# Supplementary material

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$$M_{nn'}(\mathbf{k},\mathbf{q},\mathbf{G}) = \langle n\mathbf{k}+\mathbf{q}|\mathrm{e}^{\mathrm{i}(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}|n'\mathbf{k}\rangle \tag{1}$$

$$\chi_{\mathbf{G}\mathbf{G}'}(\mathbf{q},\omega=0) = \sum_{\mathbf{k}}\sum_{n}^{\mathrm{occ}}\sum_{n'}^{\mathrm{emp}} M_{nn'}(\mathbf{k},\mathbf{q},\mathbf{G})M^*_{nn'}(\mathbf{k},\mathbf{q},\mathbf{G}')\frac{2}{E_{n\mathbf{k}+\mathbf{q}}-E_{n'\mathbf{k}}} \tag{2}$$

In the conventional pseudobands technique, the empty states are divided into one low-energy protected subspace and a series of pseudobands blocks; each of the blocks contain bands with comparable energies.

$$\chi^{\text{P.B. blocks}}_{\mathbf{G}\mathbf{G}'}(\mathbf{q},\omega=0) = \sum_{\mathbf{k}}\sum_{S}^{\text{P.B. terms}}\frac{2}{E_{n\mathbf{k}+\mathbf{q}}-\bar{E}_S}\sum_{n_1',n_2'}^{S}\sum_{n}^{\mathrm{occ}} M_{nn_1'}(\mathbf{k},\mathbf{q},\mathbf{G})M^*_{nn_2'}(\mathbf{k},\mathbf{q},\mathbf{G}') \tag{3}$$

In each block, we may see states containing a primary $\mathbf{G}$ component,

$$\langle\mathbf{r}|n'\mathbf{k}\rangle = \mathrm{e}^{\mathrm{i}\theta_{n'\mathbf{k}}}\mathrm{e}^{\mathrm{i}(\mathbf{k}+\mathbf{G}_{n'})\cdot\mathbf{r}}, \tag{4}$$

or $N$ degenerate states containing $N$ primary $\mathbf{G}$ components

$$\langle\mathbf{r}|n'\mathbf{k}\rangle = \sum_{i} c_i \mathrm{e}^{\mathrm{i}(\mathbf{k}+\mathbf{G}_i)\cdot\mathbf{r}}. \tag{5}$$

The latter case is due to symmetry.

When $n_1', n_2'$ both contain only one primary $\mathbf{G}$ component, and therefore

$$M_{nn'}(\mathbf{k},\mathbf{q},\mathbf{G}) = \mathrm{e}^{\mathrm{i}\theta_{n'\mathbf{k}}}c^*_{n\mathbf{k}+\mathbf{q}}(\mathbf{G}+\mathbf{G}_{n'}). \tag{6}$$

their contribution to $\chi$ is proportional to

$$\sum_{n}^{\mathrm{occ}} M_{nn_1'}(\mathbf{k},\mathbf{q},\mathbf{G})M^*_{nn_2'}(\mathbf{k},\mathbf{q},\mathbf{G}) = \sum_{n}^{\mathrm{occ}} c^*_{n\mathbf{k}+\mathbf{q}}(\mathbf{G}+\mathbf{G}_{n_1'})c_{n\mathbf{k}+\mathbf{q}}(\mathbf{G}+\mathbf{G}_{n_2'}). \tag{7}$$

The right hand side likely becomes $\delta_{n_1'n_2'}$ after the summation, because the subspace spanned by the dominant $\mathbf{G}$ components of the occupied states is expected to largely overlap with the subspace of the occupied states.

$$\langle\mathbf{r}|n'\mathbf{k}\rangle = \frac{1}{\sqrt{N}}\sum_{i}^{N} c^{(i)}_{n'\mathbf{k}}\mathrm{e}^{\mathrm{i}(\mathbf{k}+\mathbf{G}^{(i)}_{n'\mathbf{k}})\cdot\mathbf{r}}, \quad \left|c^{(i)}_{n'\mathbf{k}}\right|^2 = 1, \quad \sum_{i}^{N} c^{(i)}_{n_1'\mathbf{k}}c^{(i)*}_{n_2'\mathbf{k}} = \delta_{n_1'n_2'}. \tag{8}$$

Here since we assume $|n_1'\mathbf{k}\rangle$ and $n_2'\mathbf{k}$ share the same set of predominant $\mathbf{G}$ vectors, we replace $\mathbf{G}^{(i)}_{n_{1,2}'\mathbf{k}}$ by $\mathbf{G}^{(i)}_{n'\mathbf{k}}$ (and the order of the $\mathbf{G}$ vectors are also set the same for $n_1'$ and $n_2'$), and thus

$$\begin{aligned}&\sum_{n_1'n_2'}^{S}\sum_{n}^{\mathrm{occ}} M_{nn_1'}(\mathbf{k},\mathbf{q},\mathbf{G})M^*_{nn_2'}(\mathbf{k},\mathbf{q},\mathbf{G}) \\ &= \frac{1}{N}\sum_{i,j}^{N}\sum_{n}^{\mathrm{occ}} c^{(i)}_{n_1'\mathbf{k}}c^{(j)*}_{n_2'\mathbf{k}}c^*_{n\mathbf{k}+\mathbf{q}}(\mathbf{G}+\mathbf{G}^{(i)}_{n'\mathbf{k}})c_{n\mathbf{k}+\mathbf{q}}(\mathbf{G}+\mathbf{G}^{(j)}_{n'\mathbf{k}}).\end{aligned} \tag{9}$$

The $i = j$ terms evaluate as

$$\sum_{i}^{N} \sum_{n}^{\mathrm{occ}} c_{n_1'\mathbf{k}}^{(i)} c_{n_2'\mathbf{k}}^{(i)*} \left| c_{n\mathbf{k}+\mathbf{q}}^{*}(\mathbf{G} + \mathbf{G}_{n'\mathbf{k}}^{(i)}) \right|^2 \propto \delta_{n_1' n_2'}. \tag{10}$$

Note that the $\mathbf{G}_{n'\mathbf{k}}^{(i)}$ components are connected by symmetry operations, and we have

$$\left| c_{n\mathbf{k}+\mathbf{q}}^{*}(\mathbf{G} + \mathbf{G}_{n'\mathbf{k}}^{(i)}) \right|^2 = \mathrm{const}$$

for $1 \leq i \leq N$, and therefore the above equation is just a constant times the summation of $c_{n_1'\mathbf{k}}^{(i)} c_{n_2'\mathbf{k}}^{(i)*}$ over $i$, which then results in $\delta_{n_1' n_2'}$. The $i \neq j$ terms evaluate as

$$\sum_{i \neq j}^{N} c_{n_1'\mathbf{k}}^{(i)} c_{n_2'\mathbf{k}}^{(j)*} \sum_{n}^{\mathrm{occ}} c_{n\mathbf{k}+\mathbf{q}}^{*}(\mathbf{G} + \mathbf{G}_{n'\mathbf{k}}^{(i)}) c_{n\mathbf{k}+\mathbf{q}}(\mathbf{G} + \mathbf{G}_{n'\mathbf{k}}^{(j)}) \approx \sum_{i \neq j}^{N} c_{n_1'\mathbf{k}}^{(i)} c_{n_2'\mathbf{k}}^{(j)*} \delta_{ij} = 0.$$