Details in GW-BSE

Jinyuan Wu

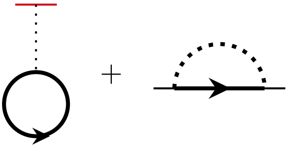
October 27, 2023

Table of contents

Infinitesimal

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

$-\mathrm{i}\,\Sigma =$



, (1)

where W is the RPA-screened potential.

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

- $G(1,2)$ is actually $G(1, 2^+)$ (so when $1 = 2$, $G = -n_{\mathrm{occ}}$: the loop in the Hartree term above)
- $\Sigma(1,2) = \mathrm{i}\, G(1, 2^+) W(1,2) = \mathrm{i}\, G(1^-, 2) W(1,2) = \mathrm{i}\, G(1,2) W(1^+, 2)$.
- 1^+ or 2^+ $\Leftrightarrow$ $\mathrm{e}^{\pm \mathrm{i}\,\omega 0^+}$ $\Leftrightarrow$ 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 (and change the form of the interaction vertex and allow broken particle conservation) but then corresponding electron modes have to be ignored.

Other tricky details in diagrammatics

Imaginary unit

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

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

Minus sign

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

Feynman rules I

Recall that we are working in a crystal – $\phi_{n\boldsymbol{k}}(\boldsymbol{r}) \neq \mathrm{e}^{\mathrm{i}\,\boldsymbol{k}\cdot\boldsymbol{r}}$
One set of rules that works:

- Propagator:

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

- Interaction:

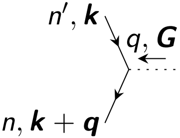
$$\overset{q,\,\boldsymbol{G}}{\cdots\cdots\cdots\cdots} \;=\; -\,\mathrm{i}\,\frac{1}{V}\,v(\boldsymbol{q}+\boldsymbol{G}). \tag{6}$$

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

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

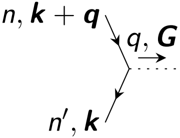
Feynman rules II

- For vertex,



$$= \left\langle n, \boldsymbol{k}+\boldsymbol{q} \middle| \mathrm{e}^{\mathrm{i}(\boldsymbol{q}+\boldsymbol{G})\cdot\boldsymbol{r}} \middle| n' \boldsymbol{k} \right\rangle =: M_{nn'}(\boldsymbol{k}, \boldsymbol{q}, \boldsymbol{G}). \tag{8}$$

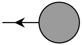
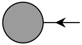
Note that the momentum arrow attached to the interaction line only controls the sign before $\boldsymbol{q}$ and $\boldsymbol{G}$; we don't sum over possible directions of the arrow. Thus



$$= \left\langle n' \boldsymbol{k} \middle| \mathrm{e}^{-\mathrm{i}(\boldsymbol{q}+\boldsymbol{G})\cdot\boldsymbol{r}} \middle| n, \boldsymbol{k}+\boldsymbol{q} \right\rangle =: M_{nn'}(\boldsymbol{k}, \boldsymbol{q}, \boldsymbol{G})^*. \tag{9}$$

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

Feynman rules III

- 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: $\boldsymbol{r}$  is $\phi_{n\boldsymbol{k}}(\boldsymbol{r})$, and  $\boldsymbol{r}'$ is $\phi^*_{n\boldsymbol{k}}(\boldsymbol{r})$, as in:

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

  $\boldsymbol{r}$ 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

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

The structure of G

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

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

  $\boldsymbol{k}$ 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 $\mathrm{i}\,0^+$ should really be), we choose to carry out $\mathrm{i}\,GW$ analytically.

Assumption: well-defined quasiparticles So we assume

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

Spectral function

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

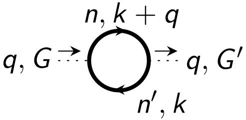
The structure of W

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)

$$\mathrm{i}\,\chi_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q}, \omega) =$$



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

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

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

The structure of W

After long and tedious contour integration . . .

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

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.

Ingredients of GW

- $\Sigma = \mathrm{i}\, GW = \mathrm{i}\, G\epsilon^{-1} v$
- G: we have spectral representation (13)
- ϵ: we have

$$\epsilon_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q}, \omega) = \delta_{\boldsymbol{G}\boldsymbol{G}'} - v(\boldsymbol{q} + \boldsymbol{G}) \chi_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q}, \omega). \tag{18}$$

  Note: in this way $\epsilon_{\boldsymbol{G}\boldsymbol{G}'}$ is not symmetric; we need to write

$$W_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q}, \omega) = \epsilon^{-1}_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q}, \omega) v(\boldsymbol{q} + \boldsymbol{G}') \tag{19}$$

  to get a symmetric screened Coulomb potential.

Next step: complex contour integral

Non-static COHSEX decomposition I

Analytic structure of *GW* Below $\boldsymbol{r}$ and $\boldsymbol{r}'$ indices are hidden; Im treats $\phi_{n\boldsymbol{k}}$ as real numbers; positivity conditions are assumed for weight functions in spectral representations:

$$\Sigma(\omega) = \mathrm{i} \int \frac{\mathrm{d}\omega'}{2\pi} \mathrm{e}^{-\mathrm{i}\,0^+ \omega'} G(\omega - \omega') W(\omega'), \tag{20}$$

$$G(\omega) = \int \mathrm{d}\omega' \frac{A(\omega')}{\omega - \omega' + \mathrm{i}\,\mathrm{sgn}(\omega)}, \quad A(\omega) = -\frac{1}{\pi} |\mathrm{Im}\, G(\omega)|, \tag{21}$$

$$W(\omega) = v + \int_0^\infty \mathrm{d}\omega' \frac{2\omega'}{\omega^2 - (\omega' - \mathrm{i}\,0^+)^2} B(\omega'), \quad \mathrm{Im}\, W(\omega) = -\pi B(\omega). \tag{22}$$

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

Non-static COHSEX decomposition II

Screened exchange term: Σ^{SEX}

- When $\mathrm{i}\,\mathrm{sgn}(\omega') < 0$ 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 $\mathrm{e}^{-\mathrm{i}0^+\omega'}$ factor). Thus:

$$
\begin{aligned}
\Sigma^{\mathrm{SEX}}(\boldsymbol{r}, \boldsymbol{r}', \omega) &= -\int_{-\infty}^{0} \mathrm{d}\omega'\, A(\boldsymbol{r}, \boldsymbol{r}', \omega') W(\boldsymbol{r}, \boldsymbol{r}', \omega - \omega') \\
&= -\sum_{n,\boldsymbol{k}}^{\mathrm{occ}} \phi_{n\boldsymbol{k}}(\boldsymbol{r}) \phi^*_{n\boldsymbol{k}}(\boldsymbol{r}') W(\boldsymbol{r}, \boldsymbol{r}', \omega - \xi_{n\boldsymbol{k}}).
\end{aligned}
\tag{23}
$$

Non-static COHSEX decomposition III

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

$$
\begin{aligned}
&\left\langle n\boldsymbol{k}\middle|\Sigma^{\mathrm{SEX}}(\omega)\middle|n'\boldsymbol{k}\right\rangle \\
&= -\sum_{n''}^{\mathrm{occ}} \sum_{\boldsymbol{q}\boldsymbol{G}\boldsymbol{G}'} M^*_{n''n}(\boldsymbol{k}, -\boldsymbol{q}, -\boldsymbol{G}) M_{n''n'}(\boldsymbol{k}, -\boldsymbol{q}, -\boldsymbol{G}') \\
&\quad \times \epsilon^{-1}_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q}, \omega - \xi_{n'', \boldsymbol{k}-\boldsymbol{q}}) v(\boldsymbol{q} + \boldsymbol{G}').
\end{aligned}
\tag{24}
$$

Comments

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

Coulomb hole term: Σ^{COH}

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

$$\begin{aligned}\Sigma^{\mathrm{COH}}(\boldsymbol{r}, \boldsymbol{r}', \omega) &= \int_0^\infty \mathrm{d}\omega'' \int_{-\infty}^\infty \mathrm{d}\omega' \, \frac{A(\boldsymbol{r}, \boldsymbol{r}', \omega') B(\boldsymbol{r}, \boldsymbol{r}', \omega'')}{\omega - \omega' - \omega'' + \mathrm{i}\,\mathrm{sgn}(\omega')} \\ &= \sum_{n, \boldsymbol{k}} \phi_{n\boldsymbol{k}}(\boldsymbol{r}) \phi^*_{n\boldsymbol{k}}(\boldsymbol{r}') \int_0^\infty \mathrm{d}\omega' \, \frac{-\operatorname{Im} W(\boldsymbol{r}, \boldsymbol{r}', \omega')/\pi}{\omega - \xi_{n\boldsymbol{k}} - \omega' + \mathrm{i}\,\mathrm{sgn}(\xi_{n\boldsymbol{k}})}.\end{aligned} \tag{25}$$

- Here the ϵ^{-1} factor in W is always the same as $\epsilon_{\mathrm{r}}^{-1}$ 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)

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

Non-static COHSEX decomposition V

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

$$
\begin{aligned}
&\left\langle n\boldsymbol{k}\middle|\Sigma^{\mathrm{COH}}(\omega)\middle|n'\boldsymbol{k}\right\rangle \\
&= \frac{\mathrm{i}}{2\pi}\sum_{n''}\sum_{\boldsymbol{q},\boldsymbol{G},\boldsymbol{G}'} M^{*}_{n''n}(\boldsymbol{k},-\boldsymbol{q},-\boldsymbol{G})M_{n''n'}(\boldsymbol{k},-\boldsymbol{q},-\boldsymbol{G}') \\
&\times \int_0^\infty \mathrm{d}\omega' \, \frac{[\epsilon^{\mathrm{r}}_{\boldsymbol{G}\boldsymbol{G}'}]^{-1}(\boldsymbol{q},\omega') - [\epsilon^{\mathrm{a}}_{\boldsymbol{G}\boldsymbol{G}'}]^{-1}(\boldsymbol{q},\omega')}{\omega - \xi_{n\boldsymbol{k}} - \omega' + \mathrm{i}\,0^+ \,\mathrm{sgn}(\xi_{n\boldsymbol{k}})} v(\boldsymbol{q}+\boldsymbol{G}').
\end{aligned}
\tag{26}
$$

Comments

- In static COHSEX,

$$
\Sigma^{\mathrm{COH}}(\boldsymbol{r},\boldsymbol{r}',\omega) = \frac{1}{2}\delta(\boldsymbol{r}-\boldsymbol{r}')(W(\boldsymbol{r},\boldsymbol{r}',\omega) - v), \tag{27}
$$

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

Non-static COHSEX decomposition VI

- Now we switching back to the normal definition of the operator Im – note that
$$\operatorname{Im} \epsilon_{\mathrm{r}}^{-1} = \frac{1}{2\,\mathrm{i}}(\epsilon_{\mathrm{r}}^{-1} - \epsilon_{\mathrm{a}}^{-1})$$
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 (24) ϵ is replaced by ϵ_{r}, and in (26)) $\mathrm{i}\,\mathrm{sgn}(\xi_{n\boldsymbol{k}})0^+$ is replaced by $\mathrm{i}\,0^+$.

A brief summary of full frequency, non-diagonal GW I

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 $\varepsilon^{GW}_{n\boldsymbol{k}}$

A brief summary of full frequency, non-diagonal GW II

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 (24) and (26)
3. Finding Z using

$$Z = \frac{\mathrm{d}\Sigma/\mathrm{d}E}{1 - \mathrm{d}\Sigma/\mathrm{d}E}. \tag{28}$$

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 $\epsilon^{-1}_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q}, \omega)$:
  - $\boldsymbol{k}$-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 expression of ϵ_2 I

- The SI version:

$$\epsilon_2 := \operatorname{Im} \epsilon_{\mathrm{r}} = \frac{\pi e^2}{\omega^2 \epsilon_0 V} \sum_S |\langle S | \boldsymbol{v} \cdot \hat{\boldsymbol{e}} | 0 \rangle|^2 \delta(\omega - \Omega_S). \tag{29}$$

- The Gaussian units version:

$$\epsilon_2 = \frac{4\pi^2 e^2}{\omega^2 V} \sum_S |\langle S | \boldsymbol{v} \cdot \hat{\boldsymbol{e}} | 0 \rangle|^2 \delta(\omega - \Omega_S). \tag{30}$$

  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

$$\epsilon_2 = \frac{16\pi^2}{\omega^2 V} \sum_S |\langle S|\boldsymbol{v} \cdot \hat{\boldsymbol{e}}|0\rangle|^2 \delta(\omega - \Omega_S), \tag{31}$$

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

$$\epsilon_2 = \frac{8\pi^2}{\omega^2 V} \sum_S |\langle S|\boldsymbol{v} \cdot \hat{\boldsymbol{e}}|0\rangle|^2 \delta(\omega - \Omega_S). \tag{32}$$

- This is the actual formula used in `absp0.f90`; but $1/\omega^2$ is not included??

Interpolation

Two sources of errors

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

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.