

Details in GW-BSE

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What's GW

To be very concise... $-i\Sigma \approx GW^{\text{RPA}} = \text{---} \overbrace{\text{---}}^{\text{---}} \text{---}$.

Assuming quasiparticles... $v(\mathbf{q}+\mathbf{G}) = \frac{4\pi}{V|\mathbf{q}+\mathbf{G}|^2} \cdot \Sigma^{\text{contour}} = \Sigma^{\text{COH}} + \Sigma^{\text{SEX}}$,
 $\epsilon_{\mathbf{G}\mathbf{G}'}(\mathbf{q}, \omega) = \delta_{\mathbf{G}\mathbf{G}'} - v(\mathbf{q}+\mathbf{G})\chi_{\mathbf{G}\mathbf{G}'}(\mathbf{q}, \omega)$, $M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) = \langle n\mathbf{k} + \mathbf{q} | e^{i(\mathbf{q}+\mathbf{G}) \cdot \mathbf{r}} | n'\mathbf{k} \rangle$

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

$$\begin{aligned} \langle n\mathbf{k} | \Sigma^{\text{COH}}(\omega) | n'\mathbf{k} \rangle &= \frac{i}{2\pi} \sum_{n''} \sum_{\mathbf{q}, \mathbf{G}, \mathbf{G}'} M_{n''n}^*(\mathbf{k}, -\mathbf{q}, -\mathbf{G}) M_{n''n'}(\mathbf{k}, -\mathbf{q}, -\mathbf{G}') \\ &\times \int_0^\infty d\omega' \frac{[\epsilon_{\mathbf{G}\mathbf{G}'}^r]^{-1}(\mathbf{q}, \omega') - [\epsilon_{\mathbf{G}\mathbf{G}'}^a]^{-1}(\mathbf{q}, \omega')}{\omega - E_{n\mathbf{k}} - \omega' + i0^+ \text{sgn}(E_{n\mathbf{k}})} v(\mathbf{q} + \mathbf{G}'). \end{aligned} \quad (2)$$

$$\begin{aligned} \chi_{\mathbf{G}\mathbf{G}'}^{r/a}(\mathbf{q}, \omega) &= \sum_{\mathbf{k}} \sum_n^{\text{occ}} \sum_{n'}^{\text{emp}} M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn'}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}') \\ &\times \left(\frac{1}{\omega + E_{n, \mathbf{k}+\mathbf{q}} - E_{n'\mathbf{k}} \pm i0^+} + \frac{1}{-\omega + E_{n, \mathbf{k}+\mathbf{q}} - E_{n'\mathbf{k}} \mp i0^+} \right). \end{aligned} \quad (3)$$

What's GW

What a splendid equation system!

In practice. . . we always use GPP $\epsilon(\omega)$ is assumed to be plasmon model-like, so – we feed

$$\chi_{\mathbf{G}\mathbf{G}'}(\mathbf{q}, \omega = 0) = \sum_{\mathbf{k}} \sum_n^{\text{occ}} \sum_{n'}^{\text{emp}} M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn'}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}') \frac{2}{E_{n, \mathbf{k}+\mathbf{q}} - E_{n'\mathbf{k}}} \quad (4)$$

to *analytic* expressions of $\Sigma^{\text{COH}}, \Sigma^{\text{SEX}}$.

Huge simplification. . . Hedin $\xrightarrow{\text{assuming GW}}$ GW $\xrightarrow{\text{QP. approx.}}$ (1), (2), (3)
 $\xrightarrow{\text{GPP}}$ we are here

But still burdensome *Summation over empty bands – 1000-30000 bands!!!*

The problem of summing over many empty bands

Empty states are important – but why?

One further simplification trick: pseudobands. For $E_{nk} \gg E_F$:

$$\begin{aligned}\{\phi_{nk}\}_{\text{adjacent energy block } n_b} &\rightarrow \sum_{n \in \text{block } n_b} \phi_{nk}, \\ \{E_{nk}\}_{\text{adjacent energy block } n_b} &\rightarrow \frac{1}{|n_b|} \sum_{n \in \text{block } n_b} E_{nk}.\end{aligned}$$

4000 bands $\rightarrow \sim 400$ to ~ 1000 bands.

... but is this snake oil? It makes no sense!!!

Understanding pseudobands: energy averaging

Observation

- $\chi \sim MM^* \times \text{some-function}(E_{\text{emp}} - E_{\text{occ}})$;
- $\Sigma^{\text{COH}} \sim MM^* \times \text{some-function}(\omega - E)$;
- We are only interested in $\omega \sim E_F$.

👉 For $E_{nk} \gg E_F$ (ω): energy-dependent factors $\sim \text{const.}$ for all k .

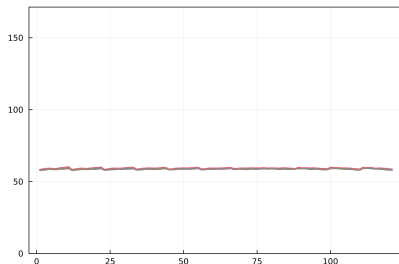
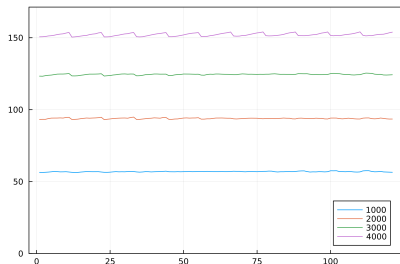
Thus for both χ and Σ^{COH} involving summation over empty bands:

high emp. bands

$$\sum_{n''} M_{n''n}^* M_{n''n'} \times \cdots = \sum_{\text{block } n_b} \cdots \times \sum_{n'' \in \text{block } n_b} M_{n''n}^* M_{n''n'}. \quad (5)$$

In RHS E_{emp} is replaced by the average energy.

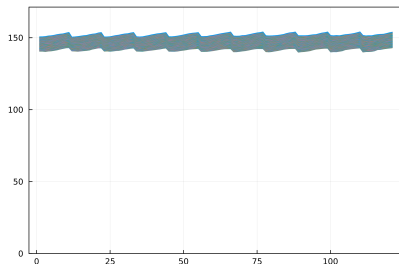
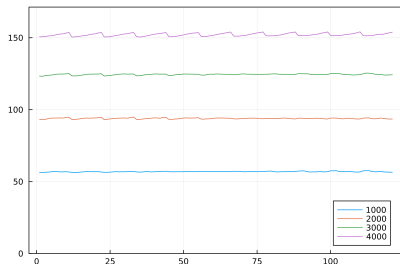
Understanding pseudobands: energy averaging



Example High-energy DFT bands of WTe₂ monolayer (ONCV-SG15, 120 electrons; 80 Ry cutoff, $20 \times 20 \times 1$ grid). x axis = k index in irreducible 1BZ; fastest varying coordinate = k_y

- 👉 Bands above 1000 are generally flat (but dispersion \uparrow as $n \uparrow$)
- 👉 Low-lying pseudobands blocks are very close in energy (but $1/(E_{\text{emp}} - E_{\text{occ}})$ more sensitive to dispersion)

Understanding pseudobands: energy averaging



Example High-energy DFT bands of WTe_2 monolayer (ONCV-SG15, 120 electrons; 80 Ry cutoff, $20 \times 20 \times 1$ grid). x axis = k index in irreducible 1BZ; fastest varying coordinate = k_y

- 👉 Bands above 1000 are generally flat (but dispersion \uparrow as $n \uparrow$)
- 👉 High-energy blocks are more dispersive (but $1/(E_{\text{emp}} - E_{\text{occ}})$ is smaller so no worry)

Understanding pseudobands: wave function averaging?

For pseudobands to work, we need

$$\begin{aligned} \sum_{n'' \in \text{block } n_b} M_{n''n}^* M_{n''n'} &\sim M_{\text{averaged band},n}^* M_{\text{averaged band},n'} \\ &= \sum_{n_1'', n_2'' \in \text{block } n_b} M_{n_1''n'} M_{n_2''n}^* \end{aligned} \quad (6)$$

The problem: it of course isn't the case in general. If

$[M_{n_1''n'} M_{n_2''n}^*]_{n_1''n_2''}$ is a random matrix: LHS : RHS ≈ 0.3 .

The question: *Then in which case is (6) correct in some sense?*

The structure of $\phi_{n\mathbf{k}}$

Plane wave basis In BerkeleyGW WFN.h5,

$$\phi_{n\mathbf{k}}(\mathbf{r}, \sigma) = \frac{1}{\sqrt{V}} \sum_{\mathbf{G}} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} c_{n\mathbf{k},\mathbf{G}\sigma}. \quad (7)$$

Thus

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

Cutoff Each \mathbf{k} has its own \mathbf{G} -grid (~ 30000 vectors for 80 Ry).

Procedure

Input

- indices of \mathbf{k}, \mathbf{q} in \mathbf{k} -grid;
- index of \mathbf{G} in \mathbf{G} -grid of \mathbf{k} (expect a \mathbf{G} in GW \mathbf{G} -grid, cutoff = say 30 Ry, not 80 Ry);
- n, n' .

Procedure

- 1 find index of \mathbf{k}
- 2 find index of $\mathbf{G} + \mathbf{G}'$ in \mathbf{G} -grid of $\mathbf{k} + \mathbf{q}$, for each \mathbf{G}' in \mathbf{G} -grid of \mathbf{k}
- 3 do summation $\sum_{\mathbf{G}', \sigma} c_{n\mathbf{k}+\mathbf{q}, \mathbf{G}+\mathbf{G}'}^* c_{n\mathbf{k}, \mathbf{G}'} \sigma$.

Performance Main bottleneck: finding $\mathbf{G} + \mathbf{G}'$. Using `StaticArrays.jl` helps a lot!

Under GPP:

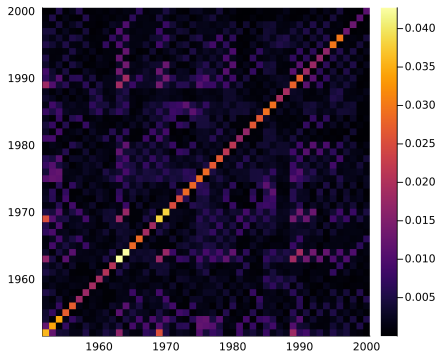
$$\begin{aligned} \chi_{\mathbf{G}\mathbf{G}'}(\mathbf{q}, \omega)^{\text{high band terms}} &\approx \sum_{\mathbf{k}} \sum_{\text{block } n_b}^{\text{emp}} \frac{2}{E_{n, \mathbf{k} + \mathbf{q}} - E_{\text{average in block } n_b}} \\ &\times \sum_{n' \in \text{block } n_b} \sum_n^{\text{occ}} M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn'}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}') \end{aligned} \quad (9)$$

Our goal *Finding how diagonal is*

$$\sum_n^{\text{occ}} M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn'}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}') \quad (10)$$

Numerical characterization of $\sum_n^{\text{occ}} M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn'}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}')$

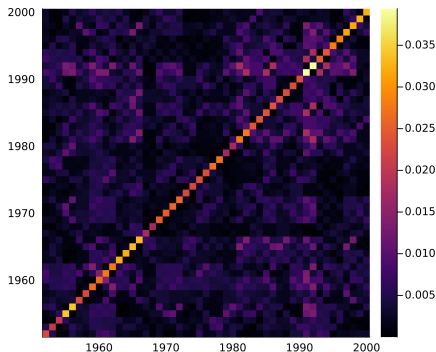
Case 1: $\mathbf{G} = \mathbf{G}'$ In this case $\sum_n^{\text{occ}} M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn'}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}')$ is large and fairly diagonal



Parameters $\mathbf{G} = (0, 1, -14)$, $\mathbf{k} = \mathbf{k}_2 = (0, 0.00, 0)$, $\mathbf{q} = (0, 0.00, 0)$

Numerical characterization of $\sum_n^{\text{occ}} M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn'}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}')$

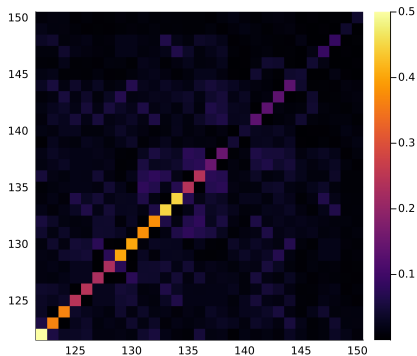
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Parameters $\mathbf{G} = (0, 1, -14)$, $\mathbf{k} = \mathbf{k}_2 = (0, 0.05, 0)$, $\mathbf{q} = (0, 0.10, 0)$

Numerical characterization of $\sum_n^{\text{occ}} M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn'}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}')$

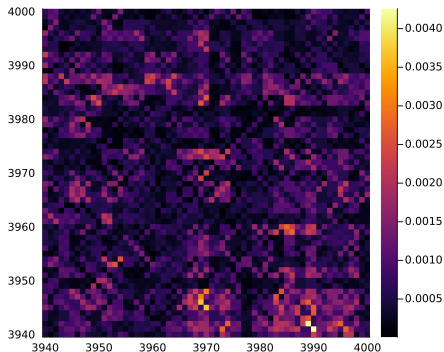
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Strikingly, $\sum_n^{\text{occ}} M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn'}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}')$ is still very diagonal for bands near Fermi surface!

Numerical characterization of $\sum_n^{\text{occ}} M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn'}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}')$

Case 2: $\mathbf{G} \neq \mathbf{G}'$ $\sum_n^{\text{occ}} M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn'}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}')$ is very non-diagonal, but since the terms's random phases cancel each other so it's small



Half-way generalization about pseudobands in χ

- 👉 pseudobands works when it's necessary to do so
- 👉 What prevents pseudobands from working around Fermi surface is the energy dispersion

...but do we have any theoretical explanation for this?

The secret of