Details in *GW*-BSE

Jinyuan Wu
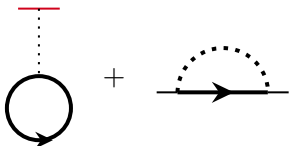
June 30, 2023

Table of contents

Infinitesimal

We all know the word "GW" means that $\Sigma = i\, GW$ (of course we have Hartree term but it's already in DFT)

$$\Sigma = \underset{}{\bigcirc} \; + \; \overset{}{\frown} \; , \tag{1}$$

where W is the RPA-screened potential.

Why some say $\Sigma(1,2) = i\, G(1,2)W(1^+,2)$?

- $G(1,2)$ is actually $G(1,2^+)$ (so when $1=2$, $G = n_{\mathrm{occ}}$: the loop in the Hartree term above)
- $\Sigma(1,2) = i\, G(1,2^+)W(1,2) = i\, G(1^-,2)W(1,2) = i\, G(1,2)(1^+,2)$.
- 1^+ or $2^+ \Leftrightarrow e^{\pm i\omega 0^+} \Leftrightarrow$ how to take contour

Other tricky details in diagrammatics

Time-reversal symmetry

- $W(-\boldsymbol{p}, -\omega) = W(\boldsymbol{p}, \omega)$ is always true (or otherwise we can symmetrize the Lagrangian)
- The real symmetry:

$$
\begin{aligned}
W(\omega, -\boldsymbol{k}) &= W(\omega, \boldsymbol{k}) \Leftrightarrow W(-\omega, \boldsymbol{k}) = W(\omega, \boldsymbol{k}) \\
\Leftrightarrow W(\boldsymbol{r}, \boldsymbol{r}', \omega) &= W(\boldsymbol{r}', \boldsymbol{r}, \omega) \Leftrightarrow W(\boldsymbol{r}, \boldsymbol{r}', \omega) = W(\boldsymbol{r}, \boldsymbol{r}', -\omega).
\end{aligned}
\tag{2}
$$

"Antiparticles" You can treat holes as antiparticles (negative energy, $i\,\mathrm{sgn}(\xi_{n\boldsymbol{k}})$ in time-ordered Green function) but then corresponding electron modes have to be ignored.

Other tricky details in diagrammatics

Imaginary unit

$$i\, G = i\, G_0 + i\, G_0 \times \underbrace{\bigcirc}_{-i\,\Sigma} \times i\, G \Rightarrow G = \frac{1}{\omega - E^0 - \Sigma}. \qquad (3)$$

$$-i\, W = -i\, v + (-i\, v) \times \underbrace{\bigcirc}_{i\,\chi} \times (-i\, W) \Rightarrow W = \epsilon^{-1} v, \quad \epsilon = 1 - v\chi. \ (4)$$

Minus sign
Note that when a closed fermionic loop is formed, a -1 factor is needed.
Example: the loop in the Hartree term
$\simeq (-1) \langle \psi \psi^\dagger \rangle \simeq \psi^\dagger \psi \simeq$ number of particle.

Feynman rules I

Recall that we are working in a crystal – we need to talk about $\boldsymbol{G}$ vectors
One set of rules that work:

- Propagator:

$$\xrightarrow{\quad n, k \quad} = \frac{\mathrm{i}}{\omega - \xi_{n\boldsymbol{k}} + \mathrm{i}\, 0^+ \operatorname{sgn}(\omega)} =: \mathrm{i}\, G^0_{n\boldsymbol{k}}(\omega). \qquad (5)$$
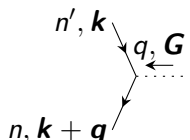
- Interaction:

$$\overset{q, \boldsymbol{G}}{\cdots\cdots\cdots} = -\mathrm{i}\,\frac{1}{V} v(\boldsymbol{q} + \boldsymbol{G}). \qquad (6)$$

But the prefactor of the interaction Hamiltonian is still $1/2V$, and

$$v(\boldsymbol{q}) = \int \mathrm{d}^3\boldsymbol{r}\, \mathrm{e}^{-\mathrm{i}\,\boldsymbol{q}\cdot\boldsymbol{r}}\, v(\boldsymbol{r}). \qquad (7)$$
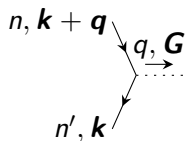
- For vertex,

$$
\begin{array}{c}
n', \boldsymbol{k} \\
\hspace{1cm} q, \boldsymbol{G} \\
n, \boldsymbol{k} + \boldsymbol{q}
\end{array}
= \langle n, \boldsymbol{k} + \boldsymbol{q} | \mathrm{e}^{\mathrm{i}(\boldsymbol{q}+\boldsymbol{G})\cdot\boldsymbol{r}} | n'\boldsymbol{k} \rangle =: M_{nn'}(\boldsymbol{k}, \boldsymbol{q}, \boldsymbol{G}). \quad (8)
$$

Note that the momentum arrow attached to the interaction line only controls the sign before $\boldsymbol{q}$ and $\boldsymbol{G}$; we don't sum over possible directions of the arrow. Thus

$$
\begin{array}{c}
n, \boldsymbol{k} + \boldsymbol{q} \\
\hspace{1cm} q, \boldsymbol{G} \\
n', \boldsymbol{k}
\end{array}
= \langle n'\boldsymbol{k} | \mathrm{e}^{-\mathrm{i}(\boldsymbol{q}+\boldsymbol{G})\cdot\boldsymbol{r}} | n, \boldsymbol{k} + \boldsymbol{q} \rangle =: M_{nn'}(\boldsymbol{k}, \boldsymbol{q}, \boldsymbol{G})^*. \quad (9)
$$

Here is where the phase factor of each $\phi_{n\boldsymbol{k}}$ enters the calculation:

- Momentum conservation is enforced by $\delta_{\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{k}_3+\boldsymbol{k}_4,0}$: no $(2\pi)^3$ factor is needed.
- For internal lines, sum over $\boldsymbol{k}$, n, $\boldsymbol{G}$; no additional $1/(2\pi)^3$ factors are needed. For frequency, do $\int \mathrm{d}\omega\,/2\pi$.
- For external lines: $\boldsymbol{r} \!-\!\!\!\triangleleft\!\bigcirc$ is $\phi_{n\boldsymbol{k}}(\boldsymbol{r})$, and $\bigcirc\!\triangleleft\!\!\!-\, \boldsymbol{r}'$ is $\phi_{n\boldsymbol{k}}^*(\boldsymbol{r})$, as in:

$$G(\boldsymbol{r},\boldsymbol{r}',\omega) = \sum_{n,\boldsymbol{k}} \frac{\phi_{n\boldsymbol{k}}(\boldsymbol{r})\phi_{n\boldsymbol{k}}(\boldsymbol{r}')^*}{\omega - \xi_{n\boldsymbol{k}} + \mathrm{i}\,\mathrm{sgn}(\xi_{n\boldsymbol{k}})}, \tag{10}$$

where $\boldsymbol{r}$ is the outgoing index and $\boldsymbol{r}'$ is the incoming index. (When going from $G(\boldsymbol{r},\boldsymbol{r}')$ to $G_{\boldsymbol{k},nn'}$, outgoing external line becomes $\phi_{n\boldsymbol{k}}^*(\boldsymbol{r})^*$ and incoming external line becomes $\phi_{n'\boldsymbol{k}}(\boldsymbol{r}')$)
The normalization condition is

$$\int \mathrm{d}^3\boldsymbol{r}\,\psi_{n\boldsymbol{k}}^*(\boldsymbol{r})\psi_{n'\boldsymbol{k}'}(\boldsymbol{r}) = \delta_{nn'}\delta_{\boldsymbol{k}\boldsymbol{k}'}, \quad \psi_{n\boldsymbol{k}} \simeq \frac{1}{\sqrt{V}}\,\mathrm{e}^{\mathrm{i}(\boldsymbol{k}+\boldsymbol{G})\cdot\boldsymbol{r}}. \tag{11}$$

The structure of G

- We *always* have Lehmann self-energy representations:

$$G(\boldsymbol{r}, \boldsymbol{r}', \omega) = \sum_n \frac{\langle \Omega | \phi(\boldsymbol{r}) | n \rangle \, \langle n | \phi^\dagger(\boldsymbol{r}') | \Omega \rangle}{\omega - E_n + i\,0^+ \operatorname{sgn}(\omega)} = \sum_{n,\boldsymbol{k}} \frac{\phi_{n\boldsymbol{k}}(\boldsymbol{r}) \phi_{n\boldsymbol{k}}(\boldsymbol{r}')^*}{\omega - \operatorname{Re} \xi_{n\boldsymbol{k}} - i \operatorname{Im} \xi_{n\boldsymbol{k}}}. \tag{12}$$

  $\boldsymbol{k}$ not necessarily good quantum number; no orthogonal conditions.

- In a Fermi liquid: since $\tau \propto 1/T^2$ near μ, for bands near the Fermi surface, approximately $\operatorname{Im} \xi_{n\boldsymbol{k}}$ is small and $\{\phi_{n\boldsymbol{k}}\}$ is a good basis.

- Note: this only means $|\Omega\rangle$ and $|n\rangle$ look like Fock states when tested with $G^{(2)}$ (hence clear-cut μ in simulated ARPES spectrum, etc.); when tested with $G^{(4)}$, correlated effects still exist ($\Rightarrow$ de-excitation terms in exciton $\chi_S(\boldsymbol{r}, \boldsymbol{r}')$)

The structure of G

To avoid directly dealing with poles numerically (and getting stuck by things like how small $i\,0^+$ should really be), we choose to carry out iGW analytically.

Assumption: well-defined quasiparticles So we assume

$$G(\boldsymbol{r}, \boldsymbol{r}', \omega) = \sum_{n,\boldsymbol{k}} \frac{\phi_{n\boldsymbol{k}}(\boldsymbol{r})\phi_{n\boldsymbol{k}}^*(\boldsymbol{r}')}{\omega - \xi_{n\boldsymbol{k}} + i\,\mathrm{sgn}(\xi_{n\boldsymbol{k}})}. \tag{13}$$

Spectral function

$$A(\boldsymbol{r}, \boldsymbol{r}', \omega) = \sum_{n,\boldsymbol{k}} \delta(\omega - \xi_{n\boldsymbol{k}})\phi_{n\boldsymbol{k}}(\boldsymbol{r})\phi_{n\boldsymbol{k}}^*(\boldsymbol{r}'). \tag{14}$$

The structure of W

Time reversal symmetry We assume

$$W(\boldsymbol{r}, \boldsymbol{r}', \omega) = W(\boldsymbol{r}, \boldsymbol{r}', -\omega). \tag{15}$$

The explicit expression in terms of $\phi_{n\boldsymbol{k}}$ (The -1 factor comes from the fermion loop)

$$\mathrm{i}\,\chi_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q}, \omega) = q, G \xrightarrow{\substack{n, k+q \\ \bigcirc \\ n', k}} q, G'$$

$$= -\int \frac{\mathrm{d}\omega'}{2\pi} \sum_{\boldsymbol{k}} \sum_{n,n'} \frac{\mathrm{i}}{\omega' - \xi_{n'\boldsymbol{k}} + \mathrm{i}\,0^+ \operatorname{sgn}(\xi_{n'\boldsymbol{k}})} \tag{16}$$

$$\times \frac{\mathrm{i}}{\omega + \omega' - \xi_{n,\boldsymbol{k}+\boldsymbol{q}} + \mathrm{i}\,0^+ \operatorname{sgn}(\xi_{n,\boldsymbol{k}+\boldsymbol{q}})}$$

$$\times M_{nn'}(\boldsymbol{k}, \boldsymbol{q}, \boldsymbol{G}) M_{nn'}^*(\boldsymbol{k}, \boldsymbol{q}, \boldsymbol{G}').$$

The structure of W

After long and tedious contour integration ...

$$
\chi_{\boldsymbol{GG'}}(\boldsymbol{q}, \omega) = \sum_{\boldsymbol{k}} \sum_{n}^{\text{occ}} \sum_{n'}^{\text{emp}} M_{nn'}(\boldsymbol{k}, \boldsymbol{q}, \boldsymbol{G}) M_{nn'}^*(\boldsymbol{k}, \boldsymbol{q}, \boldsymbol{G'})
$$
$$
\times \left(\frac{1}{\omega + \xi_{n, \boldsymbol{k}+\boldsymbol{q}} - \xi_{n'\boldsymbol{k}} + \mathrm{i}\,0^+} + \frac{1}{-\omega + \xi_{n, \boldsymbol{k}+\boldsymbol{q}} - \xi_{n'\boldsymbol{k}} + \mathrm{i}\,0^+} \right).
$$
$$(17)$$

Sketch of steps:

- When the signs of $\xi_{n, \boldsymbol{k}+\boldsymbol{q}}$ and $\xi_{n'\boldsymbol{k}}$ are different, the poles of the two propagators don't cancel.
- Time reversal symmetry allows swapping n and n' and adding necessary minus signs to momenta
- So now we can fix n to the occupied band and n' to the empty band and still have the shared MM^* factor for the two terms.

Non-static COHSEX decomposition I

Analytic structure of GW Below r and r' indices are hidden; Im treats ϕ_{nk} as real numbers; positivity conditions are assumed for weight functions in spectral representations:

$$\Sigma(\omega) = \mathrm{i} \int \frac{\mathrm{d}\omega'}{2\pi} \, \mathrm{e}^{-\mathrm{i}0^+\omega'} \, G(\omega - \omega')W(\omega'), \tag{18}$$

$$G(\omega) = \int \mathrm{d}\omega' \frac{A(\omega')}{\omega - \omega' + \mathrm{i}\,\mathrm{sgn}(\omega)}, \quad A(\omega) = -\frac{1}{\pi}|\mathrm{Im}\, G(\omega)|, \tag{19}$$

$$W(\omega) = v + \int_0^\infty \mathrm{d}\omega' \frac{2\omega'}{\omega^2 - (\omega' - \mathrm{i}0^+)^2} B(\omega'), \quad \mathrm{Im}\, W(\omega) = -\pi B(\omega). \tag{20}$$

The decomposition So in $G(\omega - \omega')$ and $W(\omega')$ we both have poles ...

- $\Sigma^{\mathrm{COH}} = \Sigma^{GW}$ from poles of W
- $\Sigma^{\mathrm{SEX}} = \Sigma^{GW}$ from poles of G

Screened exchange term: Σ^{SEX}

- When $i\,\mathrm{sgn}(\omega') < 0$ in $G(\omega)$, we have one pole in the lower plane, otherwise no pole exists. We need to integrate on the lower plane (due to $e^{-i0^+\omega'}$ factor). Thus:

$$
\begin{aligned}
\Sigma^{\mathsf{SEX}}(\boldsymbol{r}, \boldsymbol{r}', \omega) &= -\int_{-\infty}^{0} \mathrm{d}\omega'\, A(\boldsymbol{r}, \boldsymbol{r}', \omega') W(\boldsymbol{r}, \boldsymbol{r}', \omega - \omega') \\
&= -\sum_{n,\boldsymbol{k}}^{\mathrm{occ}} \phi_{n\boldsymbol{k}}(\boldsymbol{r})\phi_{n\boldsymbol{k}}^{*}(\boldsymbol{r}') W(\boldsymbol{r}, \boldsymbol{r}', \omega - \xi_{n\boldsymbol{k}}).
\end{aligned}
\tag{21}
$$

- Inserting the definition of W, and switching to the $n, \mathbf{k}$ basis:

$$
\begin{aligned}
&\langle n\mathbf{k} | \Sigma^{\text{SEX}}(\omega) | n'\mathbf{k} \rangle \\
&= -\sum_{n''}^{\text{occ}} \sum_{\mathbf{q}\mathbf{G}\mathbf{G}'} M_{n''n}^*(\mathbf{k}, -\mathbf{q}, -\mathbf{G}) M_{n''n'}(\mathbf{k}, -\mathbf{q}, -\mathbf{G}') \\
&\quad \times \epsilon_{\mathbf{G}\mathbf{G}'}^{-1}(\mathbf{q}, \omega - \xi_{n'', \mathbf{k}-\mathbf{q}}) v(\mathbf{q} + \mathbf{G}').
\end{aligned}
\tag{22}
$$

Comments

- Σ^{SEX} is the only term in Hartree-Fock approx.

Coulomb hole term: $\Sigma^{\mathbf{COH}}$

- Consider the poles from W, and insert the definition of A:

$$
\begin{aligned}
\Sigma^{\mathsf{COH}}(\boldsymbol{r}, \boldsymbol{r}', \omega) &= \int_0^\infty \mathrm{d}\omega'' \int_{-\infty}^\infty \mathrm{d}\omega' \, \frac{A(\boldsymbol{r}, \boldsymbol{r}', \omega') B(\boldsymbol{r}, \boldsymbol{r}', \omega'')}{\omega - \omega' - \omega'' + \mathrm{i}\,\mathrm{sgn}(\omega')} \\
&= \sum_{n, \boldsymbol{k}} \phi_{n\boldsymbol{k}}(\boldsymbol{r}) \phi_{n\boldsymbol{k}}^*(\boldsymbol{r}') \int_0^\infty \mathrm{d}\omega' \, \frac{-\operatorname{Im} W(\boldsymbol{r}, \boldsymbol{r}', \omega')/\pi}{\omega - \xi_{n\boldsymbol{k}} - \omega' + \mathrm{i}\,\mathrm{sgn}(\xi_{n\boldsymbol{k}})}.
\end{aligned}
\tag{23}
$$

- Here the ϵ^{-1} factor in W is always the same as $\epsilon_{\mathsf{r}}^{-1}$ since $\omega' > 0$.

- We can verify (recall that here Im treats $\phi_{n\boldsymbol{k}}$ as a real number and only considers the positions of the poles)

$$
2\,\mathrm{i}\operatorname{Im} \frac{1}{a + b\,\mathrm{i}} = \frac{1}{a + b\,\mathrm{i}} - \frac{1}{a - b\,\mathrm{i}} \Rightarrow \operatorname{Im} \epsilon^{-1}(\omega') = \frac{1}{2\,\mathrm{i}}(\epsilon_{\mathsf{r}}^{-1} - \epsilon_{\mathsf{a}}^{-1}).
$$

- Switching to the $n, \boldsymbol{k}$ basis:

$$
\begin{aligned}
&\left\langle n\boldsymbol{k}\middle|\Sigma^{\text{COH}}(\omega)\middle|n'\boldsymbol{k}\right\rangle \\
&= \frac{\mathrm{i}}{2\pi}\sum_{n''}\sum_{\boldsymbol{q},\boldsymbol{G},\boldsymbol{G}'}M_{n''n}^{*}(\boldsymbol{k},-\boldsymbol{q},-\boldsymbol{G})M_{n''n'}(\boldsymbol{k},-\boldsymbol{q},-\boldsymbol{G}') \\
&\times \int_{0}^{\infty}\mathrm{d}\omega'\,\frac{[\epsilon_{\boldsymbol{G}\boldsymbol{G}'}^{\mathrm{r}}]^{-1}(\boldsymbol{q},\omega')-[\epsilon_{\boldsymbol{G}\boldsymbol{G}'}^{\mathrm{a}}]^{-1}(\boldsymbol{q},\omega')}{\omega-\xi_{n\boldsymbol{k}}-\omega'+\mathrm{i}\,0^{+}\,\mathrm{sgn}(\xi_{n\boldsymbol{k}})}v(\boldsymbol{q}+\boldsymbol{G}').
\end{aligned}
\tag{24}
$$

Comments

- In static COHSEX,

$$
\Sigma^{\text{COH}}(\boldsymbol{r},\boldsymbol{r}',\omega) = \frac{1}{2}\delta(\boldsymbol{r}-\boldsymbol{r}')(W(\boldsymbol{r},\boldsymbol{r}',\omega)-v),
\tag{25}
$$

which tells us how an electron is dragged away from positions with large charge concentration – the origin of the name "Coulomb hole"?

- Now we switching back to the normal definition of the operator Im – note that

$$\text{Im}\,\epsilon_r^{-1} = \frac{1}{2\,i}(\epsilon_r^{-1} - \epsilon_a^{-1})$$

  is only true for systems with inversion symmetry (real wave function, etc.).

- In Deslippe et al. 2012, Σ^{COH} and Σ^{SEX} are actually the retarded version (note that in (22) ϵ is replaced by ϵ_r, and in (24)) $i\,\text{sgn}(\xi_{n\boldsymbol{k}})0^+$ is replaced by $i\,0^+$.

Key assumptions

- Well-defined quasiparticles labeled by $\boldsymbol{k}$ and n (Fermi liquid theory; used everywhere)
- Time-reversal symmetry (used when deriving χ and doing spectral representation of W)

Input $\{\phi_{n\boldsymbol{k}}\}$, $\{\varepsilon_{n\boldsymbol{k}}\}$, occupation (from which μ and hence $\xi_{n\boldsymbol{k}} = \varepsilon_{n\boldsymbol{k}} - \mu$ are decided)

Main procedures

- `epsilon`: input $\{\phi_{n\boldsymbol{k}}\}$ and $\{\varepsilon_{n\boldsymbol{k}}\}$, output $\epsilon^{-1}_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q}, \omega)$
  1. From $\{\phi_{n\boldsymbol{k}}\}$ to $M_{nn'}(\boldsymbol{k}, \boldsymbol{q}, \boldsymbol{G})$ using (8).
  2. From $\varepsilon_{n\boldsymbol{k}}$ to $\chi_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q}, \omega)$ using (17).
  3. From χ to ϵ.
  4. Finding ϵ^{-1}.
- `sigma`: input $\phi_{n\boldsymbol{k}}$, V_{xc} and $\epsilon^{-1}_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q}, \omega)$, output $\langle n\boldsymbol{k}|\Sigma^G W(E)|n'\boldsymbol{k}\rangle$ and $\varepsilon^{GW}_{n\boldsymbol{k}}$

1. From $\{\phi_{n\boldsymbol{k}}\}$ to $M_{nn'}(\boldsymbol{k}, \boldsymbol{q}, \boldsymbol{G})$ using (8).
2. From $M_{nn'}(\boldsymbol{k}, \boldsymbol{q}, \boldsymbol{G})$ to $\langle n\boldsymbol{k}|\Sigma^{\text{COH,SEX}}|n'\boldsymbol{k}\rangle$ using (22) and (24)
3. Finding Z using TODO

Cutoff parameters

- In $\phi_{n\boldsymbol{k}}$:
  - N_{bands} (i.e. max n),
  - $\boldsymbol{k}$-grid density,
  - E_{cut} (i.e. $\boldsymbol{G}$-grid size, i.e. spatial resolution)
- In $\epsilon_{\boldsymbol{G}\boldsymbol{G}'}^{-1}(\boldsymbol{q}, \omega)$:
  - $\boldsymbol{k}$-grid from $\{\phi_{n\boldsymbol{k}}\}$
  - N_{bands} (i.e. max n in summation in (17))
  - E_{cut} (used to reduce the $\boldsymbol{G}$-grid in $\{\phi_{n\boldsymbol{k}}\}$, which may be too large)
  - ω-grid

Overview

Three levels of frequency dependence:

1. Static COHSEX
2. Generalized plasmon-pole model (GPP)
3. Full frequency

- The SI version:

$$\epsilon_2 := \mathsf{Im}\, \epsilon_{\mathsf{r}} = \frac{\pi e^2}{\omega^2 \epsilon_0 V} \sum_S |\langle S|\mathbf{v} \cdot \hat{\mathbf{e}}|0\rangle|^2 \delta(\omega - \Omega_S). \qquad (26)$$

- The Gaussian units version:

$$\epsilon_2 = \frac{4\pi^2 e^2}{\omega^2 V} \sum_S |\langle S|\mathbf{v} \cdot \hat{\mathbf{e}}|0\rangle|^2 \delta(\omega - \Omega_S). \qquad (27)$$

   The value of ϵ doesn't change in unit conversion, but e^2/ϵ_0 should be replaced by $4\pi e^2$.

- With spin degeneracy we have an additional 2 factor (magnetic field not strong, no mechanism of spin splitting, so the input and output spins are the same)

The expression of ϵ_2 II

- In Rydberg units, $e^2 = 2$
- So with spin degeneracy we have

$$\epsilon_2 = \frac{16\pi^2}{\omega^2 V} \sum_S |\langle S|\boldsymbol{v} \cdot \hat{\boldsymbol{e}}|0\rangle|^2 \delta(\omega - \Omega_S), \qquad (28)$$

- and without spin degeneracy (or when SOC is strong and the spin index has been incorporated into S) we have

$$\epsilon_2 = \frac{8\pi^2}{\omega^2 V} \sum_S |\langle S|\boldsymbol{v} \cdot \hat{\boldsymbol{e}}|0\rangle|^2 \delta(\omega - \Omega_S). \qquad (29)$$

- This is the actual formula used in `absp0.f90`.

Interpolation

Two sources of errors

- k-grid sampling
- Finite number of bands (this can be systematically reduced: for *each* k, $\{u_{nk}\}_n$ is a complete basis of the space of possible u_{nk}.)

References I

Deslippe, Jack et al. (2012). "BerkeleyGW: A massively parallel computer package for the calculation of the quasiparticle and optical properties of materials and nanostructures". In: *Computer Physics Communications* 183.6, pp. 1269–1289. ISSN: 0010-4655. DOI: https://doi.org/10.1016/j.cpc.2011.12.006. URL: https://www.sciencedirect.com/science/article/pii/S0010465511003912.