Details in GW-BSE

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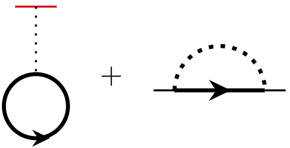
Infinitesimal

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

$\Sigma =$



(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:

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

Imaginary unit

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

“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.

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:

$$\xrightarrow{\quad n, k \quad} \quad = \frac{\mathrm{i}}{\omega - \xi_{n\boldsymbol{k}} + \mathrm{i}\, 0^+ \operatorname{sgn}(\omega)} =: \mathrm{i}\, G^0_{n\boldsymbol{k}}(\omega). \tag{4}$$

- Interaction:

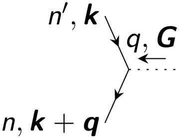
$$\overset{q, \boldsymbol{G}}{\cdots\cdots\cdots\cdots} \quad = -\mathrm{i}\, \frac{1}{V} v(\boldsymbol{q} + \boldsymbol{G}). \tag{5}$$

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

$$v(\boldsymbol{q}) = \int \mathrm{d}^3 \boldsymbol{r}\, \mathrm{e}^{-\mathrm{i}\, \boldsymbol{q} \cdot \boldsymbol{r}}\, v(\boldsymbol{r}). \tag{6}$$

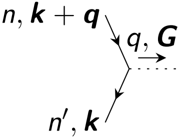
Feynman rules II

- For vertex,



$$= \left\langle n, \boldsymbol{k}+\boldsymbol{q} \middle| \mathrm{e}^{\mathrm{i}(\boldsymbol{q}+\boldsymbol{G})\cdot\boldsymbol{r}} \middle| n' \boldsymbol{k} \right\rangle =: M_{nn'}(\boldsymbol{k}, \boldsymbol{q}, \boldsymbol{G}). \tag{7}$$

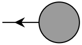
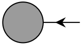
Note that the momentum arrow attached to the interaction line only controls the sign before $\boldsymbol{q}$ and $\boldsymbol{G}$; we don't sum over possible directions of the arrow. Thus



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

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 normalization factors are needed.
- For external lines: $\boldsymbol{r}$  is $\phi_{n\boldsymbol{k}}(\boldsymbol{r})$, and  $\boldsymbol{r}'$ is $\phi^*_{n\boldsymbol{k}}(\boldsymbol{r})$, as in:

$$G(\boldsymbol{r}, \boldsymbol{r}', \omega) = \sum_{n,\boldsymbol{k}} \frac{\phi_{n\boldsymbol{k}}(\boldsymbol{r})\phi_{n\boldsymbol{k}}(\boldsymbol{r})^*}{\omega - \xi_{n\boldsymbol{k}} + \mathrm{i}\,\mathrm{sgn}(\xi_{n\boldsymbol{k}})}, \tag{9}$$

  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

$$\int \mathrm{d}^3\boldsymbol{r}\, \psi^*_{n\boldsymbol{k}}(\boldsymbol{r})\psi_{n'\boldsymbol{k}'}(\boldsymbol{r}) = \delta_{nn'}\delta_{\boldsymbol{k}\boldsymbol{k}'}, \quad \psi_{n\boldsymbol{k}} \simeq \frac{1}{\sqrt{V}}\,\mathrm{e}^{\mathrm{i}(\boldsymbol{k}+\boldsymbol{G})\cdot\boldsymbol{r}}\,. \tag{10}$$

GW without G

To avoid directly dealing with poles, we choose to

Overview

Three levels of frequency dependence:

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

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 $u_{n\boldsymbol{k}}$.)

The expression of ϵ_2