k}}}(E+\mathrm{i}\delta)$$

$$\langle H_{\mathrm{el}} \rangle = \sum_{\substack{\mathbf{k}\in Q \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\}}} \epsilon_{m\mathbf{k}\sigma} \langle n_{m\mathbf{k}\sigma} \rangle = \frac{-1}{\pi} \lim_{\delta\to 0} \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}\in Q \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\ldots,\infty\} \\ E\in(-\infty,+\infty)}} \epsilon_{m\mathbf{k}\sigma}\, \mathrm{F}_{\beta}(E)\, \mathrm{Im}\, G^{\mathrm{ret}}_{\substack{m,m \\ \sigma,\sigma}}(E+\mathrm{i}\delta,\mathbf{k})$$

Problem (e.g. for the Phononic Contribution):

- the self-energy is no longer diagonal in k
- the displacement Green-function D (with polarization Pi) can in the interacting case no longer be related to the particle number

Cats in physics:

Cats in physics:

- Schrödingers cat

Cats in physics:

- Schrödingers cat
- F.D.C. Willard

Who was this physics-guy that made his cat a coauthor?

Ah, an inquiry both whimsical and rooted in the annals of our learned sciences—let me illuminate this curious tale for you:

In the year 1975, a distinguished physicist by the name of **Jack H. Hetherington** found himself in a most peculiar scholarly predicament. He had completed a theoretical paper on low-temperature physics destined for *Physical Review Letters*, only to discover, alas, that he had inadvertently written his manuscript in the plural ("we" and "our") despite being the sole contributor. In that era of typewriters and painstaking manual revision, altering every pronoun was no small task. Futility Closet +1

Rather than rewrite the work, this erudite gentleman chose a path of clever legerdemain: he added a second author… his beloved Siamese cat. The feline, christened **Chester**, was bestowed with the elegant academic pseudonym **F.D.C. Willard**—an abbreviation of *Felis Domesticus Chester Willard*, the latter name being that of the cat's sire. Under this name, the cat was listed as co-author on the published physics paper. Wikipedia

Thus did Chester the cat, under his dignified nom de plume, stride into scientific literature, not as a mere observer of human endeavour but as a celebrated co-signatory on a peer-reviewed work. Futility Closet

Cats in physics:

- Schrödingers cat
- F.D.C. Willard
- Ket-vectors

Cats in physics:

- Schrödingers cat
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- … another one!

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Cure: **Computer-Assisted Thermal Quantum Field Theory! (CAT-QFT)**

Theorem 17.23 One can rewrite the mixed partition function Z as a functional field integral

$$Z = \mathrm{Tr}_{\mathscr{H}} \exp -\beta \left(H_{m>0} - \mu N_{m>0} + H_{m=0} \right) = \int \mathscr{D}(\chi, \overline{\chi}) \, \mathrm{e}^{-S[\chi, \overline{\chi}]}$$

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$$\begin{aligned} S[\chi,\overline{\chi}] \equiv \quad & S_0[\chi,\overline{\chi}] && + \quad S_{\substack{m>0 \\ \mathrm{int}}}[\psi,\overline{\psi}] + S_{\substack{m=0 \\ \mathrm{int}}}[\phi,\overline{\phi}] + S_{\mathrm{int}}[\chi,\overline{\chi}] \\ = & \int_0^{\hbar\beta} \mathrm{d}\tau \begin{pmatrix} \overline{\psi} \\ \overline{\phi} \end{pmatrix}^{\mathrm{T}} \cdot \begin{pmatrix} \partial_\tau + \dfrac{H_{m>0} - \mu}{\hbar} & 0 \\ 0 & \partial_\tau + \dfrac{H_{m=0}}{\hbar} \end{pmatrix} \cdot \begin{pmatrix} \psi \\ \phi \end{pmatrix} && + \quad \int_0^{\hbar\beta} \mathrm{d}\tau\, \frac{V_{m>0}(\overline{\psi},\psi) + V_{m=0}(\overline{\phi},\phi) + V_{\mathrm{int}}(\overline{\chi},\chi)}{\hbar} \end{aligned}$$

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Theorem 17.17 For $\tau_1, \ldots, \tau_n, \tau_1', \ldots, \tau_n' \in (0, \hbar\beta)$ one finds for the imaginary-time n-body Green-Functions

$$\begin{aligned} \mathscr{G}(A_1, \ldots, A_n \mid A_n', \ldots, A_1') &= \left(-\frac{1}{\hbar}\right)^n \frac{1}{Z} \int \mathscr{D}_\zeta(\psi,\overline{\psi})\, \mathrm{e}^{-S[\psi,\overline{\psi}]}\, \psi_{\alpha_1}(\tau_1) \cdots \psi_{\alpha_n}(\tau_n)\, \overline{\psi}_{\alpha_1'}(\tau_1') \cdots \overline{\psi}_{\alpha_n'}(\tau_n') \\ &\equiv \left(-\frac{1}{\hbar}\right)^n \left\langle\, \psi(A_1) \cdots \psi(A_n)\, \overline{\psi}(A_1') \cdots \overline{\psi}(A_n') \,\right\rangle . \end{aligned}$$

Fact 21.4 Going over to the field-integral-description of the problem gives the action

$$S[\chi, \overline{\chi}] = S_{\text{el}}[\psi, \overline{\psi}] + S_{\text{ph}}[\phi, \overline{\phi}] + S_{\text{el-ph-int}}[\chi, \overline{\chi}]$$

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- $$S_{\text{el}}[\psi,\overline{\psi}] = \sum_{\substack{\mathbf{k}\in Q \\ \sigma\in\{\downarrow,\uparrow\} \\ \tau\in(0,\hbar\beta) \\ m\in\{1,2,\ldots,\infty\}}} \overline{\psi}_{m\sigma}(\tau,\mathbf{k})\left(\partial_\tau + \frac{\epsilon_{m\sigma}(\mathbf{k})-\mu}{\hbar}\right)\psi_{m\sigma}(\tau,\mathbf{k})$$

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Notation 21.5 We implement external sources into the partition-function as

$$Z \mapsto Z[j_{\text{el}},\overline{j}_{\text{el}},j_{\text{ph}},\overline{j}_{\text{ph}}] \equiv \int \mathscr{D}(\overline{\chi},\chi)\,\exp\left[-\left(S_{\text{el}}[\psi,\overline{\psi}] + S_{\text{ph}}[\phi,\overline{\phi}] + S_{\text{el-ph-int}}[\chi,\overline{\chi}]\right) + \sum_{\bullet\in\{\text{el,ph}\}} \overline{j}_\bullet\chi_\bullet + \overline{\chi}_\bullet j_\bullet\right] \tag{21.6}$$

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with abbreviations

- $$\overline{j}_{\text{el}}\chi_{\text{el}} \equiv \sum\!\!\!\!\!\!\int_{\substack{\mathbf{k}\in Q\\ \sigma\in\{\downarrow,\uparrow\}\\ \tau\in(0,\hbar\beta)\\ m\in\{1,2,\ldots,\infty\}}} \overline{j}_{m\sigma}(\tau,\mathbf{k})\psi_{m\sigma}(\tau,\mathbf{k})$$
- $$\overline{j}_{\text{ph}}\chi_{\text{ph}} \equiv \sum\!\!\!\!\!\!\int_{\substack{\mathbf{q}\in Q\\ \tau\in(0,\hbar\beta)\\ \nu\in\{1,2,\ldots,rd_{\mathbf{x}}\}}} \overline{j}_\nu(\tau,\mathbf{q})\phi_\nu(\tau,\mathbf{q})$$
- etc...

Lemma 21.16 For the phononic occupation numbers of the interacting system we have the identity

$$\langle H_{\mathrm{ph}} \rangle \approx -\frac{1}{\beta} \sum_{\substack{q \in \mathrm{i}\Omega_{+1} \times Q \\ \nu \in \{1,2,\ldots,rd_{\mathbf{x}}\}}} \mathrm{e}^{+\mathrm{i}\omega_q 0^+} \Omega_\nu(\mathbf{q}) \mathscr{G}_{0,\nu}(q)$$

Corollary 21.17 Evaluating the Matsubara-sums simplifies the individual terms as

$$\langle H_{\mathrm{ph}} \rangle \approx \sum_{\substack{\mathbf{q} \in Q \\ \nu \in \{1,2,\ldots,rd_{\mathbf{x}}\}}} \Omega_\nu(\mathbf{q}) \, \mathrm{B}_\beta(\Omega_\nu(\mathbf{q}))$$

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Corollary 21.17 Evaluating the Matsubara-sums simplifies the individual terms as

$$\begin{aligned}\langle H_{\mathrm{ph}}\rangle \approx & \sum_{\substack{\mathbf{q}\in Q\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}}}\Omega_\nu(\mathbf{q})\,\mathrm{B}_\beta(\Omega_\nu(\mathbf{q})) \quad + \quad \sum_{\nu\in\{1,2,\dots,rd_{\mathbf{x}}\}} A_\nu B_\nu^2\\ & -\sum_{\substack{\mathbf{k},\mathbf{q}\in Q\\ \sigma\in\{\downarrow,\uparrow\}\\ \nu\in\{1,2,\dots,rd_{\mathbf{x}}\}\\ n,n'\in\{1,\dots,\infty\}}}\frac{\Omega_\nu(\mathbf{q})}{N_p}|g_{n'n\nu}(\mathbf{k},\mathbf{q})|^2\left(\mathrm{F}_\beta(\xi_{n,\sigma,\mathbf{k}})-\mathrm{F}_\beta(\xi_{n',\sigma,\mathbf{k}+\mathbf{q}})\right)\left[\frac{\mathrm{B}_\beta(\Omega_\nu(\mathbf{q}))-\mathrm{B}_\beta(\xi_{n',\sigma,\mathbf{k}+\mathbf{q}}-\xi_{n,\sigma,\mathbf{k}})}{\left(\Omega_\nu(\mathbf{q})+\xi_{n,\sigma,\mathbf{k}}-\xi_{n',\sigma,\mathbf{k}+\mathbf{q}}\right)^2}+\frac{1}{4}\frac{\beta\,\mathrm{csch}(\beta\Omega_\nu(\mathbf{q})/2)^2}{\Omega_\nu(\mathbf{q})+\xi_{n,\sigma,\mathbf{k}}-\xi_{n',\sigma,\mathbf{k}+\mathbf{q}}}\right]\\ & +\mathcal{O}(g^4)\end{aligned}$$

with real coefficients A_ν and B_ν defined as

$$A_\nu=\Omega_\nu(\mathbf{q}=\mathbf{0})\mathscr{G}^2_{0,\nu}(q=0)=\Omega_\nu^{-1}(\mathbf{q}=\mathbf{0}),\qquad B_\nu=\frac{1}{\sqrt{N_p}}\sum_{\substack{\mathbf{k}\in Q\\ \sigma\in\{\downarrow,\uparrow\}\\ n\in\{1,\dots,\infty\}}} g_{nn\nu}(\mathbf{k},0)\,\mathrm{F}_\beta(\xi_{n\mathbf{k}\sigma}) \tag{21.24}$$

Workflow of the FPW-Project

Workflow of the FPW-Project

CIF-File

Workflow of the FPW-Project

CIF-File

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Detailed View Entry 1 of 1

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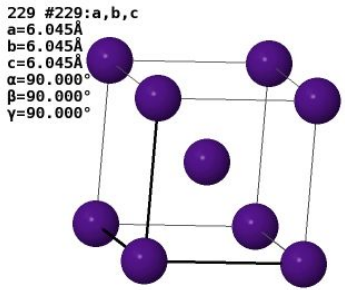
Summary Collection Code 196974

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Cell volume	220.90 [Å³]	Z	2
Temperature	5 [K]	Pressure	atmospheric
Data quality	Standard quality		
Author	Barrett, C.S.;	Title	X-ray study of the alkali metals at low temperatures
Reference	Acta Crystallographica (1956) 9, (8) p. 671-677 (12 structures)	Fulltext	Get full text by DOI Search full text by Google Scholar
See also	CCDC structures depot		

Details Expand all | Collapse all

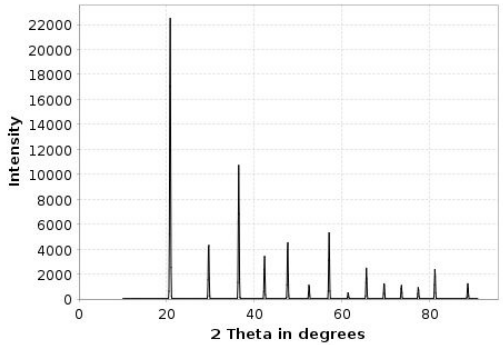
Visualization

Published Crystal Structure



Interactive Visualization

Powder Pattern



Interactive Visualization

Workflow of the EPW-Project

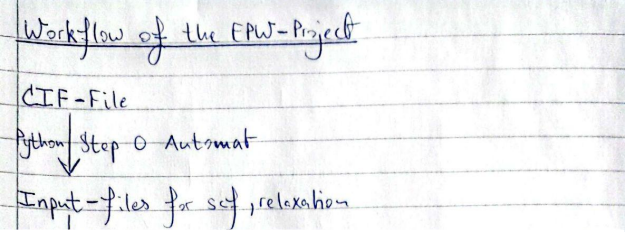
CIF-File

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  Au_Fm3m.cif                                       5431 Feb 13 18:20
  CIF-Files for the heat-capacities.pdf          2146399 Feb 13 19:09
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  Cu_Fm3m.cif                                       5345 Mai  5  2025
  Diamond_Fd3m.cif                                  6178 Feb 13 18:08
  KCl_Fm3m.cif                                      5570 Feb 13 17:30
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  Rb_Im3m.cif                                       3326 Feb 13 17:22
  Si_Fd3m1.cif                                      5854 Okt  2  2024

 Cs_Im3m.cif
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_cell_length_b 6.045(2)
_cell_length_c 6.045(2)
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_cell_angle_beta 90.
_cell_angle_gamma 90.
_cell_volume 220.9
_cell_formula_units_Z 2
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_space_group_IT_number 229
loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 'z, y, -x'
2 'y, x, -z'
3 'x, z, -y'
4 'z, x, -y'

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b_main_0.py

```python
import a_input_file as input
import z_utilities as utils

# Jobs
cif2cell_raw    = True
cell2clean_cell = True
AA_scf          = True
AB_relax        = True

# Step 0
tasks = [
    cif2cell_raw,
    cell2clean_cell,
    AA_scf,
    AB_relax
]

utils.print_intro()

utils.clean_directory(input.cif, cif2cell_raw)

utils.prepare_input_files_Step0(input.cif, tasks)

utils.add_further_templates(input.cif)

utils.print_outro()
```

Workflow of the EPW-Project

CIF-File

Python Step 0 Automat

Input-files for scf, relaxation

```
<-  ...ns_Box/BC_My_Codes/D_EPW_Project/A_Python/BA_Generated_Files/Cs_Im3m  -.[^]>-
.n                          Name                    Size   Modify time
/..                                                UP--DIR Feb 23 11:22
/Dispersions                                          4096 Feb  4 12:07
 AA_basic.in                                           965 Feb 23 11:22
 AB_vcrelax.in                                        1087 Feb 23 11:22
 Cs.upf                                             420444 Feb 23 11:22
 Step0.py                                             1726 Feb 23 11:22
 cell.in                                              1088 Feb 23 11:22

 AA_basic.in
                                                  387G / 724G (53%)
```

```
/home/sebastian/04_SL_D~les/Cs_Im3m/AA_basic.in       541/965                  56%
&CONTROL
  outdir       = './'
  prefix       = 'basic'
  pseudo_dir   = './'
  wf_collect   = .true.
  verbosity    = 'high'
  tprnfor      = .true.
  tstress      = .true.
  restart_mode = 'from_scratch'
  calculation  = 'scf'
/
&SYSTEM
  ibrav       = 0
  A           = 6.04500
  nat         = 1
  ntyp        = 1
  occupations = 'smearing'
  smearing    = 'gaussian'
  degauss     = 0.2d0
  input_dft   = 'pbe'
  ecutwfc     = 140
  ecutrho     = 600
  nbnd        = 50
/
&ELECTRONS
  conv_thr         = 1d-16
  mixing_beta      = 0.7d0
```

Workflow of the FPW-Project

CIF-File

Python Step 0 Automat

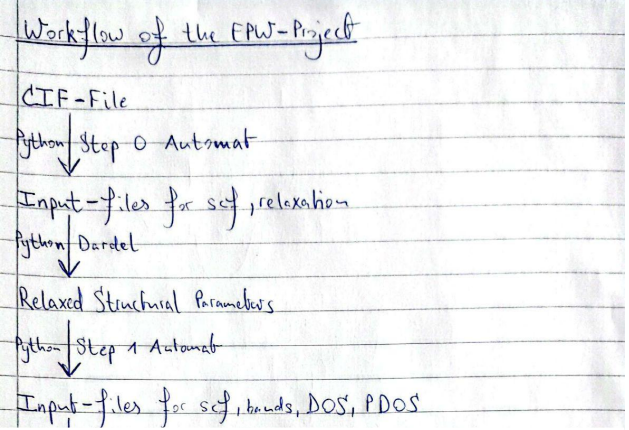
↓

Input-files for scf, relaxation

Python Dardel

↓

Relaxed Structural Parameters



b_main_1.py × a_input_file.py

b_main_1.py > ...

```python
import a_input_file as input
import z_utilities as utils


# Jobs
cif2cell_raw     = True
cell2clean_cell  = True
use_relaxed_cell = True
AA_scf           = True
CD_bands         = True
PDOS             = True
DOS              = True # Remark: if DOS = True, then PDOS must also be True, because the the other option is not implemented yet.

# Step 1
tasks = [
    cif2cell_raw,
    cell2clean_cell,
    use_relaxed_cell,
    AA_scf,
    CD_bands,
    PDOS,
    DOS
]

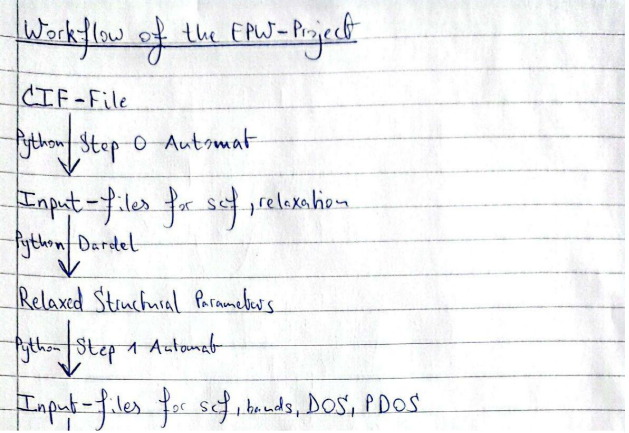
utils.print_intro()

utils.clean_directory(input.cif, cif2cell_raw)

utils.prepare_input_files_Step1(input.cif, tasks)

utils.add_further_templates(input.cif)

utils.print_outro()
```




```
SK ~/Storage/Dropbox/AA_Sebastians_Box/BC_My_Codes/D_EPW_Project/A_Python $ /bin/python /home/sebastian/Storage
/Dropbox/AA_Sebastians_Box/BC_My_Codes/D_EPW_Project/A_Python/b_main_1.py

Selected Structure in the Input-File:  Cs_Im3m

================================================================================
==================== Input Generator for S.K. ==================================
================================================================================


 - Old Material-Folder 'BA_Generated_Files/Cs_Im3m' has been deleted.
 - Created the Material-Folder Cs_Im3m with cell.in-file generated by cif2cell
 - Moved the Material-Folder Cs_Im3m to ./BA_Generated_Files/Cs_Im3m

 - Preparing the basic blocks for the DFT-Calculations

 - AA_basic.in      (   scf-file) saved to BA_Generated_Files/Cs_Im3m/AA_basic.in
 - CD_basicbands.in ( bands-file) saved to BA_Generated_Files/Cs_Im3m/CD_basicbands.in
 - CE_bands.in      ( bands-file) saved to BA_Generated_Files/Cs_Im3m/CE_bands.in
 - DA_basicdos.in   (  nscf-file) saved to BA_Generated_Files/Cs_Im3m/DA_basicdos.in
 - DD_basicdos.in   (   dos-file) generation is integrated in Step1.py.
 - StepX.py              (python-file) saved to BA_Generated_Files/Cs_Im3m/Step1.py


--------------------------------------------------------------------------------


 - After running the python-script on Dardel as python3.12 StepX.py, the following files are generated:

 - In the folder Dispersions one can find the file AA_basic.out, from which one gets the Fermi energy.

 - In the folder Dispersions one can find the files ...
   ...  the band-structure as a plot in QE_bands_Eref_eq_0.ps,
   ...  the band-structure as a dataset in basicbands.dat,
        which can be post-processed with c_post_processing.py

 - In the folder Dispersions one can find the PDOS by running plot_pdos.gnu.
   ... or one uses the python-script c_post_processing.py

 - In the folder Dispersions one can find the the DOS in basic.dos.dat.
   ... which can be post-processed (e.g. visualised) with c_post_processing.py


================================================================================
==================== Input Successfully Generated ==============================
================================================================================
```

Workflow of the EPW-Project

CIF-File

Python | Step 0 Automat

↓

Input-files for scf, relaxation

Python | Dardel

↓

Relaxed Structural Parameters

Python | Step 1 Automat

↓

Input-files for scf, bands, DOS, PDOS

```
 Above     File     Command     Options     Below
┌<-  ...ns_Box/BC_My_Codes/D_EPW_Project/A_Python/BA_Generated_Files/Cs_Im3m -.[^]>-
 .n                        Name                        Size   Modify time
 /Dispersions                                          4096  Feb  4 12:07
  AA_basic.in                                           970  Feb 23 11:25
  CD_basicbands.in                                     1120  Feb 23 11:25
  CE_bands.in                                            96  Feb 23 11:25
  Cs.upf                                             420444  Feb 23 11:25
  DA_basicdos.in                                        971  Feb 23 11:25
  Step1.py                                            12550  Feb 23 11:25
  cell.in                                              1088  Feb 23 11:25
  cell_clean.in                                         400  Feb 23 11:25
  job_AA.sh                                             394  Dez 30 01:24
  job_AB.sh                                             400  Feb 13 19:44
  job_BA.sh                                             382  Jan 20 21:33
  job_CA.sh                                             391  Jul  1  2025
  job_CB.sh                                             409  Jul  1  2025
  job_CD.sh                                             410  Jul  1  2025
  job_CE.sh                                             403  Jul  1  2025
```

Workflow of the FPW-Project

CIF-File

Python | Step 0 Automat

↓

Input-files for scf, relaxation

Python | Dardel

↓

Relaxed Structural Parameters

Python | Step 1 Automat

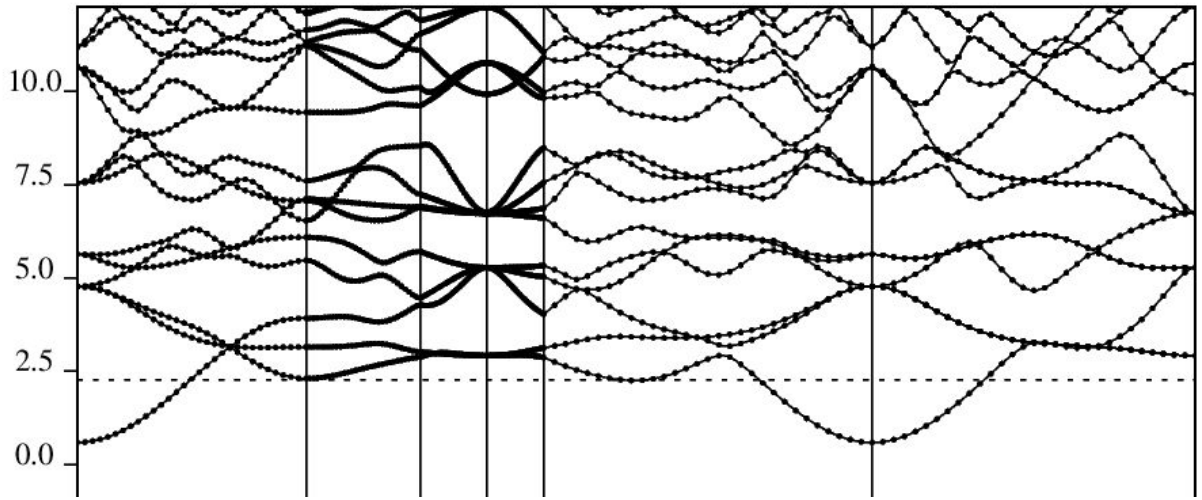
↓

Input-files for scf, bands, DOS, PDOS

Python | Dardel

↓

Output-files ⟶ Evaluation (Python)



Workflow of the FPW-Project

CIF-File

Python | Step 0 Automat

↓

Input-files for scf, relaxation

Python | Dardel

↓

Relaxed Structural Parameters

Python | Step 1 Automat

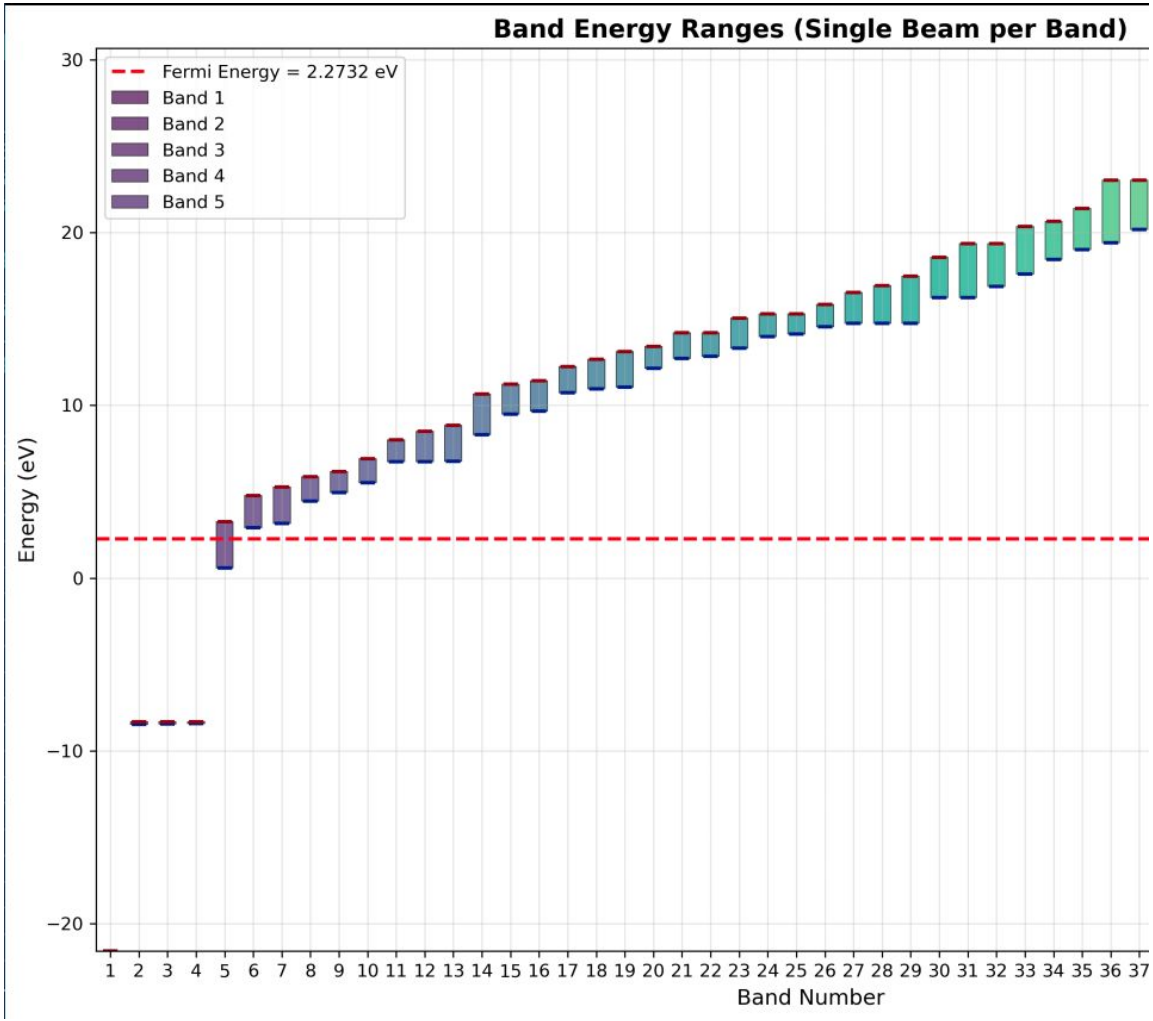
↓

Input-files for scf, bands, DOS, PDOS

Python | Dardel

↓

Output-files ⟶ Evaluation (Python)



Workflow of the FPW-Project

CIF-File

Python | Step 0 Automat

Input-files for scf, relaxation

Python | Dardel

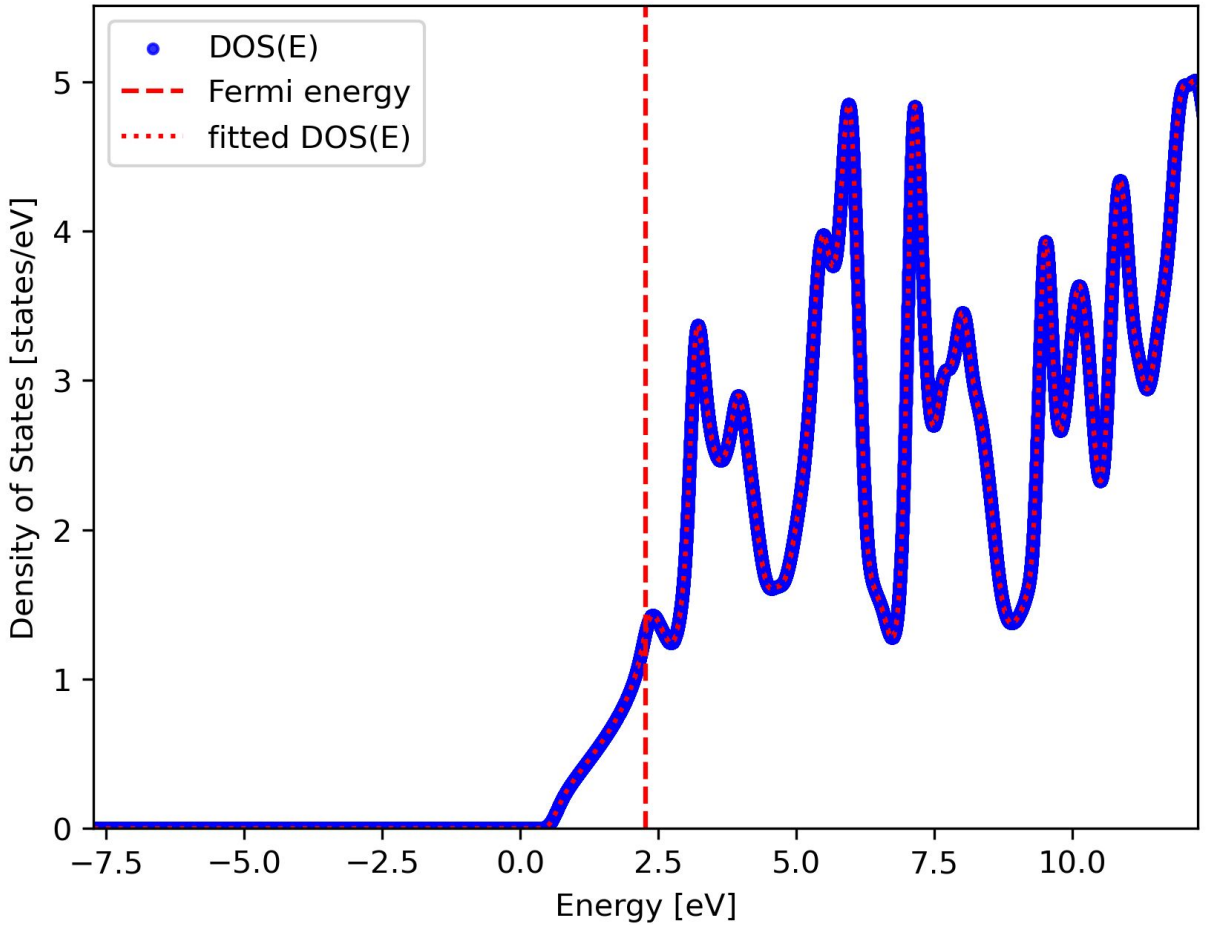
Relaxed Structural Parameters

Python | Step 1 Automat

Input-files for scf, bands, DOS, PDOS

Python | Dardel

Output-files ⟶ Evaluation (Python)



Workflow of the FPW-Project

CIF-File

Python | Step 0 Automat

↓

Input-files for scf, relaxation

Python | Dardel

↓

Relaxed Structural Parameters

Python | Step 1 Automat

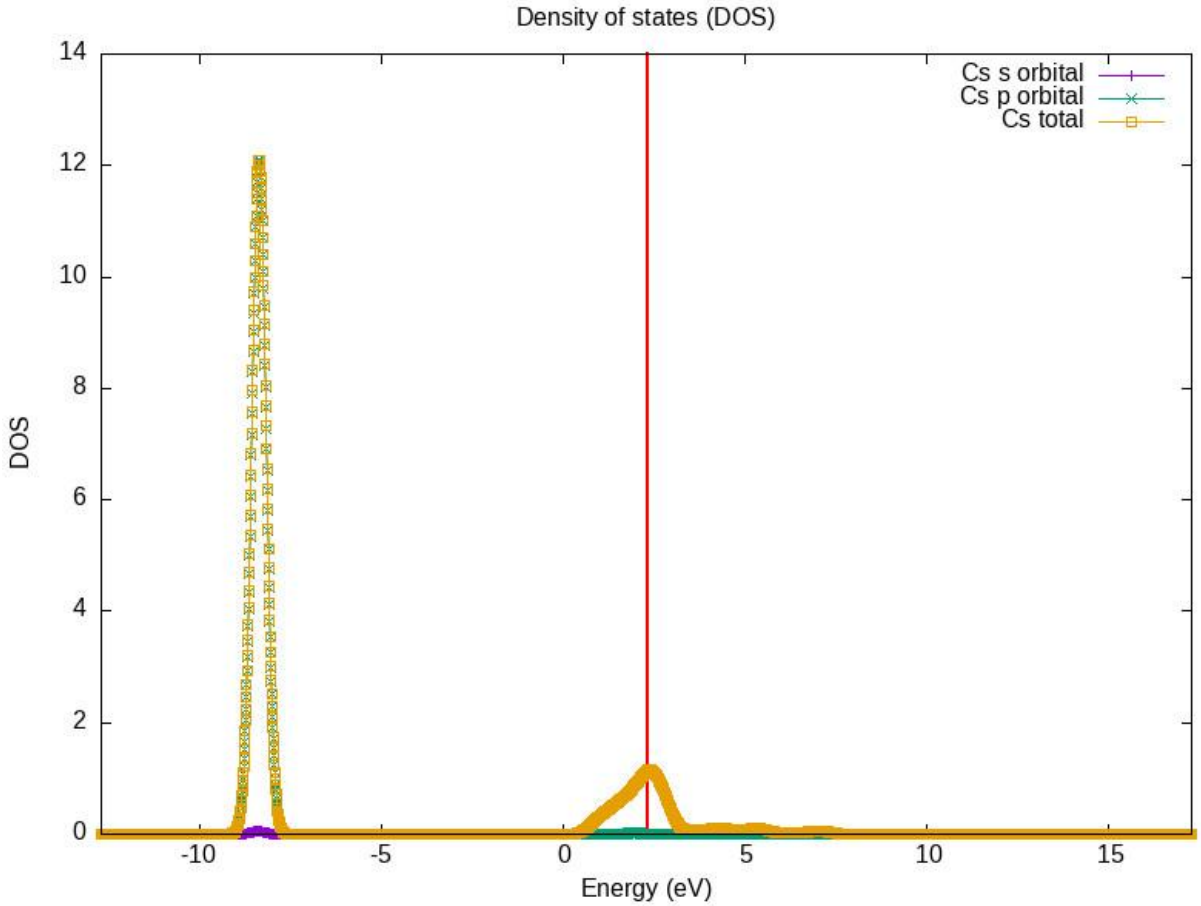
↓

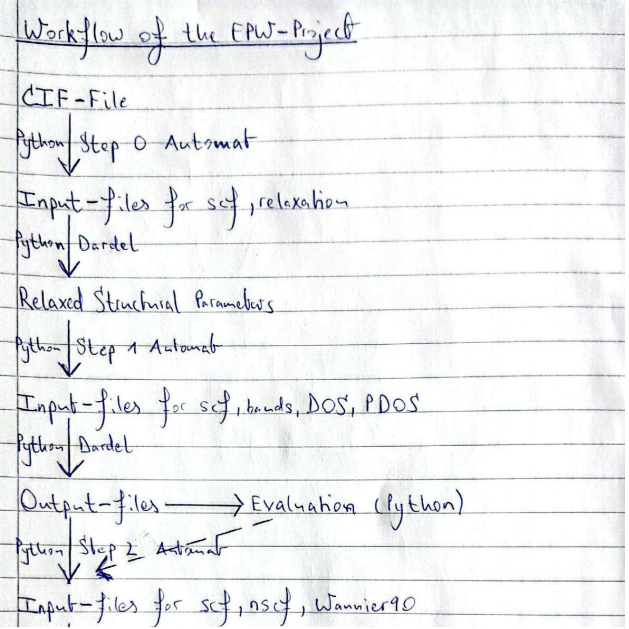
Input-files for scf, bands, DOS, PDOS

Python | Dardel

↓

Output-files ⟶ Evaluation (Python)





b_main_2.py × a_input_file.py

b_main_2.py > ...

```python
import a_input_file as input
import z_utilities as AB


# Jobs
cif2cell_raw      = True
cell2clean_cell   = True
use_relaxed_cell  = True
AA_scf            = True
DC_Wannierization = True

# Step 2
tasks = [
    cif2cell_raw,
    cell2clean_cell,
    use_relaxed_cell,
    AA_scf,
    DC_Wannierization
    ]

AB.print_intro()
AB.clean_directory(input.cif, cif2cell_raw)

AB.prepare_input_files_Step2(input.cif, tasks)

AB.add_further_templates(input.cif)

AB.print_outro()
```

Workflow of the EPW-Project

CIF-File

Python | Step 0 Automat

Input-files for scf, relaxation

Python | Dardel

Relaxed Structrual Parameters

Python | Step 1 Automat

Input-files for scf, bands, DOS, PDOS

Python | Dardel

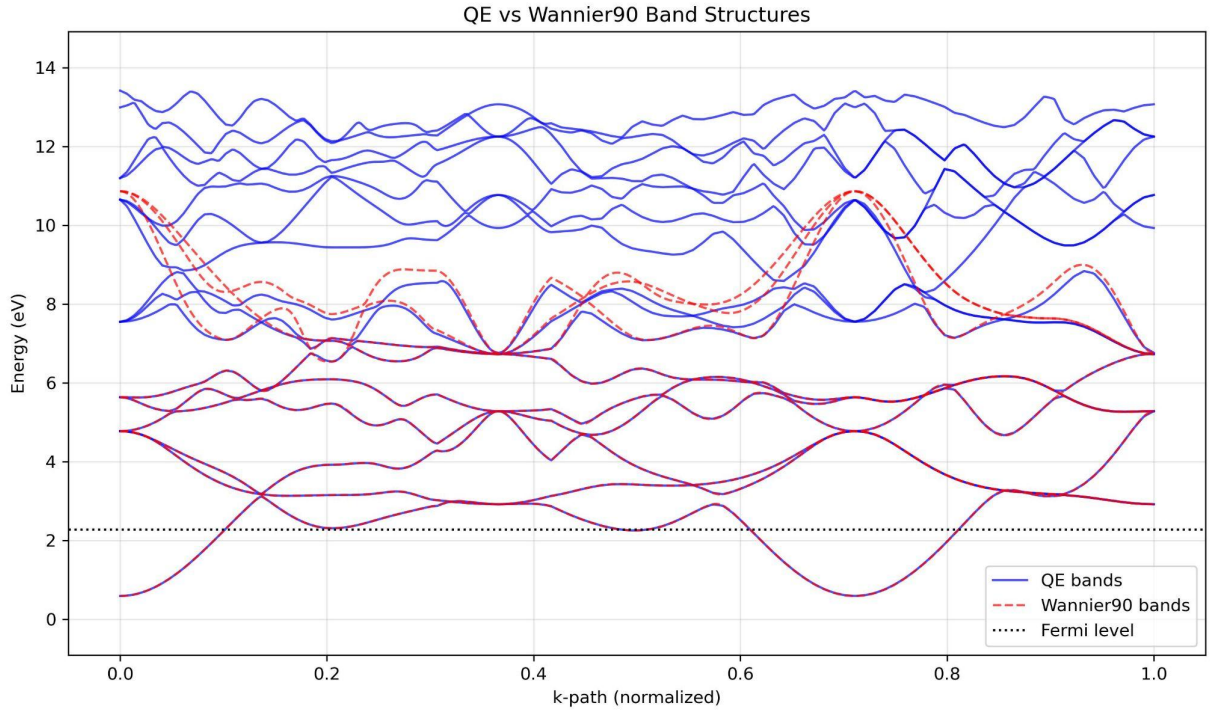
Output-files ⟶ Evaluation (Python)

Python | Step 2 ~~Automat~~

Input-files for scf, nscf, Wannier90

Python | Dardel

Output-files ⟶ Comparison w. QE-BS.



Workflow of the FPW-Project

CIF-File

Python | Step 0 Automat

↓

Input-files for scf, relaxation

Python | Dardel

↓

Relaxed Structural Parameters

Python | Step 1 Automat

↓

Input-files for scf, bands, DOS, PDOS

Python | Dardel

↓

Output-files ⟶ Evaluation (Python)

Python | Step 2 ~~Automat~~

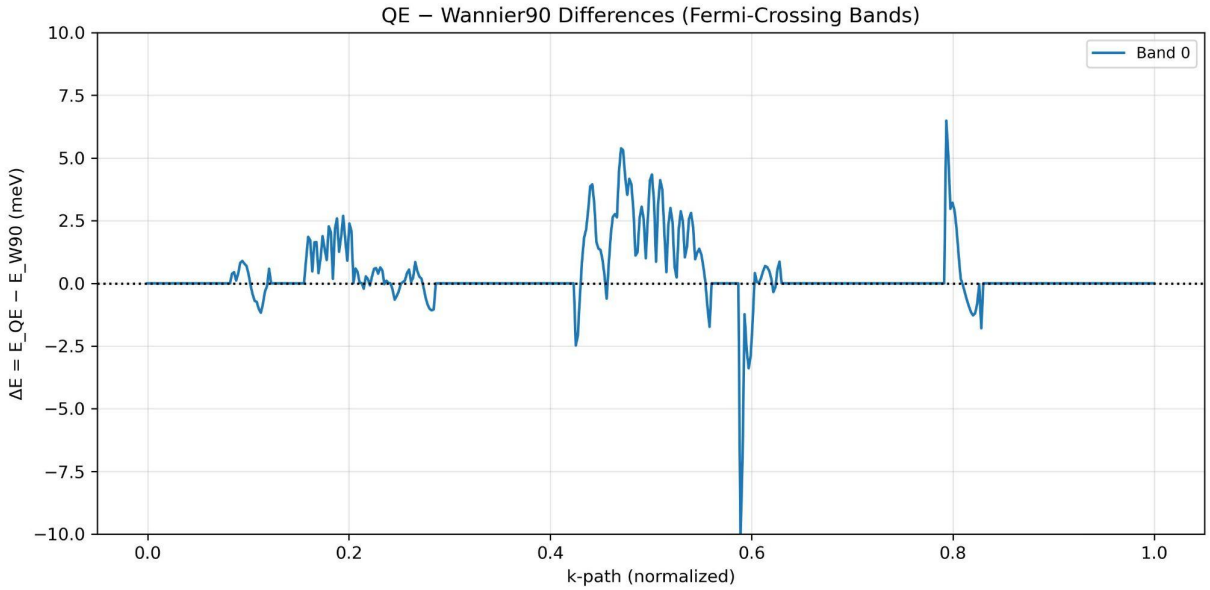
↓

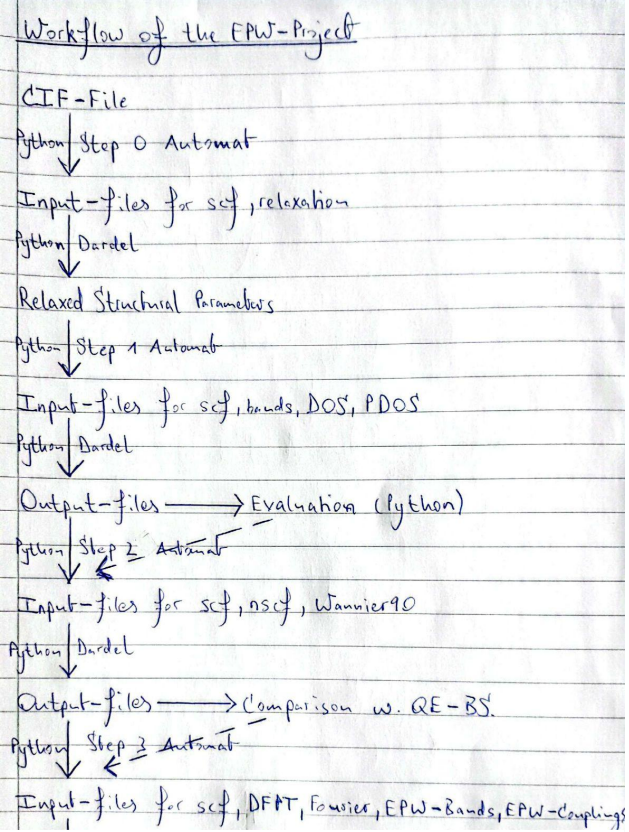
Input-files for scf, nscf, Wannier90

Python | Dardel

↓

Output-files ⟶ Comparison w. QE-BS.





b_main_3.py × a_input_file.py

b_main_3.py > ...

```python
import a_input_file as input
import z_utilities as AB


# Jobs
cif2cell_raw         = True
cell2clean_cell      = True
use_relaxed_cell     = True
AA_scf               = True
BA_ph                = True
CA_CB_ph_dispersion  = True
DC_Wannierization    = False
EA_bands             = True
EB_fine0_el          = True
EC_fine0_ph          = True
ED_SE_couplings      = True
EE_uniform_couplings = True

# Step 3
tasks = [
    cif2cell_raw,
    cell2clean_cell,
    use_relaxed_cell,
    AA_scf,
    BA_ph,
    CA_CB_ph_dispersion,
    EA_bands,
    EB_fine0_el,
    EC_fine0_ph,
    ED_SE_couplings,
    EE_uniform_couplings
    ]

AB.print_intro()
AB.clean_directory(input.cif, cif2cell_raw)

AB.prepare_input_files_Step3(input.cif, tasks)

AB.add_further_templates(input.cif)

AB.print_outro()
```

Workflow of the EPW-Project

CIF-File

Python | Step 0 Automat

↓

Input-files for scf, relaxation

Python | Dardel

↓

Relaxed Structural Parameters

Python | Step 1 Automat

↓

Input-files for scf, bands, DOS, PDOS

Python | Dardel

↓

Output-files ⟶ Evaluation (Python)

Python | Step 2 ~~Automat~~

↓

Input-files for scf, nscf, Wannier90

Python | Dardel

↓

Output-files ⟶ Comparison w. QE-BS.

Python | Step 3 ~~Automat~~

↓

Input-files for scf, DFPT, Fourier, EPW-Bands, EPW-Couplings

...ns_Box/BC_My_Codes/D_EPW_Project/A_Python/BA_Generated_Files/Cs_Im3m

.n	Name	Size	Modify time
/..		UP--DIR	Feb 23 11:35
/Dispersions		4096	Feb 4 12:07
AA_basic.in		965	Feb 23 11:35
BA_ph.in		267	Feb 23 11:35
CA_q2r.in		81	Feb 23 11:35
CB_matdyn.in		352	Feb 23 11:35
Cs.upf		420444	Feb 23 11:35
DC_nscf.in		89078	Feb 23 11:35
EA_bands.in		1026	Feb 23 11:35
EB_fine0_el.in		1240	Feb 23 11:35
EC_fine0_ph.in		1242	Feb 23 11:35
ED_SE_couplings.in		1265	Feb 23 11:35
EE_uniform_couplings.in		1173	Feb 23 11:35
Step3.py		12160	Feb 23 11:35
cell.in		1088	Feb 23 11:35
cell_clean.in		400	Feb 23 11:35
job_AA.sh		394	Dez 30 01:24
job_AB.sh		400	Feb 13 19:44
job_BA.sh		382	Jan 20 21:33
job_CA.sh		391	Jul 1 2025
job_CB.sh		409	Jul 1 2025
job_CD.sh		410	Jul 1 2025
job_CE.sh		403	Jul 1 2025
job_DA.sh		403	Dez 7 15:20
job_DB.sh		421	Dez 30 01:25
job_DC.sh		391	Dez 30 01:25
job_DD.sh		406	Nov 20 23:55
job_DE.sh		502	Dez 30 21:24
job_EA.sh		409	Feb 20 11:21
job_EB.sh		441	Feb 15 21:29
job_EC.sh		417	Jan 11 00:46
job_ED.sh		452	Feb 14 21:18
job_EE.sh		444	Feb 14 21:18
path.dat		7752	Jan 28 18:01
pw2wan.in		131	Apr 3 2025

Workflow of the EPW-Project

CIF-File

Python | Step 0 Automat

Input-files for scf, relaxation

Python | Dardel

Relaxed Structrual Parameters

Python | Step 1 Automat

Input-files for scf, bands, DOS, PDOS

Python | Dardel

Output-files ⟶ Evaluation (Python)

Python | Step 2 ~~Automat~~

Input-files for scf, nscf, Wannier90

Python | Dardel

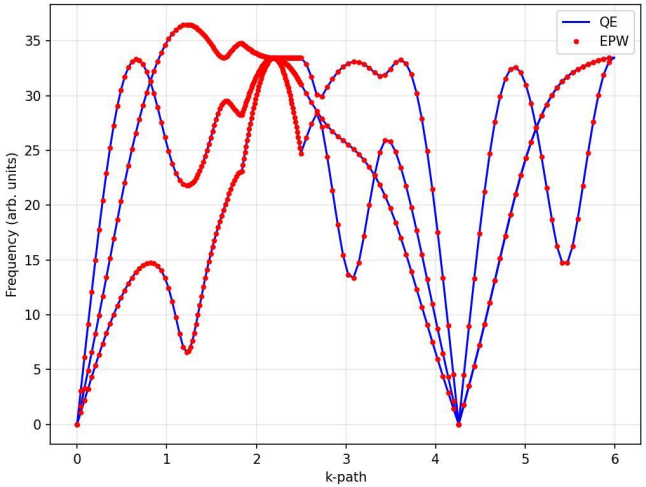
Output-files ⟶ Comparison w. QE-BS

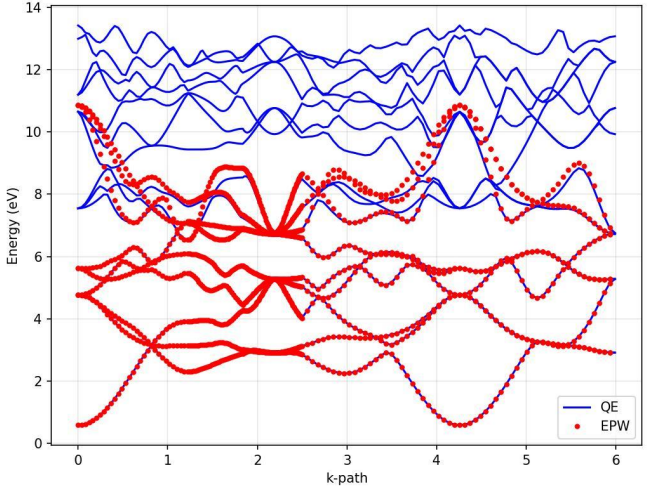
Python | Step 3 ~~Automat~~

Input-files for scf, DFPT, Fourier, EPW-Bands, EPW-Couplings

Python | Dardel

Output-files ⟶ Evaluation: • Comparison of Bands & Brand





Workflow of the EPW-Project

CIF-File

Python | Step 0 Automat

↓

Input-files for scf, relaxation

Python | Dardel

↓

Relaxed Structural Parameters

Python | Step 1 Automat

↓

Input-files for scf, bands, DOS, PDOS

Python | Dardel

↓

Output-files ⟶ Evaluation (Python)

Python | Step 2 ~~Automat~~

↓

Input-files for scf, nscf, Wannier90

Python | Dardel

↓

Output-files ⟶ Comparison w. QE-BS

Python | Step 3 ~~Automat~~

↓

Input-files for scf, DFPT, Fourier, EPW-Bands, EPW-Couplings

Python | Dardel

↓

Output-files ⟶ Evaluation: • Comparison of Bands & Bra
• Symmetries

$$H = H_0 + V$$

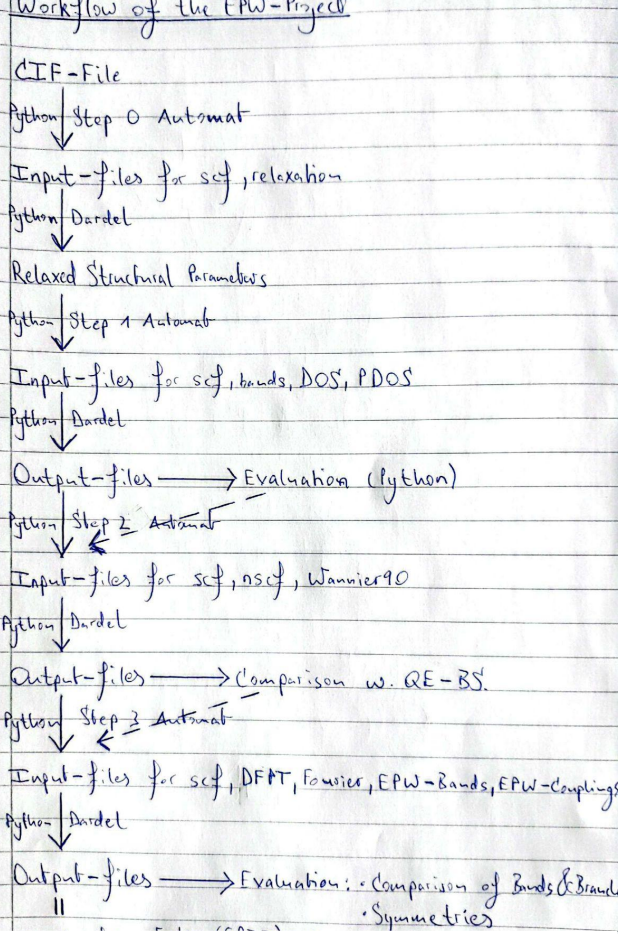
$$= \sum_{\substack{\mathbf{k}\in Q \\ \sigma\in\{\uparrow,\downarrow\} \\ m\in\{1,\dots,\infty\}}} \epsilon_{m\mathbf{k}\sigma} c^\dagger_{m\mathbf{k}\sigma} c_{m\mathbf{k}\sigma} + \sum_{\substack{\mathbf{q}\in Q \\ \nu\in\{1,\dots,rd_x\}}} \hbar\omega_{\mathbf{q},\nu} b^\dagger_{\mathbf{q}\nu} b_{\mathbf{q}\nu} + \sum_{\substack{\mathbf{k},\mathbf{q}\in Q \\ \sigma\in\{\uparrow,\downarrow\} \\ \nu\in\{1,\dots,rd_x\} \\ m,n\in\{1,\dots,\infty\}}} \frac{g_{mn\nu}(\mathbf{k},\mathbf{q})}{\sqrt{N_p}} c^\dagger_{\mathbf{k}+\mathbf{q}m\sigma} c_{\mathbf{k}n\sigma} \left(b_{\mathbf{q}\nu} + b^\dagger_{-\mathbf{q}\nu} \right)$$

Lemma 8.28 The hermiticity of the Hamiltonian implies for the coupling

$$g_{mn\nu}(\mathbf{k},\mathbf{q}) = g^*_{nm\nu}(\mathbf{k}+\mathbf{q},-\mathbf{q}).$$

Lemma 8.29 Notice that for inversion-symmetric crystals one has the additional symmetry

$$g_{mn\nu}(\mathbf{k},\mathbf{q}) = g^*_{mn\nu}(-\mathbf{k},-\mathbf{q}).$$




```
+=========================================+
|| Symmetry-Checker for the EPW-Couplings ||
+=========================================+

 - The wavevector-array was successfully loaded.
   Note: wavevector_arr[i] = k_i = q_i in reciprocal coordinates.

   The coupling-array was successfully loaded.
   Note: g_arr[m, n, nu, i_k, i_q] = g_{m n nu} ( k_i, q_i )


+-----------------------------------------------------------------------------------------------------+
|  Assessing the Quality of the Couplings by plotting the Hermiticity- and Inversion-Symmetry-Conditions  |
+-----------------------------------------------------------------------------------------------------+

 10% completed
    < g_{m n nu} (k,q) / g_{n m nu}^* (k + q, -q) >_avg = 1.141,
    < g_{m n nu} (k,q) / g_{m n nu}^* ( -k, -q ) >_avg  = 1.000
 20% completed
    < g_{m n nu} (k,q) / g_{n m nu}^* (k + q, -q) >_avg = 1.158,
    < g_{m n nu} (k,q) / g_{m n nu}^* ( -k, -q ) >_avg  = 1.000
 30% completed
    < g_{m n nu} (k,q) / g_{n m nu}^* (k + q, -q) >_avg = 1.159,
    < g_{m n nu} (k,q) / g_{m n nu}^* ( -k, -q ) >_avg  = 1.000
 40% completed
    < g_{m n nu} (k,q) / g_{n m nu}^* (k + q, -q) >_avg = 1.153,
    < g_{m n nu} (k,q) / g_{m n nu}^* ( -k, -q ) >_avg  = 1.000
 50% completed
    < g_{m n nu} (k,q) / g_{n m nu}^* (k + q, -q) >_avg = 1.151,
    < g_{m n nu} (k,q) / g_{m n nu}^* ( -k, -q ) >_avg  = 1.000
 60% completed
    < g_{m n nu} (k,q) / g_{n m nu}^* (k + q, -q) >_avg = 1.148,
    < g_{m n nu} (k,q) / g_{m n nu}^* ( -k, -q ) >_avg  = 1.000
 70% completed
    < g_{m n nu} (k,q) / g_{n m nu}^* (k + q, -q) >_avg = 1.148,
    < g_{m n nu} (k,q) / g_{m n nu}^* ( -k, -q ) >_avg  = 1.000
 80% completed
    < g_{m n nu} (k,q) / g_{n m nu}^* (k + q, -q) >_avg = 1.146,
    < g_{m n nu} (k,q) / g_{m n nu}^* ( -k, -q ) >_avg  = 1.000
 90% completed
    < g_{m n nu} (k,q) / g_{n m nu}^* (k + q, -q) >_avg = 1.148,
    < g_{m n nu} (k,q) / g_{m n nu}^* ( -k, -q ) >_avg  = 1.000
100% completed
    < g_{m n nu} (k,q) / g_{n m nu}^* (k + q, -q) >_avg = 1.150,
    < g_{m n nu} (k,q) / g_{m n nu}^* ( -k, -q ) >_avg  = 1.000
```

Workflow of the EPW-Project

CIF-File

Python | Step 0 Automat

↓

Input-files for scf, relaxation

Python | Dardel

↓

Relaxed Structural Parameters

Python | Step 1 Automat

↓

Input-files for scf, bands, DOS, PDOS

Python | Dardel

↓

Output-files ⟶ Evaluation (Python)

Python | Step 2 ~~Automat~~

↓ ↔

Input-files for scf, nscf, Wannier90

Python | Dardel

↓

Output-files ⟶ Comparison w. QE-BS

Python | Step 3 ~~Automat~~

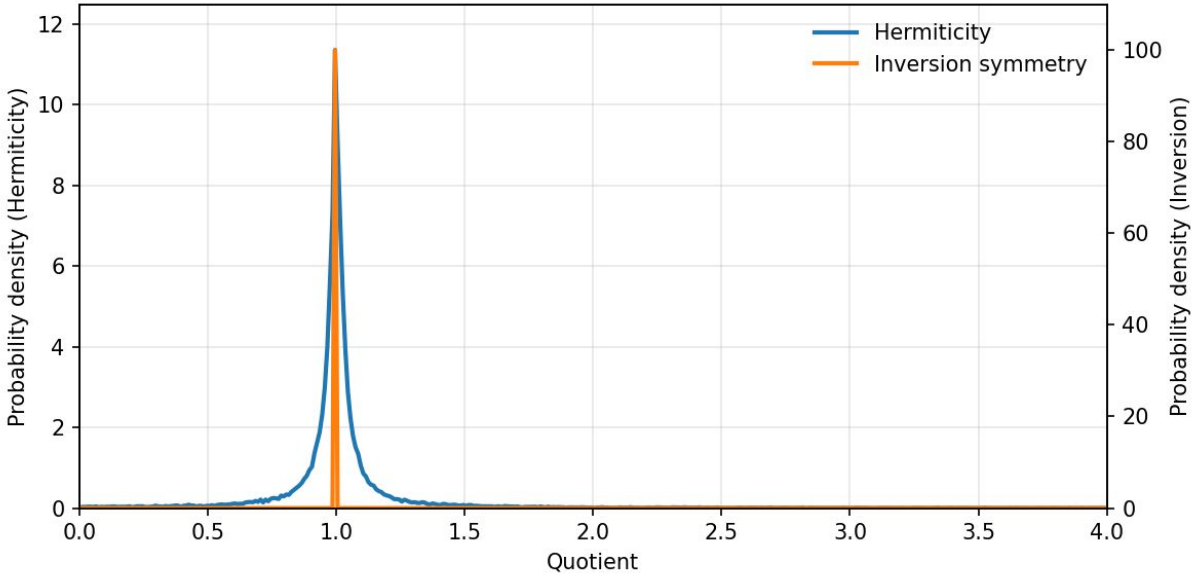
↓ ↔

Input-files for scf, DFPT, Fourier, EPW-Bands, EPW-Couplings

Python | Dardel

↓

Output-files ⟶ Evaluation: • Comparison of Bands & Brand
• Symmetries



Workflow of the EPW-Project

CIF-File

Python → Step 0 Automat

Input-files for scf, relaxation

Python → Dardel

Relaxed Structural Parameters

Python → Step 1 Automat

Input-files for scf, bands, DOS, PDOS

Python → Dardel

Output-files ⟶ Evaluation (Python)

Python → Step 2 ~~Automat~~

Input-files for scf, nscf, Wannier90

Python → Dardel

Output-files ⟶ Comparison w. QE-BS.

Python → Step 3 ~~Automat~~

Input-files for scf, DFPT, Fourier, EPW-Bands, EPW-Couplings

Python → Dardel

Output-files ⟶ Evaluation: • Comparison of Bands & Bands
• Symmetries

Input-files → Fortran (GRIT) / Dardel → Specific Heat vs T.

```
    ================================================================================
   ||                                                                              ||
   ||  GGGGGGGGGGGGGG    RRRRRRRRRRRR       IIIIIIIIIIIII    TTTTTTTTTTTTTTTTT  ||
   ||  GGGGGGGGGGGGGG    RRRRRRRRRRRRR      IIIIIIIIIIIII    TTTTTTTTTTTTTTTTT  ||
   ||  GGG               RRRR       RRRR         IIII              TTTT         ||
   ||  GGG               RRRR       RRRR         IIII              TTTT         ||
   ||  GGG      GGGG     RRRRRRRRRRRRR           IIII              TTTT         ||
   ||  GGG      GGGGG    RRRRRRRRRRRRR           IIII              TTTT         ||
   ||  GGG          GG   RRRR      RRRR          IIII              TTTT         ||
   ||  GGG          GG   RRRR       RRRR         IIII              TTTT         ||
   ||  GGGGGGGGGGGGGG    RRRR        RRRR   IIIIIIIIIIIII         TTTT         ||
   ||  GGGGGGGGGGGGGG    RRRR         RRRR  IIIIIIIIIIIII         TTTT         ||
   ||                                                                           ||
    ================================================================================

            [Gr]een-Functions for [I]nteracting [T]hermodynamics
            (Post-Processing Tool for the Electron-Phonon-Calculations)



+====================================+
|| Information about Input-Parameters ||
+====================================+


+---------+
|  Modes  |
+---------+

 - Fine k-grid near Fermi surface    = F
 - Fine q-grid near the Gamma-point  = F
 - Interacting Electrons and phonons = T
 - Debug mode enabled                = F

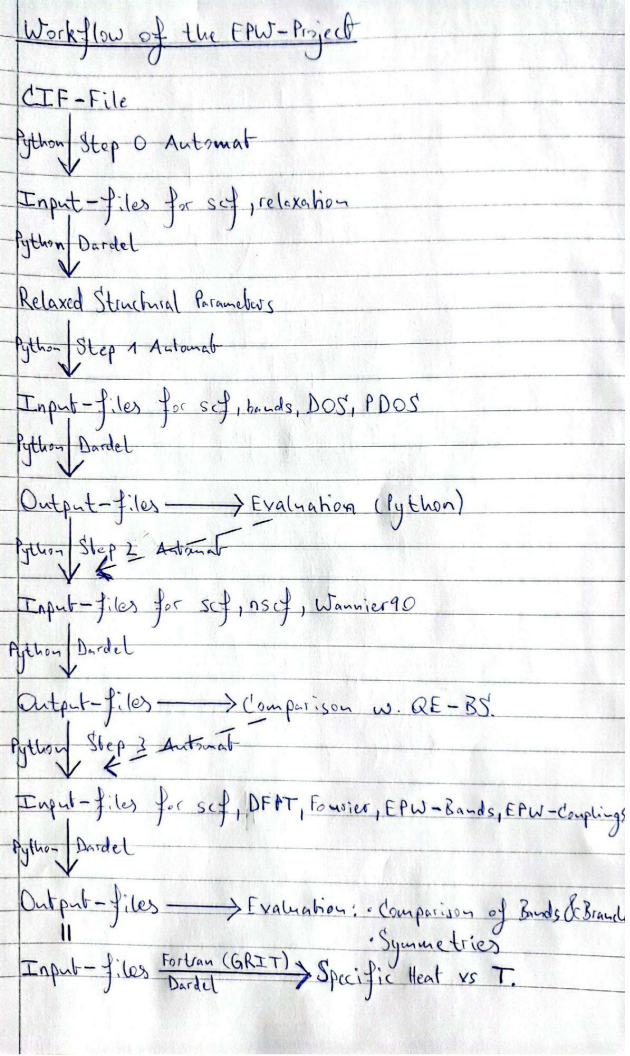

+---------+
|  Tasks  |
+---------+

 - Create binary files                    = T
 - Calc N_states_per_UC (mu = E_F, T = 0) = T
 - Calc N_per_UC (mu = E_F, T = 0)        = T
 - Calc mu vs Temperature                 = T
 - Calc specific heat per UC              = T
 - Calc Sommerfeld gamma from linear fit  = F


+--------------------------+
|  Temperature parameters  |
+--------------------------+

 - Number of temperature points = 20
 - Minimum temperature (K)   =      20.0000
 - Maximum temperature (K)   =     125.0000
```

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```
+=====================================================+
|| Task = calc_N_states_per_UC_mu_eq_E_F_T_eq_zero ||
+=====================================================+

 - Computing the number of states per UC at T = 0 K for mu = E_F.
   ===> Calculating integrand for i_E =     1 /  1000 at energy E_i =     -9.484 eV
   ===> Calculating integrand for i_E =   101 /  1000 at energy E_i =     -7.654 eV
   ===> Calculating integrand for i_E =   201 /  1000 at energy E_i =     -5.825 eV
   ===> Calculating integrand for i_E =   301 /  1000 at energy E_i =     -3.995 eV
   ===> Calculating integrand for i_E =   401 /  1000 at energy E_i =     -2.166 eV
   ===> Calculating integrand for i_E =   501 /  1000 at energy E_i =     -0.336 eV
   ===> Calculating integrand for i_E =   601 /  1000 at energy E_i =      1.493 eV
   ===> Calculating integrand for i_E =   701 /  1000 at energy E_i =      3.323 eV
   ===> Calculating integrand for i_E =   801 /  1000 at energy E_i =      5.153 eV
   ===> Calculating integrand for i_E =   901 /  1000 at energy E_i =      6.982 eV
   ===> Calculating integrand for i_E =  1000 /  1000 at energy E_i =      8.793 eV

 - The computed number of states per UC at T = 0 K for mu = E_F is <N_states_per_UC> =        1.963
 - The expected number of states per UC is                                N_bnd * 2 =        2.000
 - The ratio is                          <N_states_per_UC> / (N_bnd * 2) =        0.982


 - States calculation took   0.0001 days,   0.0024 hours,   0.1413 minutes,   8.4790 seconds
 - Approximated runtime for the remaining tasks: TBImplemented.

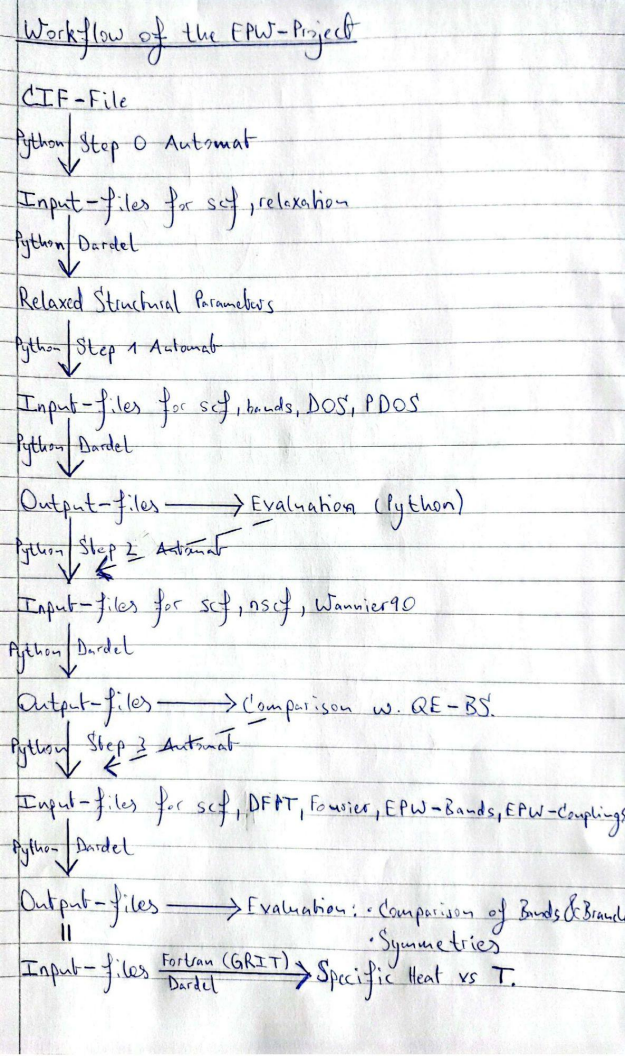


+=============================================+
|| Task = calc_N_per_UC_mu_eq_E_F_T_eq_zero ||
+=============================================+

 - Computing the number of electrons per UC at T = 0 K for mu = E_F.
   ===> Calculating integrand for i_E =     1 /  1000 at energy E_i =     -9.484 eV
   ===> Calculating integrand for i_E =   101 /  1000 at energy E_i =     -7.654 eV
   ===> Calculating integrand for i_E =   201 /  1000 at energy E_i =     -5.825 eV
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   ===> Calculating integrand for i_E =   801 /  1000 at energy E_i =      5.153 eV
   ===> Calculating integrand for i_E =   901 /  1000 at energy E_i =      6.982 eV
   ===> Calculating integrand for i_E =  1000 /  1000 at energy E_i =      8.793 eV

 - The computed particle-number per UC is n_UC =  1.01037 (electrons).
 - The expected particle-number per UC is n_UC = 1
```

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```
+==========================+
|| Task = calc_c_V_per_UC ||
+==========================+

 - Computing the specific heat capacity for different temperatures.
 - Chemical potential values for different temperatures read from: ../B_QE_n_EPW_Files/Step3_EPW/Rb_Im3m/Dispersions_




 - Temperature:    20.00 K
=============================================================================================================
Electrons:
 - The 1st electronic contribution  is                    \partial_T H_el      / n_moles =    51.00 mJ / K mol
 - The 2nd electronic contribution  is           dT mu * \partial_mu H_el      / n_moles =   -37.82 mJ / K mol
 - The tot electronic contribution  is c_V_molar_el     =        d/dT H_el      / n_moles =    13.18 mJ / K mol

Phonons:
 - The free phononic contribution   is c_V_molar_ph_0   = \partial_T  H_ph_0    / n_moles = 16684.50 mJ / K mol
 - The 1st  phononic correction     is                    \partial_T  H_ph_corr / n_moles =  3309.74 mJ / K mol
 - The 2nd  phononic correction     is           dT mu * \partial_mu H_ph_corr / n_moles =    -0.43 mJ / K mol
 - The tot  phononic contribution   is c_V_molar_ph     =        d/dT H_ph      / n_moles = 19993.80 mJ / K mol

Interactions:
 - The interaction    contribution  is c_V_molar_int     =       d/dT H_int     / n_moles =     0.00 mJ / K mol

Total Specific Heat Capacity:
 - The total specific heat capacity is c_V_molar_T       =       d/dT H_tot     / n_moles = 20006.98 mJ / K mol
=============================================================================================================




 - Temperature:    25.53 K
=============================================================================================================
Electrons:
 - The 1st electronic contribution  is                    \partial_T H_el      / n_moles =    49.64 mJ / K mol
 - The 2nd electronic contribution  is           dT mu * \partial_mu H_el      / n_moles =   -38.60 mJ / K mol
 - The tot electronic contribution  is c_V_molar_el     =        d/dT H_el      / n_moles =    11.04 mJ / K mol

Phonons:
 - The free phononic contribution   is c_V_molar_ph_0   = \partial_T  H_ph_0    / n_moles = 19237.86 mJ / K mol
 - The 1st  phononic correction     is                    \partial_T  H_ph_corr / n_moles =  3435.55 mJ / K mol
 - The 2nd  phononic correction     is           dT mu * \partial_mu H_ph_corr / n_moles =    -0.83 mJ / K mol
 - The tot  phononic contribution   is c_V_molar_ph     =        d/dT H_ph      / n_moles = 22672.58 mJ / K mol

Interactions:
 - The interaction    contribution  is c_V_molar_int     =       d/dT H_int     / n_moles =     0.00 mJ / K mol

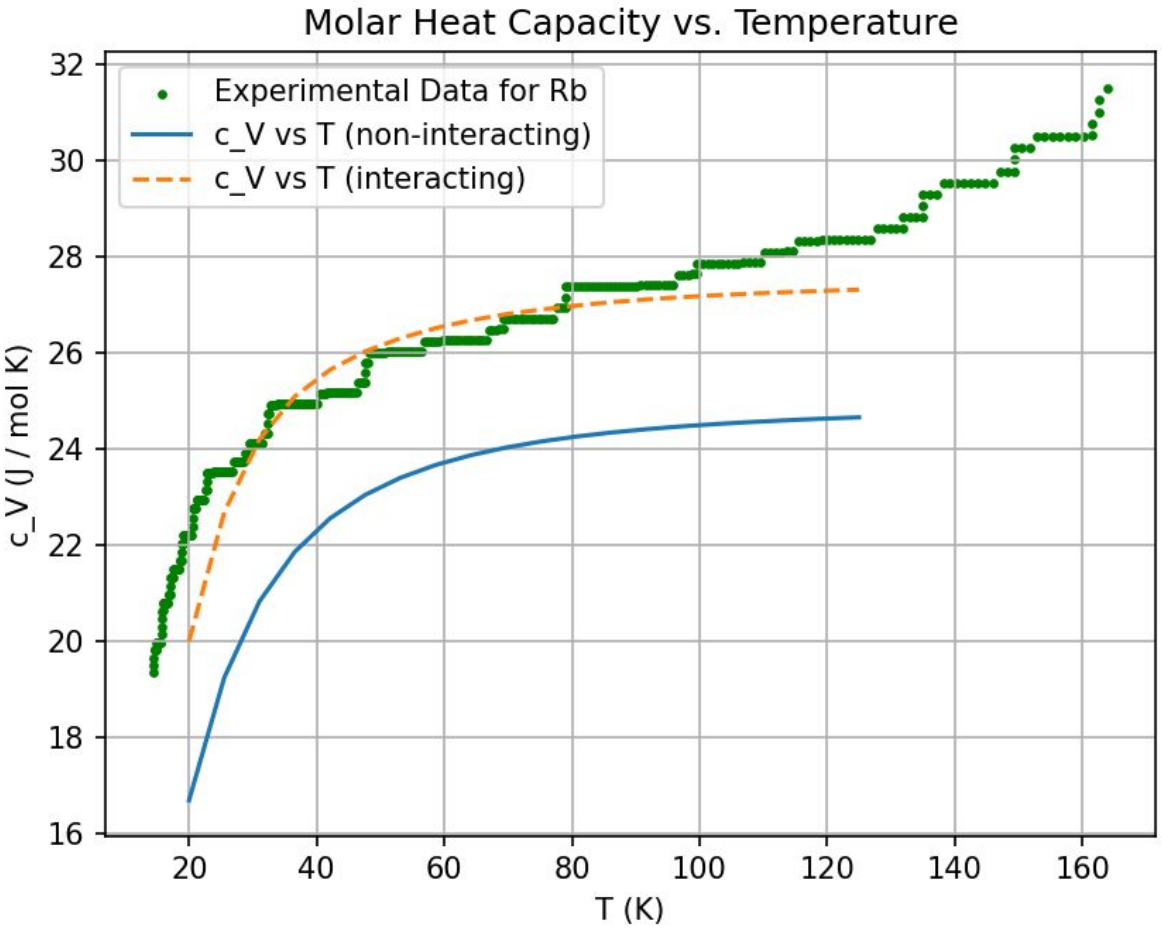
Total Specific Heat Capacity:
 - The total specific heat capacity is c_V_molar_T       =       d/dT H_tot     / n_moles = 22683.61 mJ / K mol
=============================================================================================================

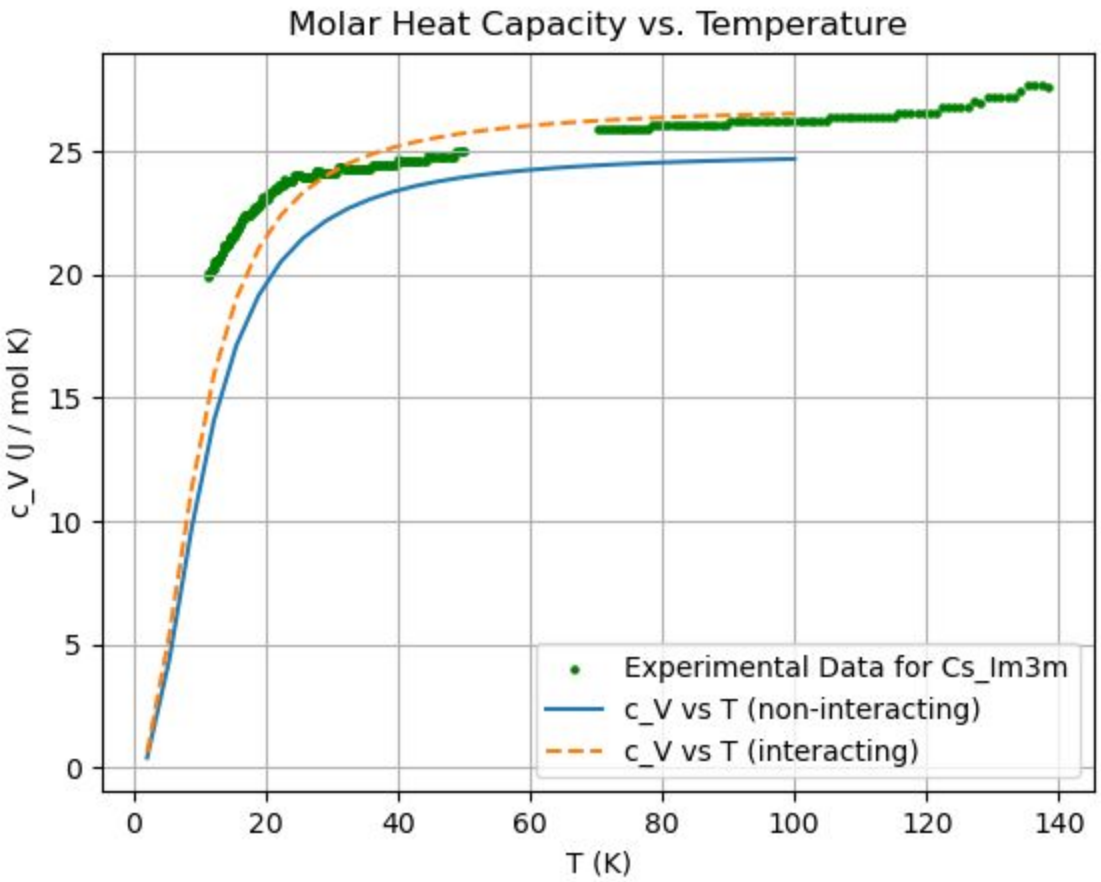


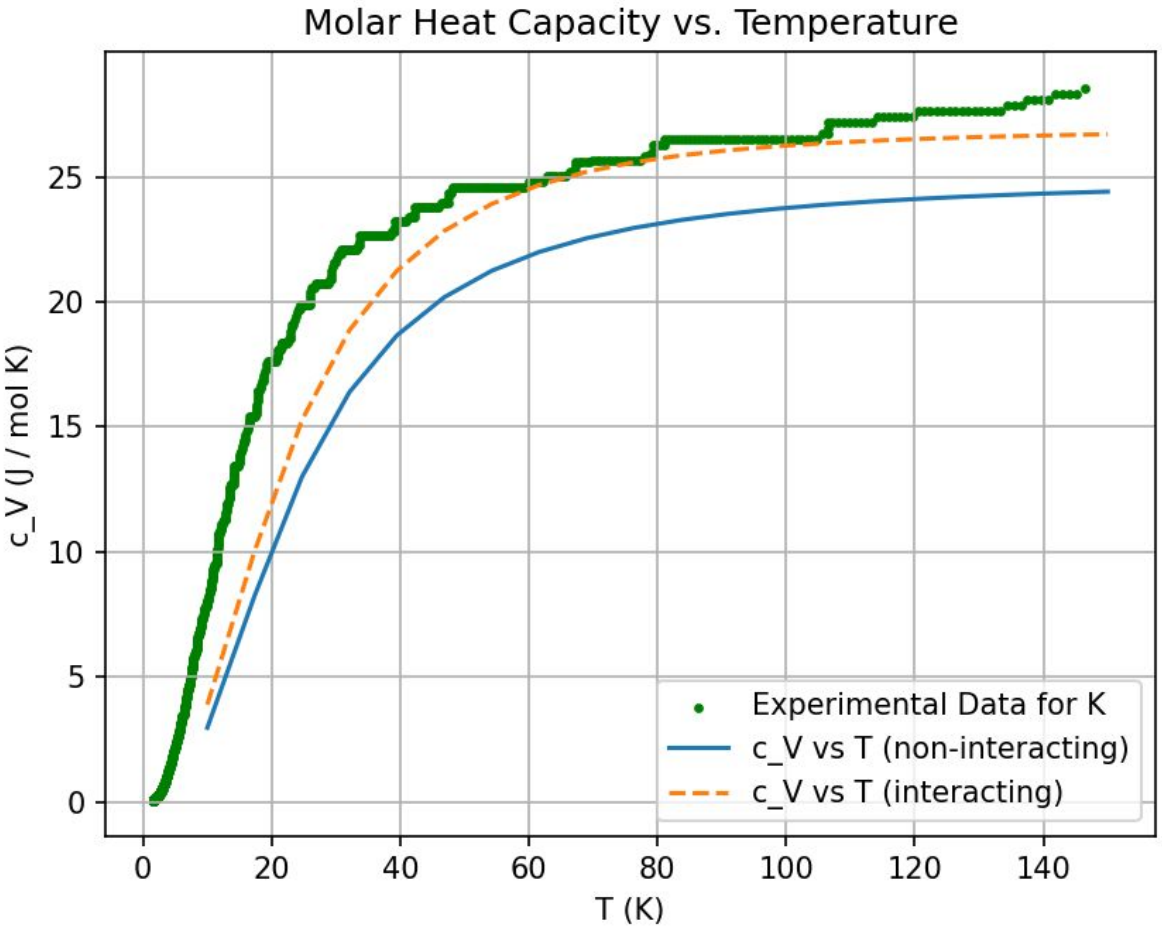

 - Temperature:    31.05 K
=============================================================================================================
Electrons:
 - The 1st electronic contribution  is                    \partial_T H_el      / n_moles =    47.15 mJ / K mol
```

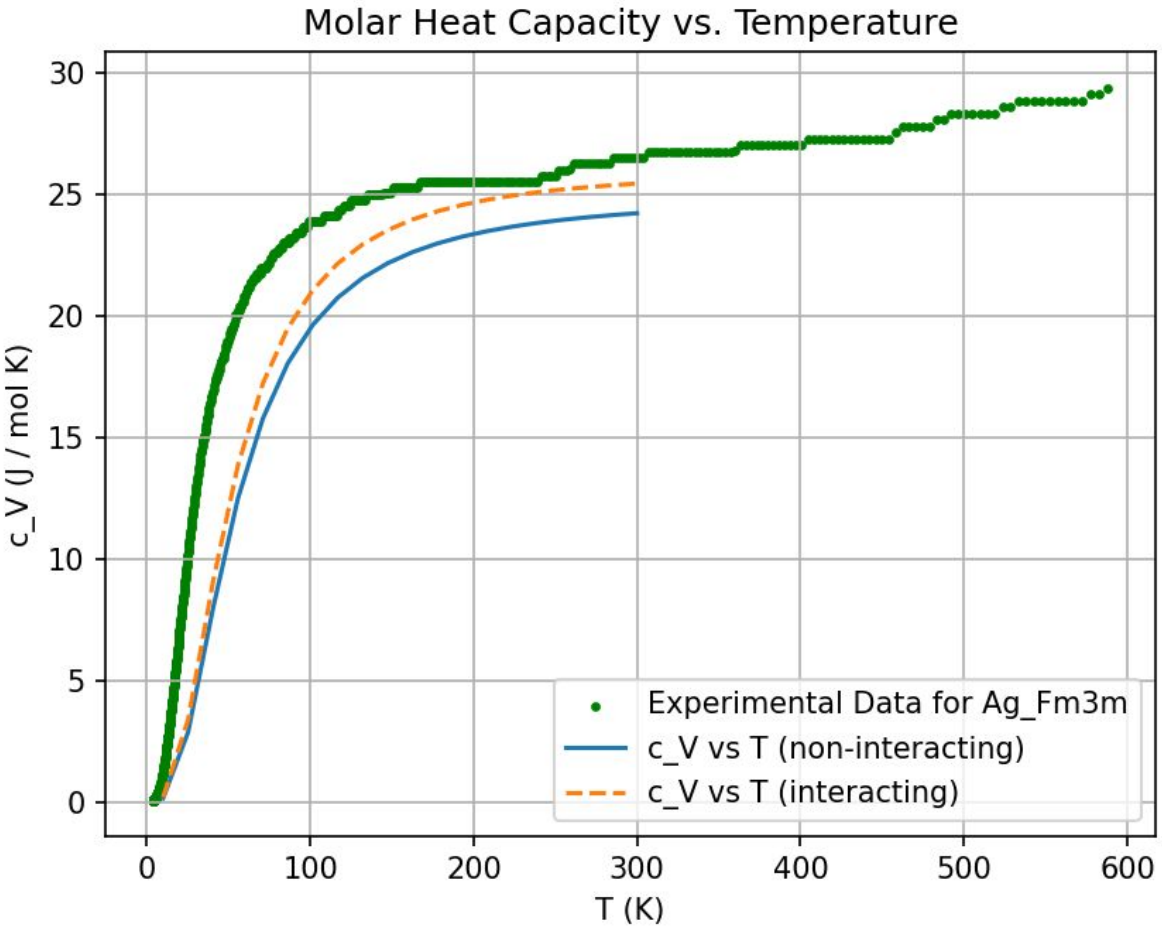
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Results:

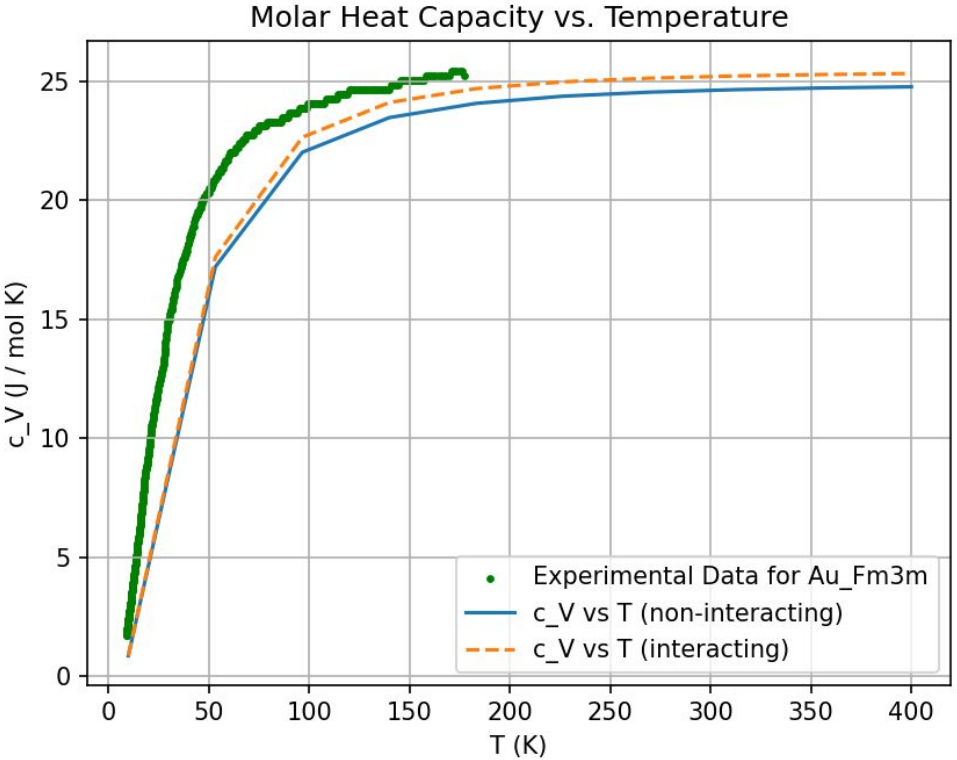

Molar Heat Capacity vs. Temperature
Experimental Data for Rb
c_V vs T (non-interacting)
c_V vs T (interacting)
c_V (J / mol K)
T (K)
32
30
28
26
24
22
20
18
16
20
40
60
80
100
120
140
160


Molar Heat Capacity vs. Temperature
c_V (J / mol K)
T (K)
0
5
10
15
20
25
0
20
40
60
80
100
120
140
Experimental Data for Cs_Im3m
c_V vs T (non-interacting)
c_V vs T (interacting)

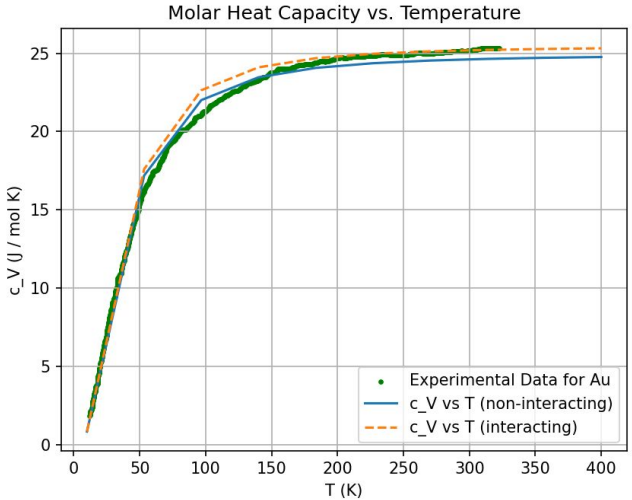

Molar Heat Capacity vs. Temperature
c_V (J / mol K)
T (K)
0
5
10
15
20
25
0
20
40
60
80
100
120
140
Experimental Data for K
c_V vs T (non-interacting)
c_V vs T (interacting)


Molar Heat Capacity vs. Temperature
c_V (J / mol K)
T (K)
0
5
10
15
20
25
30
0
100
200
300
400
500
600
Experimental Data for Ag_Fm3m
c_V vs T (non-interacting)
c_V vs T (interacting)

Experimental-Data 1



Experimental-Data 2



Sanity-Checks:

- Bands from QE reproduced by Wannier90 and EPW.
- DOSes from QE reproduced by EPW.
- Normalizations are fulfilled.
- Non-Interacting results are close to Experimental Values
  (... also in the low-temperature-limit)

Lessons learned:

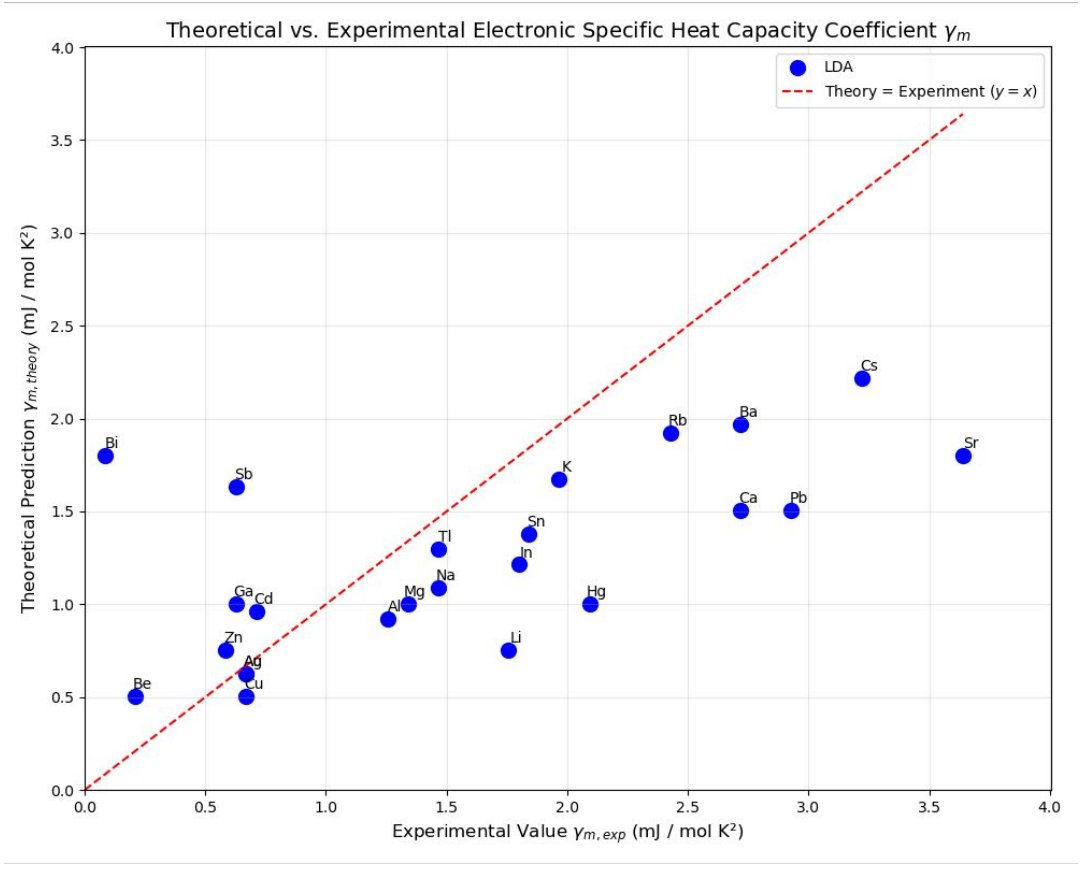
- Electron-Phonon-Interactions can represent essential corrections in the medium temperature limit

- CAT-QFT provides a technique to compute these corrections

Outlook (maybe…):

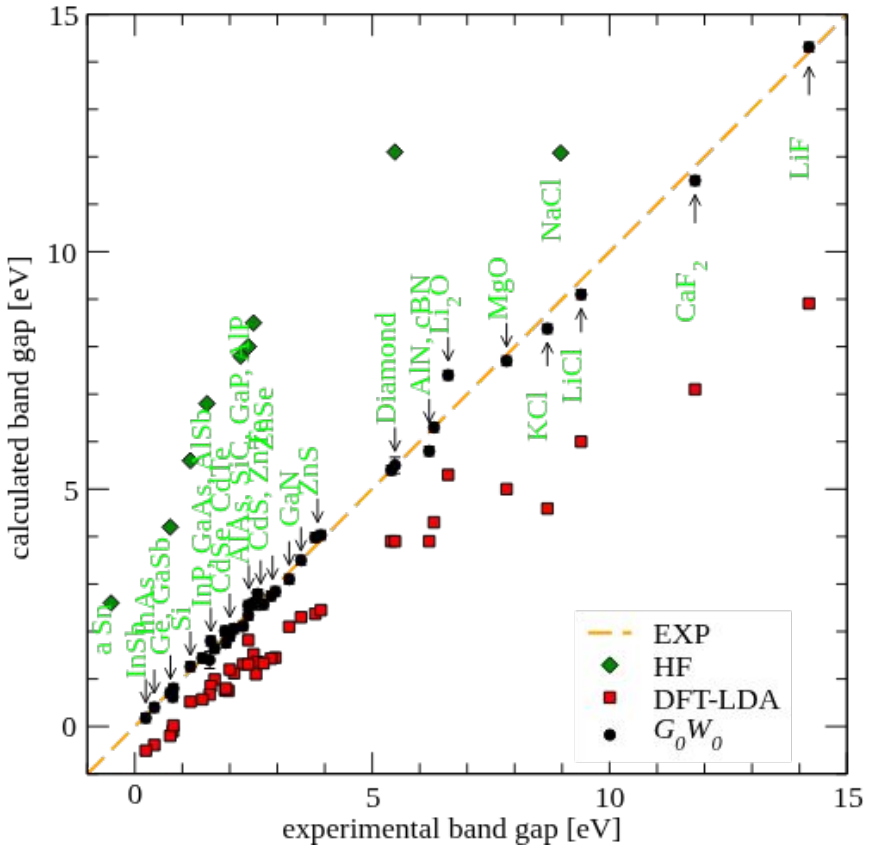
- Finer Grids, more bands and more complicated structures (...)
- High-Temperature limits with phonon-phonon-interactions (...)
- Low-Temperature limits with smearing and ultrafine grids (...)

$$C_{V,N,\text{molar}}(T) = \frac{1}{n} \cdot C_{V,N}(T) \approx \gamma_m \cdot T + A \cdot T^3$$



Initial thought:

“Imitate” the GW-Propaganda-Picture under the inclusion of interactions



Outlook (maybe…):

- Finer Grids, more bands and more complicated structures (...)
- High-Temperature limits with phonon-phonon-interactions (...)
- Low-Temperature limits with smearing and ultrafine grids (...)
- (Prediction of Structural Phase-Transitions (P-T-Phase-Diagrams) with the computation of the grand canonical partition function in the hybrid ensemble)
- (Spin-Triplet Superconductivity by decoupling in the Functional Field Integral Formalism)

Finishing comments (on how the project emerged…)

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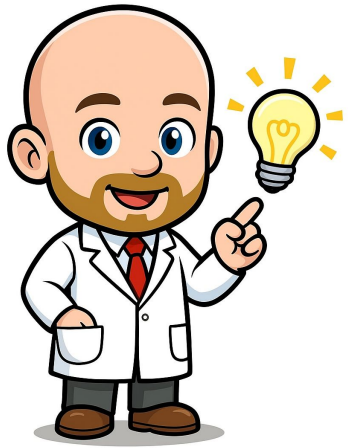
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Acknowledgements

- Jonas (Green-Functions and Phonons)
- Johan (EPW on Dardel (!!!))
- Lucas (First EPW-manipulation)
- Lars (“How to steal data”)
- Biplab (DFT-course-project)
- Ralph (Quantum Materials Course)
- Soheil (Wannier90)
- Prathibha (Encouragement and SQL)
- Moa (Encouragement and Moral Support)
- Chin (Encouragement and Quantum-Espresso)
- Oscar (Encouragement, Computing Power, Article and first DFT-contact)

Thank you for your Attention!

Questions / Suggestions / Comments?