# Details in *GW*-BSE

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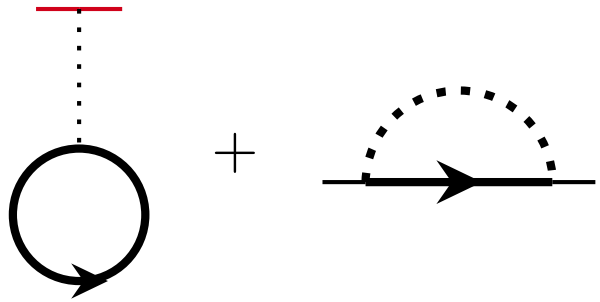
# Infinitesimal

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

$$\Sigma = \quad + \quad , \tag{1}$$



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)
- $\Sigma(1,2) = \mathrm{i}\, G(1,2^+)W(1,2) = \mathrm{i}\, G(1^-,2)W(1,2) = \mathrm{i}\, G(1,2)(1^+,2)$.
- $1^+$ 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 (negative energy, $\mathrm{i}\,\mathrm{sgn}(\xi_{n\boldsymbol{k}})$ in time-ordered Green function) but then corresponding electron modes have to be ignored.

# Other tricky details in diagrammatics

**Imaginary unit**

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

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

**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 – we need to talk about $\boldsymbol{G}$ vectors
One set of rules that work:

- Propagator:

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

- Interaction:

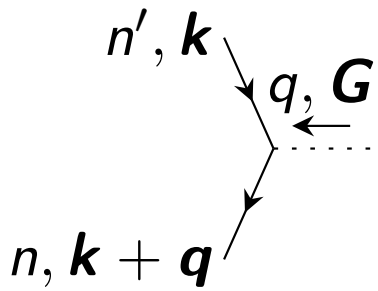
$$\cdots\cdots\cdots \overset{q,\boldsymbol{G}}{} \cdots\cdots\cdots = -\mathrm{i}\,\frac{1}{V} v(\boldsymbol{q}+\boldsymbol{G}). \tag{6}$$

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

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

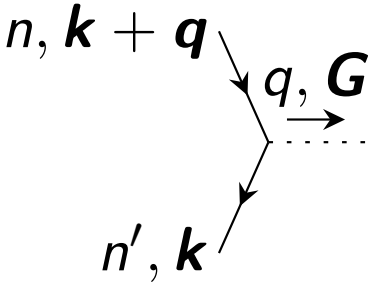
# Feynman rules II

- For vertex,




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

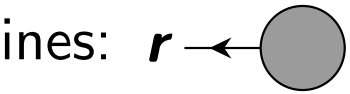
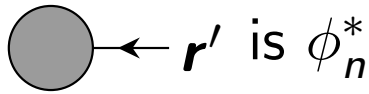
Note that the momentum arrow attached to the interaction line only controls the sign before $\boldsymbol{q}$ and $\boldsymbol{G}$; we don't sum over possible directions of the arrow. Thus




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

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:

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

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:

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

  $\boldsymbol{k}$ not necessarily good quantum number; no orthogonal conditions.
- In a Fermi liquid: since $\tau\propto 1/T^2$ near $\mu$, for bands near the Fermi surface, approximately $\mathrm{Im}\,\xi_{n\boldsymbol{k}}$ 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 $\mu$ 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**

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

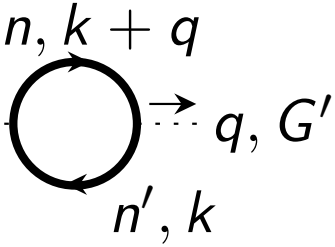
# The structure of $W$

**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)

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




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

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

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

# 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.

# Non-static COHSEX decomposition I

**Analytic structure of** *GW* Below $\boldsymbol{r}$ and $\boldsymbol{r}'$ indices are hidden; Im treats $\phi_{\boldsymbol{nk}}$ 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 $G$

# Non-static COHSEX decomposition II

**Screened exchange term: $\Sigma^{\mathrm{SEX}}$**

- 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:

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

# Non-static COHSEX decomposition III

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

$$\begin{aligned}
&\left\langle n\boldsymbol{k}\middle|\Sigma^{\mathrm{SEX}}(\omega)\middle|n'\boldsymbol{k}\right\rangle \\
&= -\sum_{n''}^{\mathrm{occ}}\sum_{\boldsymbol{q}\boldsymbol{G}\boldsymbol{G}'} M^{*}_{n''n}(\boldsymbol{k},-\boldsymbol{q},-\boldsymbol{G})M_{n''n'}(\boldsymbol{k},-\boldsymbol{q},-\boldsymbol{G}') \\
&\quad\times \epsilon^{-1}_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q},\omega-\xi_{n'',\boldsymbol{k}-\boldsymbol{q}})v(\boldsymbol{q}+\boldsymbol{G}').
\end{aligned} \tag{22}$$

**Comments**

- $\Sigma^{\mathrm{SEX}}$ is the only term in Hartree-Fock approx.

# Non-static COHSEX decomposition IV

**Coulomb hole term: $\Sigma^{\mathrm{COH}}$**

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

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

- Here the $\epsilon^{-1}$ 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)

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

# Non-static COHSEX decomposition V

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

$$\begin{aligned}
&\left\langle n\boldsymbol{k}\middle|\Sigma^{\mathrm{COH}}(\omega)\middle|n'\boldsymbol{k}\right\rangle \\
&= \frac{\mathrm{i}}{2\pi}\sum_{n''}\sum_{\boldsymbol{q},\boldsymbol{G},\boldsymbol{G}'} M^{*}_{n''n}(\boldsymbol{k},-\boldsymbol{q},-\boldsymbol{G})M_{n''n'}(\boldsymbol{k},-\boldsymbol{q},-\boldsymbol{G}') \\
&\times \int_0^\infty \mathrm{d}\omega' \frac{[\epsilon^{\mathrm{r}}_{\boldsymbol{G}\boldsymbol{G}'}]^{-1}(\boldsymbol{q},\omega') - [\epsilon^{\mathrm{a}}_{\boldsymbol{G}\boldsymbol{G}'}]^{-1}(\boldsymbol{q},\omega')}{\omega - \xi_{n\boldsymbol{k}} - \omega' + \mathrm{i}\,0^{+}\,\mathrm{sgn}(\xi_{n\boldsymbol{k}})} v(\boldsymbol{q}+\boldsymbol{G}').
\end{aligned} \tag{24}$$

**Comments**

- In static COHSEX,

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

  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

$$\mathrm{Im}\,\epsilon_{\mathrm{r}}^{-1} = \frac{1}{2\,\mathrm{i}}(\epsilon_{\mathrm{r}}^{-1} - \epsilon_{\mathrm{a}}^{-1})$$

  is only true for systems with inversion symmetry (real wave function, etc.).
- In Deslippe et al. 2012, $\Sigma^{\mathrm{COH}}$ and $\Sigma^{\mathrm{SEX}}$ are actually the retarded version (note that in (22) $\epsilon$ is replaced by $\epsilon_{\mathrm{r}}$, and in (24)) $\mathrm{i}\,\mathrm{sgn}(\xi_{n\boldsymbol{k}})0^{+}$ 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 $\chi$ and doing spectral representation of $W$)

**Input** $\{\phi_{n\boldsymbol{k}}\}$, $\{\varepsilon_{n\boldsymbol{k}}\}$, occupation (from which $\mu$ 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 $\chi$ to $\epsilon$.
  4. Finding $\epsilon^{-1}$.
- `sigma`: input $\phi_{n\boldsymbol{k}}$, $V_{\mathrm{xc}}$ 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 $\langle n\boldsymbol{k}|\Sigma^{\mathrm{COH,SEX}}|n'\boldsymbol{k}\rangle$ using (22) and (24)
3. Finding $Z$ using

$$Z = \frac{\mathrm{d}\Sigma/\mathrm{d}E}{1 - \mathrm{d}\Sigma/\mathrm{d}E}. \tag{26}$$

**Cutoff parameters**

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

# Overview

Three levels of frequency dependence:

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

# The expression of $\epsilon_2$ I

- The SI version:

$$\epsilon_2 := \mathrm{Im}\,\epsilon_r = \frac{\pi e^2}{\omega^2 \epsilon_0 V} \sum_S |\langle S|\boldsymbol{v}\cdot\hat{\boldsymbol{e}}|0\rangle|^2 \delta(\omega - \Omega_S). \tag{27}$$

- The Gaussian units version:

$$\epsilon_2 = \frac{4\pi^2 e^2}{\omega^2 V} \sum_S |\langle S|\boldsymbol{v}\cdot\hat{\boldsymbol{e}}|0\rangle|^2 \delta(\omega - \Omega_S). \tag{28}$$

  The value of $\epsilon$ doesn't change in unit conversion, but $e^2/\epsilon_0$ 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 $\epsilon_2$ II

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

$$\epsilon_2 = \frac{16\pi^2}{\omega^2 V} \sum_S |\langle S|\boldsymbol{v} \cdot \hat{\boldsymbol{e}}|0\rangle|^2 \delta(\omega - \Omega_S), \tag{29}$$

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

$$\epsilon_2 = \frac{8\pi^2}{\omega^2 V} \sum_S |\langle S|\boldsymbol{v} \cdot \hat{\boldsymbol{e}}|0\rangle|^2 \delta(\omega - \Omega_S). \tag{30}$$

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

# 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.