

# Why pseudobands works?

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## **A review of *GW***

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# GW in momentum space

$$-i\Sigma \approx GW^{\text{RPA}} = \text{diagram} . \text{ In } \mathbf{k} \text{ space, } M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) = \underbrace{\langle n\mathbf{k} + \mathbf{q} | e^{i(\mathbf{q} + \mathbf{G}) \cdot \mathbf{r}} | n'\mathbf{k} \rangle}_{\text{quasiparticle approx.}}; \quad v(\mathbf{q} + \mathbf{G}) = \frac{4\pi}{V|\mathbf{q} + \mathbf{G}|^2}.$$

$$\text{In epsilon } \epsilon_{\mathbf{G}\mathbf{G}'}(\mathbf{q}, \omega) = \delta_{\mathbf{G}\mathbf{G}'} - v(\mathbf{q} + \mathbf{G}) \chi_{\mathbf{G}\mathbf{G}'}(\mathbf{q}, \omega),$$

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

$$\text{In sigma } \Sigma^{\text{contour}} = \Sigma^{\text{CH}} + \Sigma^{\text{SX}},$$

$$\langle n\mathbf{k} | \Sigma^{\text{SX}}(\omega) | n'\mathbf{k} \rangle = - \sum_{n''}^{\text{occ}} \sum_{\mathbf{q}, \mathbf{G}, \mathbf{G}'} M_{n''n}^*(\mathbf{k}, -\mathbf{q}, -\mathbf{G}) M_{n''n'}(\mathbf{k}, -\mathbf{q}, -\mathbf{G}') \epsilon_{\mathbf{G}\mathbf{G}'}^{-1}(\mathbf{q}, \omega - E_{n'', \mathbf{k} - \mathbf{q}}) v(\mathbf{q} + \mathbf{G}')$$

$$\langle n\mathbf{k} | \Sigma^{\text{CH}}(\omega) | n'\mathbf{k} \rangle = \frac{i}{2\pi} \sum_{n''} \sum_{\mathbf{q}, \mathbf{G}, \mathbf{G}'} M_{n''n}^*(\mathbf{k}, -\mathbf{q}, -\mathbf{G}) M_{n''n'}(\mathbf{k}, -\mathbf{q}, -\mathbf{G}') \int_0^\infty \frac{[\epsilon^r(\mathbf{q}, \omega') - \epsilon^a(\mathbf{q}, \omega')]_{\mathbf{G}\mathbf{G}'}^{-1} d\omega'}{\omega - E_{n\mathbf{k}} - \omega' + i0^+ \text{sgn}(E_{n\mathbf{k}})} v(\mathbf{q} + \mathbf{G}').$$

Infinite  $\sum^{\text{emp.}}$  in  $\chi$  and  $\Sigma_{nn'}^{\text{CH}}$ : **A major bottleneck of GW in momentum space**

# The problem of summing over many empty bands

**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  $\sim 1000$  bands.

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

pseudobands, **and when it works**

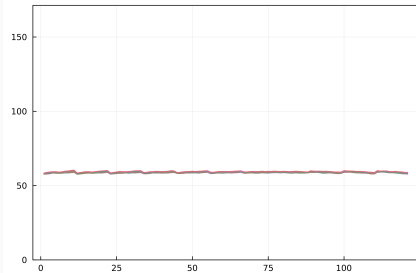
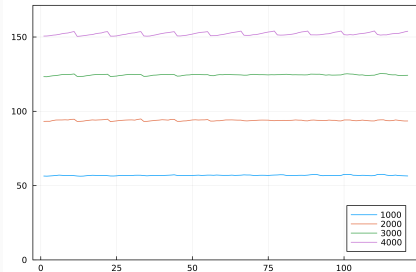
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# Understanding pseudobands: energy averaging

## Flatness of high energy bands

High-energy DFT bands of  $\text{WTe}_2$  monolayer (ONCV-SG15, 120 electrons; 80 Ry cutoff,  $20 \times 20 \times 1$  grid).  $x$  axis =  $\mathbf{k}$  index in irreducible 1BZ; fastest varying coordinate =  $k_y$

👉  $n \sim 1000$ : bands are generally flat

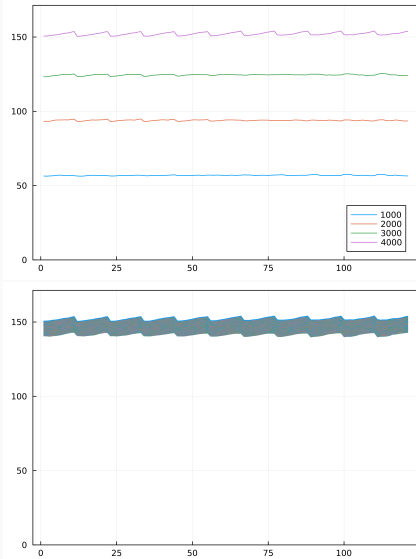


# Understanding pseudobands: energy averaging

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👉 High-lying bands are more dispersive but since they are high,  $1/(E_{\text{emp}} - E_{\text{occ}})$  is still flat

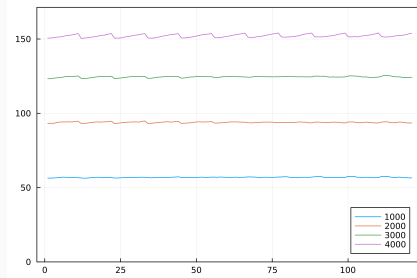


# Understanding pseudobands: energy averaging

## Flatness of high energy bands

- $\chi \sim MM^* \times f_1(E_{\text{emp}} - E_{\text{occ}});$
- $\Sigma^{\text{CH}} \sim MM^* \times f_2(\omega - E), \quad \omega \sim E_F.$

For  $E_{nk} \gg E_F$  ( $\omega$ ):  $f_{1,2} \sim \text{const.}$  for all  $\mathbf{k}$ .



Thus in both  $\chi$  and  $\Sigma^{\text{CH}}$ :

$$\sum_{n''}^{\text{high emp.}} M_{n''n}^* M_{n''n'} \times f(E_{n''\mathbf{k}}) = \sum_{\text{block } n_b}^{\text{high emp.}} f(\bar{E}_{n_b}) \sum_{n''}^{\text{block } n_b} M_{n''n}^* M_{n''n'}.$$



# Understanding pseudobands: wave function averaging?

For pseudobands to work, we need

$$\underbrace{\sum_{n'' \in \text{block } n_b} M_{n''n}^* M_{n''n'}}_{\text{normal}} \sim M_{\text{averaged band},n}^* M_{\text{averaged band},n'} \quad (1)$$
$$= \underbrace{\sum_{n_1'', n_2'' \in \text{block } n_b} M_{n_1''n'} M_{n_2''n}^*}_{\text{pseudobands}}$$

**The question:** is  $[M_{n_1''n'} M_{n_2''n}^*]_{n_1''n_2''}$  **diagonal**? Easy to verify: it's not.

**Then in which case is (1) correct in some sense?**

## Technical issues in calculating $M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G})$

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

**Plane wave basis** In BerkeleyGW WFN.h5,

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

Thus

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

**Cutoff** Each  $\mathbf{k}$  has its own  $\mathbf{G}$ -grid ( $\sim 30000$  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!

pseudobands **for**  $\chi$

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Under GPP:

$$\begin{aligned} & \chi_{\mathbf{G}\mathbf{G}'}(\mathbf{q}, \omega = 0)^{\text{high band terms}} \\ & \approx \sum_{\mathbf{k}} \sum_{\text{block } n_b}^{\text{emp}} \frac{2}{E_{n,\mathbf{k}+\mathbf{q}} - E_{\text{average in block } n_b}} \\ & \times \sum_{n' \in \text{block } n_b} \sum_n^{\text{occ}} M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn'}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}') \end{aligned}$$

**Our goal** Show that

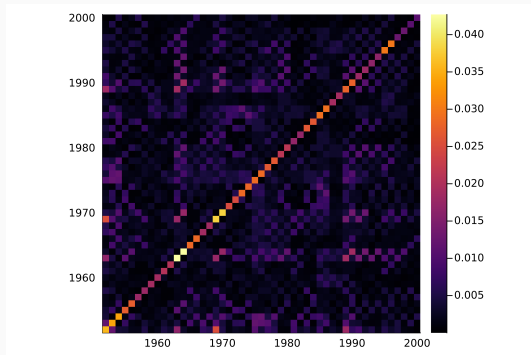
$$\sum_n^{\text{occ}} M_{nn'_1}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn'_2}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}')$$

is diagonal for pseudobands to work.

Under GPP:

$$\begin{aligned} & \chi_{\mathbf{G}\mathbf{G}'}(\mathbf{q}, \omega = 0)^{\text{high band terms}} \\ & \approx \sum_{\mathbf{k}} \sum_{\text{block } n_b}^{\text{emp}} \frac{2}{E_{n,\mathbf{k}+\mathbf{q}} - E_{\text{average in block } n_b}} \\ & \times \sum_{n' \in \text{block } n_b}^{\text{occ}} \sum_n M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn'}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}') \end{aligned}$$

For  $\mathbf{G} = \mathbf{G}'$ ,  $\sum_n M_{nn'_1}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn'_2}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}')$  is diagonal.



The same WTe<sub>2</sub> run,  $\mathbf{G} = (0, 1, -14)$ ,  $\mathbf{k} = \mathbf{k}_2 = (0, 0.00, 0)$ ,  $\mathbf{q} = (0, 0.00, 0)$

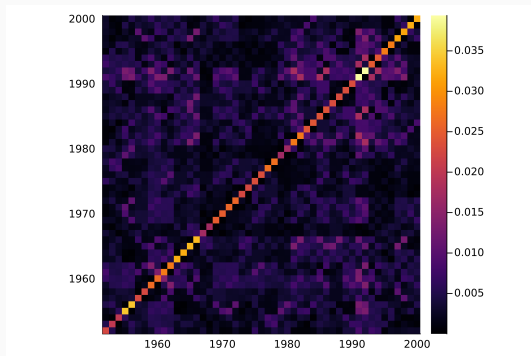
Under GPP:

$$\chi_{\mathbf{G}\mathbf{G}'}(\mathbf{q}, \omega = 0)^{\text{high band terms}}$$

$$\approx \sum_{\mathbf{k}} \sum_{\text{block } n_b}^{\text{emp}} \frac{2}{E_{n,\mathbf{k}+\mathbf{q}} - E_{\text{average in block } n_b}}$$

$$\times \sum_{n' \in \text{block } n_b}^{\text{occ}} \sum_n M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn'}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}')$$

For  $\mathbf{G} = \mathbf{G}'$ ,  $\sum_n M_{nn_1'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn_2'}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}')$  is diagonal.



The same WTe<sub>2</sub> run,  $\mathbf{G} = (0, 1, -14)$ ,  $\mathbf{k} = \mathbf{k}_2 = (0, 0.05, 0)$ ,  $\mathbf{q} = (0, 0.10, 0)$

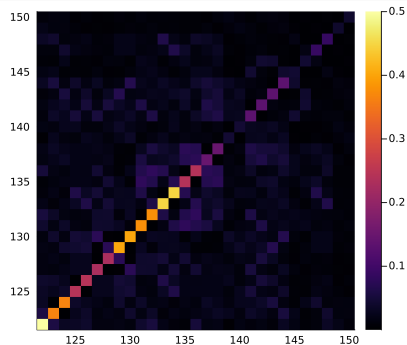


Under GPP:

$$\begin{aligned} & \chi_{\mathbf{G}\mathbf{G}'}(\mathbf{q}, \omega = 0)^{\text{high band terms}} \\ & \approx \sum_{\mathbf{k}} \sum_{\text{block } n_b}^{\text{emp}} \frac{2}{E_{n,\mathbf{k}+\mathbf{q}} - E_{\text{average in block } n_b}} \\ & \times \sum_{n' \in \text{block } n_b} \sum_n^{\text{occ}} M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn'}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}') \end{aligned}$$

For  $\mathbf{G} = \mathbf{G}'$ ,  $\sum_n^{\text{occ}} M_{nn_1'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn_2'}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}')$  is diagonal.

Strikingly,  $\sum_n^{\text{occ}} M_{nn_1'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn_2'}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}')$  is still very diagonal for bands near Fermi surface!

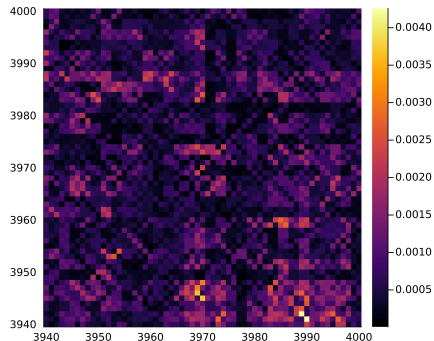


Under GPP:

$$\begin{aligned} & \chi_{\mathbf{G}\mathbf{G}'}(\mathbf{q}, \omega = 0)^{\text{high band terms}} \\ & \approx \sum_{\mathbf{k}} \sum_{\text{block } n_b}^{\text{emp}} \frac{2}{E_{n,\mathbf{k}+\mathbf{q}} - E_{\text{average in block } n_b}} \\ & \times \sum_{n' \in \text{block } n_b} \sum_n^{\text{occ}} M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn'}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}') \end{aligned}$$

When  $\mathbf{G} \neq \mathbf{G}'$ ,

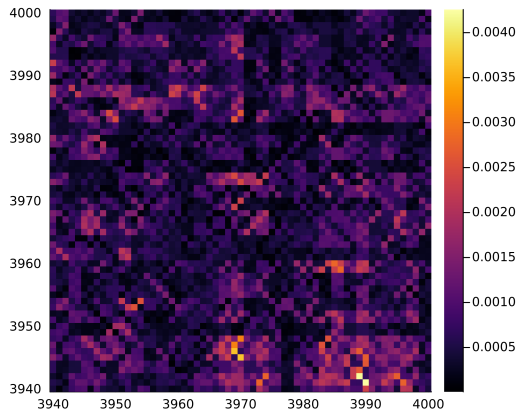
$\sum_n^{\text{occ}} M_{nn'_1}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn'_2}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}')$  is not diagonal at all.



# Numerical characterization of

**Case 2:**  $\mathbf{G} \neq \mathbf{G}'$   $\sum_n^{\text{occ}} M_{nn'_1}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn'_2}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}')$  is very non-diagonal, but since the terms's random phases cancel each other so the overall sum after  $\sum_{n'}^{\text{emp}}$  is small

# Numerical characterization of



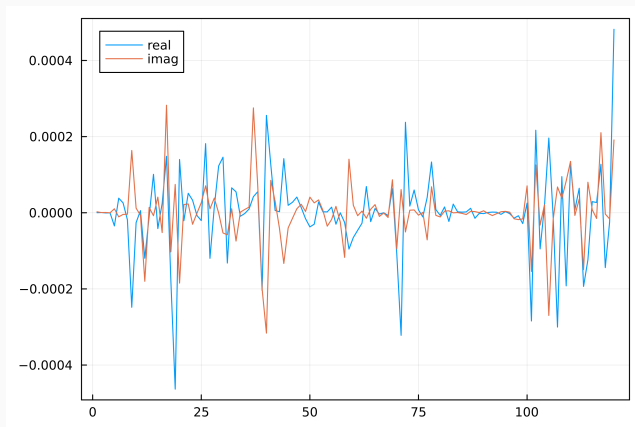
## Half-way generalization about pseudobands in $\chi$

- 👉 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?

# Cancellation of cross-terms in $\chi$

$M_{nn'_1}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn'_2}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}')$  and  $n$  (occupied band index), when  $n'_1 \neq n'_2$ :



## Cancellation of cross-terms in $\chi$

👉 Although for a single  $n$ , the value can be large, as we sum over  $n$  the terms cancel each other  $\Rightarrow$  diagonal  $\sum_n^{\text{occ}} M_{nn_1}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn_2}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}')$

**Why is this the case?**

**Case 1:**  $|n\mathbf{k}\rangle \propto e^{i(\mathbf{G}_n + \mathbf{k}) \cdot \mathbf{r}}$  For high-energy bands primarily containing only one  $\mathbf{G}$  components, unwanted terms are:

$$\sum_n^{\text{occ}} M_{nn_1}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn_2}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}) = \sum_n^{\text{occ}} c_{n\mathbf{k}+\mathbf{q}}(\mathbf{G} + \mathbf{G}_1)^* c_{n\mathbf{k}+\mathbf{q}}(\mathbf{G} + \mathbf{G}_2)$$

The terms rapid fast when  $\mathbf{G}_1 \neq \mathbf{G}_2$ :

## Cancellation of cross-terms in $\chi$

**Case 2:**  $|nk\rangle$  contains several  $\mathbf{G}$  components suppose high-energy bands  $n_{1,2}$  primarily contain two  $\mathbf{G}$  components:

$$|n_i\mathbf{k}\rangle = (c_{i1}|\mathbf{G}_1\rangle + c_{i2}|\mathbf{G}_2\rangle)e^{i\mathbf{k}\cdot\mathbf{r}}, \quad i = 1, 2. \quad (2)$$

In this way

$$\begin{aligned} & \sum_n^{\text{occ}} M_{nn_1}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{nn_2}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}) \\ &= \sum_n^{\text{occ}} (c_{11}c_{nk+\mathbf{q}}^*(\mathbf{G} + \mathbf{G}_1) + c_{12}c_{nk+\mathbf{q}}^*(\mathbf{G} + \mathbf{G}_2)) \times \\ & \quad (c_{21}^*c_{nk+\mathbf{q}}(\mathbf{G} + \mathbf{G}_1) + c_{22}^*c_{nk+\mathbf{q}}(\mathbf{G} + \mathbf{G}_2)). \end{aligned}$$



## Cancellation of cross-terms in $\chi$

The following terms vanish:

$$\sum_n^{\text{occ}} (c_{11}c_{21}^* |c_{n\mathbf{k}+\mathbf{q}}(\mathbf{G} + \mathbf{G}_1)|^2 + c_{12}c_{22}^* |c_{n\mathbf{k}+\mathbf{q}}(\mathbf{G} + \mathbf{G}_2)|^2)$$

1. After summation over  $n$ ,  $\sum_n |c_{n\mathbf{k}+\mathbf{q}}(\mathbf{G} + \mathbf{G}_1)|^2 = \sum_n |c_{n\mathbf{k}+\mathbf{q}}(\mathbf{G} + \mathbf{G}_2)|^2$
2. Orthogonal relation:  $c_{11}c_{21}^* + c_{12}c_{22}^* = 0$ .

The other terms

$$\sum_n^{\text{occ}} (c_{11}c_{22}^* c_{n\mathbf{k}+\mathbf{q}}^*(\mathbf{G} + \mathbf{G}_1) c_{n\mathbf{k}+\mathbf{q}}(\mathbf{G} + \mathbf{G}_2) + c_{12}c_{21}^* c_{n\mathbf{k}+\mathbf{q}}^*(\mathbf{G} + \mathbf{G}_2) c_{n\mathbf{k}+\mathbf{q}}(\mathbf{G} + \mathbf{G}_1))$$

oscillate in the same way in the first case.

pseudobands **for**  $\Sigma$

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Only  $\Sigma^{\text{CH}}$  involves  $\Sigma^{\text{emp}}$ :

$$\langle n\mathbf{k} | \Sigma^{\text{CH, GPP}} | n'\mathbf{k} \rangle = \frac{1}{2} \sum_{n''} \sum_{\mathbf{q}\mathbf{G}\mathbf{G}'} M_{n''n}^*(\mathbf{k}, -\mathbf{q}, -\mathbf{G}) M_{n''n'}(\mathbf{k}, -\mathbf{q}, -\mathbf{G}') \times$$

something about  $\mathbf{q}, \mathbf{k}, \mathbf{G}, \mathbf{G}'$

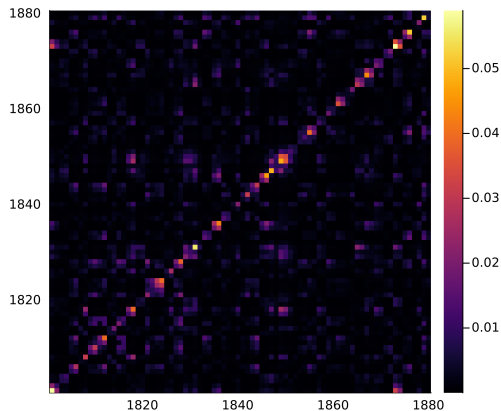
## Problems

- No summation over occupied states  $\Rightarrow$  ~~X~~the aforementioned cancellation mechanism
- Summation over  $\mathbf{G}$  very complicated  $\Rightarrow$  analysis based on  $\mathbf{G}$  very hard.

## Some tentative ideas

- It has been verified that a single  $M_{n_1''n}^* M_{n_2''n}$  term is never diagonal
- But it seems naively summing over  $\mathbf{G} = \mathbf{G}'$  (without considering the weight factor) makes it diagonal. . .

## Some tentative ideas



- $M_{n_1''n}^*(\mathbf{G}_1)M_{n_2''n}(\mathbf{G}_2)$  is not diagonal at all when  $\mathbf{G}_1 \neq \mathbf{G}_2$ ;

## Some tentative ideas

- but probably only the  $\mathbf{G}_1 = \mathbf{G}_2$  terms matter?

## **Comments from Felipe H. Jornada's recent paper**

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# “Stochastic” pseudobands

Energy averaging is also done in their paper:

$$G = \sum_{n \text{ near F.S.}} \frac{|\phi_{n\mathbf{k}}\rangle\langle\phi_{n\mathbf{k}}|}{\omega - E_{n\mathbf{k}}} + \sum_{\text{pseudobands block}} \frac{1}{\omega - \bar{E}} \sum_{n \in \text{block}} |\phi_{n\mathbf{k}}\rangle\langle\phi_{n\mathbf{k}}|.$$

**Their procedure** Replace each pseudobands block by *several bands*:

$$\{|\phi_{n\mathbf{k}}\rangle\}_{n \text{ in block}} \longrightarrow \left\{ |\phi_{\xi\mathbf{k}}\rangle = \sum_{n \text{ in block}} e^{i\theta_{n\xi}} |\phi_{n\mathbf{k}}\rangle \right\}_{\xi}$$

**Justification** When  $N_{\xi} \rightarrow \infty$ ,  $\langle e^{-i\theta_{n'\xi}} e^{i\theta_{n\xi}} \rangle_{\xi} = \delta_{nn'}$

**Comparison with the current script** When  $N_{\xi} = 1$ ,  $e^{i\theta_{n\xi}}$  comes from DFT diagonalization



# FHJ's justification of pseudobands

**Convergence conditions** When  $N_{\text{pseudobands blocks}} \rightarrow \infty$  and in each block  $N_{\xi} \rightarrow \infty$ ,

- the expectations of  $\chi$  and  $\Sigma$  goes to the true value;
- the standard error goes to zero.

**Is this result enough as a justification?** My answer: no; because the limits = not doing pseudobands at all. (And their recommended values are not large enough anyway.)

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**Additional justification** “the polarizability tends to converge much faster than  $G$ , partially due to the *rapidly oscillating nature* of the matrix elements involving Kohn-Sham states used in the evaluation of the polarizability”

## Compressing the bands even harder: size of blocks

Recall that band dispersion is the main problem. . .

$$\Delta\chi \sim \frac{\Delta E}{E^2}, \quad \chi \sim \frac{1}{E} \Rightarrow \frac{\Delta\chi}{\chi} \simeq \frac{\Delta E}{E}$$
$$\Rightarrow \frac{\Delta\chi}{\chi} \lesssim \text{const} \Leftrightarrow \boxed{\frac{\Delta E}{E} \lesssim \text{const}}$$

**Exponential growth of the energy spread of blocks!**

## Compressing the bands even harder: pseudobands near $E_F$ ?

They claim that for `epsilon`, bands near Fermi surface can also be pseudo-ized

*It somehow goes against my own numerical experiments; but they are quite sure about that hmm...*

They also claim that for `sigma`, only the bands near Fermi surface shouldn't be pseudo-ized.

**Important claim: protection window is not a convergence parameter.**

## Discussion

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**Implications to GW acceleration** There are lots of garbage in the giant input files we feed to GW

**Implications to machine learning** There exists a *analytic* relation between  $\Sigma^{GW}$  and  $\{\bar{E}, |\phi_{\mathbf{k}}\rangle^{\text{pseudo}}\}_{\text{blocks}}$

- Starting from pseudobands is *not* feature engineering
- Pseudobands (with further compression of autoencoders) should be the starting point of all ML tasks