

Details in *GW*-BSE

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Infinitesimal

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

$$\Sigma = \text{Hartree term} + \text{exchange term}, \quad (1)$$

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 $1 = 2$, $G = n_{\text{occ}}$: 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

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

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

“Antiparticles” You can treat holes as antiparticles (negative energy, $\text{isgn}(\xi_{n\mathbf{k}})$ in time-ordered Green function) but then corresponding electron modes have to be ignored.

Other tricky details in diagrammatics

Imaginary unit

$$iG = iG_0 + iG_0 \times \underbrace{\text{circle}}_{-i\Sigma} \times iG \Rightarrow G = \frac{1}{\omega - E^0 - \Sigma}. \quad (3)$$

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

Minus sign

Note that when a closed fermionic loop is formed, a -1 factor is needed.

Example: the loop in the Hartree term

$$\simeq (-1) \langle \psi \psi^\dagger \rangle \simeq \psi^\dagger \psi \simeq \text{number of particle}.$$

Feynman rules I

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

- Propagator:

$$\text{---}\overrightarrow{\hspace{1.5cm}}_{n,k} \text{---} = \frac{i}{\omega - \xi_{n\mathbf{k}} + i0^+ \text{sgn}(\omega)} =: i G_{n\mathbf{k}}^0(\omega). \quad (5)$$

- Interaction:

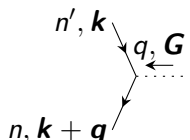
$$\text{.....}^{q, \mathbf{G}} \text{.....} = -i \frac{1}{V} v(\mathbf{q} + \mathbf{G}). \quad (6)$$

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

$$v(\mathbf{q}) = \int d^3\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} v(\mathbf{r}). \quad (7)$$

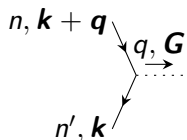
Feynman rules II

- For vertex,



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

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



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

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

Feynman rules III

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

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

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

The normalization condition is

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

The structure of G

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

$$G(\mathbf{r}, \mathbf{r}', \omega) = \sum_n \frac{\langle \Omega | \phi(\mathbf{r}) | n \rangle \langle n | \phi^\dagger(\mathbf{r}') | \Omega \rangle}{\omega - E_n + i0^+ \text{sgn}(\omega)} = \sum_{n, \mathbf{k}} \frac{\phi_{n\mathbf{k}}(\mathbf{r}) \phi_{n\mathbf{k}}(\mathbf{r}')^*}{\omega - \text{Re} \xi_{n\mathbf{k}} - i \text{Im} \xi_{n\mathbf{k}}}. \quad (12)$$

\mathbf{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 $\text{Im} \xi_{n\mathbf{k}}$ is small and $\{\phi_{n\mathbf{k}}\}$ 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 $\chi_S(\mathbf{r}, \mathbf{r}')$)

The structure of G

To avoid directly dealing with poles numerically (and getting stuck by things like how small $i0^+$ should really be), we choose to carry out i GW analytically.

Assumption: well-defined quasiparticles So we assume

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

Spectral function

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

The structure of W

Time reversal symmetry We assume

$$W(\mathbf{r}, \mathbf{r}', \omega) = W(\mathbf{r}, \mathbf{r}', -\omega). \quad (15)$$

The explicit expression in terms of ϕ_{nk} (The -1 factor comes from the fermion loop)

$$\begin{aligned} i\chi_{\mathbf{G}\mathbf{G}'}(\mathbf{q}, \omega) &= q, G \rightarrow \text{loop} \rightarrow q, G' \\ &= - \int \frac{d\omega'}{2\pi} \sum_{\mathbf{k}} \sum_{n, n'} \frac{i}{\omega' - \xi_{n'\mathbf{k}} + i0^+ \text{sgn}(\xi_{n'\mathbf{k}})} \\ &\quad \times \frac{i}{\omega + \omega' - \xi_{n, \mathbf{k}+\mathbf{q}} + i0^+ \text{sgn}(\xi_{n, \mathbf{k}+\mathbf{q}})} \\ &\quad \times M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn'}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}'). \end{aligned} \quad (16)$$

The structure of W

After long and tedious contour integration ...

$$\chi_{\mathbf{G}\mathbf{G}'}(\mathbf{q}, \omega) = \sum_{\mathbf{k}} \sum_n^{\text{occ}} \sum_{n'}^{\text{emp}} M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn'}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}') \\ \times \left(\frac{1}{\omega + \xi_{n, \mathbf{k}+\mathbf{q}} - \xi_{n' \mathbf{k}} + i0^+} + \frac{1}{-\omega + \xi_{n, \mathbf{k}+\mathbf{q}} - \xi_{n' \mathbf{k}} + i0^+} \right). \quad (17)$$

Sketch of steps:

- When the signs of $\xi_{n, \mathbf{k}+\mathbf{q}}$ and $\xi_{n' \mathbf{k}}$ 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

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

$$\Sigma(\omega) = i \int \frac{d\omega'}{2\pi} e^{-i0^+\omega'} G(\omega - \omega') W(\omega'), \quad (18)$$

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

$$W(\omega) = v + \int_0^\infty d\omega' \frac{2\omega'}{\omega^2 - (\omega' - i0^+)^2} B(\omega'), \quad \text{Im } W(\omega) = -\pi B(\omega). \quad (20)$$

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

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

Non-static COHSEX decomposition

Screened exchange term: Σ^{SEX}

A brief summary of full frequency, one-shot GW I

Key assumptions

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

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

Main procedures

- epsilon: input $\{\phi_{n\mathbf{k}}\}$ and $\{\varepsilon_{n\mathbf{k}}\}$, output $\epsilon_{\mathbf{G}\mathbf{G}'}^{-1}(\mathbf{q}, \omega)$
 - 1 From $\{\phi_{n\mathbf{k}}\}$ to $M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G})$ using (8).
 - 2 From $\varepsilon_{n\mathbf{k}}$ to $\chi_{\mathbf{G}\mathbf{G}'}(\mathbf{q}, \omega)$ using (17).
 - 3 From χ to ϵ .
 - 4 Finding ϵ^{-1} .
- sigma: input $\phi_{n\mathbf{k}}$, V_{xc} and $\epsilon_{\mathbf{G}\mathbf{G}'}^{-1}(\mathbf{q}, \omega)$, output $\varepsilon_{n\mathbf{k}}^{GW}$
 - 1 From $\{\phi_{n\mathbf{k}}\}$ to $M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G})$ using (8).

A brief summary of full frequency, one-shot GW II

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Cutoff parameters

- In $\phi_{n\mathbf{k}}$:
 - N_{bands} (i.e. $\max n$),
 - \mathbf{k} -grid density,
 - E_{cut} (i.e. \mathbf{G} -grid size, i.e. spatial resolution)
- In $\epsilon_{\mathbf{G}\mathbf{G}'}^{-1}(\mathbf{q}, \omega)$:
 - N_{bands} and \mathbf{k} -grid from $\{\phi_{n\mathbf{k}}\}$
 -

Overview

Three levels of frequency dependence:

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

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} .)

The expression of ϵ_2