1 From Tight-Binding Wannier Hamiltonian to Dipole Elements

Starting from the Tight-Binding hamiltonian in the Wannier basis set

$$H_{ij}(\boldsymbol{R}\sigma) = \langle w_{i\sigma}| \hat{H} |w_{j\sigma}\boldsymbol{R}\rangle \tag{1}$$

wher $|w_{i\sigma}\boldsymbol{R}\rangle$ is the wannier function i of the σ spin channel in the unitary cell $\boldsymbol{R}$. A Fourier transform of the hamiltonian allows us to consider only the wannier functions in the unitary cell 0; in the collinear case, the hamiltonians in the two spin channels are considered separately:

$$H_{ij}(\boldsymbol{k}\sigma) = \sum_{\boldsymbol{R}} H_{ij}(\boldsymbol{R}\sigma)e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \tag{2}$$

At this point, the hamiltonian is diagonalized in order to obtain Bloch states

$$H_{ij}(\boldsymbol{k}\sigma)|n\sigma\boldsymbol{k}\rangle = \epsilon_{n\sigma}(\boldsymbol{k})|n\sigma\boldsymbol{k}\rangle = \sum_j H_{ij}(\boldsymbol{k}\sigma)C^{n\boldsymbol{k}}_{j\sigma}|w_{j\sigma}\boldsymbol{0}\rangle = \epsilon_{n\sigma}(\boldsymbol{k})C^{n\boldsymbol{k}}_{i\sigma}|w_{i\sigma}\boldsymbol{0}\rangle \tag{3}$$

where $|n\sigma\boldsymbol{k}\rangle$ is the Bloch state n of the spin channel σ at the $\boldsymbol{k}$ point of the Brillouin zone, and $C^{n\boldsymbol{k}}_{j\sigma}$ is its projection over the j wannier function of the basis set. From the Bloch states in the two spin channel a spinor is built

$$|n\boldsymbol{k}\rangle = |n\uparrow\boldsymbol{k}\rangle|n\downarrow\boldsymbol{k}\rangle = \sum_{i\sigma} C^{n\boldsymbol{k}}_{i\sigma}|w_{i\sigma}\boldsymbol{0}\rangle \tag{4}$$

At this point, the Bloch states allow to define a generalized dipole element

$$\begin{aligned}\rho_{\sigma(n1,\boldsymbol{k1})(n2,\boldsymbol{k2})}(\boldsymbol{G};\boldsymbol{r1},\boldsymbol{r2},\boldsymbol{q}) = \langle n1\boldsymbol{k1}-\boldsymbol{r1}|\, e^{i(\boldsymbol{q}+\boldsymbol{G})\cdot\boldsymbol{r}}(|n2\boldsymbol{k2}-\boldsymbol{r2}\rangle)^c = \\ \sum_j (C^{n1\boldsymbol{k1}-\boldsymbol{r1}}_{j\sigma})^* e^{i(\boldsymbol{q}+\boldsymbol{G})\cdot\boldsymbol{r}_j} C^{n2\boldsymbol{k2}-\boldsymbol{r2}}_{j\sigma}\end{aligned} \tag{5}$$

where $n1, n2, \boldsymbol{k1}, \boldsymbol{k2}, \boldsymbol{G}$ are considered as variables, while $\boldsymbol{q}, \boldsymbol{r1}, \boldsymbol{r2}$,$c$ are considered as parameters (obviously the two states $n1$ and $n2$ have spin σ). The following notation for ρ will be used:

$$\rho_{\sigma(n1,\boldsymbol{k1}-\boldsymbol{r1})(n2,\boldsymbol{k2}-\boldsymbol{r2})}(\boldsymbol{G},\boldsymbol{q}) \equiv \rho_{\sigma(n1,\boldsymbol{k1})(n2,\boldsymbol{k2})}(\boldsymbol{G};\boldsymbol{r1},\boldsymbol{r2},\boldsymbol{q}) \tag{6}$$

2 From Dipole Elements to BSE Hamiltonian

Before building the BSE hamiltonian, we need to construct our screening potential, which we will consider in this preliminary code at the IPA level

$$(\epsilon^{(IPA)})^{-1}_{\boldsymbol{GG'}}(\boldsymbol{q}\omega) = \delta_{\boldsymbol{GG'}} + v(\boldsymbol{q}+\boldsymbol{G})\chi^{(IPA)}_{\boldsymbol{GG'}}(\boldsymbol{q}\omega) \tag{7}$$

where $v(\boldsymbol{q})$ is the Coulomb potential (in case of 2D systems a cutoff has been considered along the non-periodic direction) and χ is the response function

$$\begin{aligned}\chi^{(IPA)}_{\boldsymbol{GG'}}(\boldsymbol{q}\omega) = \sum_{\sigma cv\boldsymbol{k}} (\rho_{\sigma(c\boldsymbol{k})(v\boldsymbol{k}-\boldsymbol{q})}(\boldsymbol{G},\boldsymbol{q}))^* \rho_{\sigma(c\boldsymbol{k})(v\boldsymbol{k}-\boldsymbol{q})}(\boldsymbol{G'},\boldsymbol{q})\times \\ \times\left[\frac{1}{\omega+\epsilon_{v\sigma}(\boldsymbol{k}-\boldsymbol{q})-\epsilon_{c\sigma}(\boldsymbol{k})+i\eta} - \frac{1}{\omega-\epsilon_{v\sigma}(\boldsymbol{k}-\boldsymbol{q})+\epsilon_{c\sigma}(\boldsymbol{k})-i\eta}\right]\end{aligned} \tag{8}$$

The BSE hamiltonian projected on a basis of electron-hole transitions $t : (n1\boldsymbol{k1}) \rightarrow (n2\boldsymbol{k2})$ can be written as

$$\langle t|\, H_{BSE}\, |t'\rangle = E_t\delta_{tt'} + \langle t|\,(v-W)\,|t'\rangle \tag{9}$$

where W is the screened potential. The screened potential W can be written in reciprocal space ($\boldsymbol{k}$) as:

$$\begin{aligned} W_{\boldsymbol{kk'}} &= \epsilon^{-1}_{\boldsymbol{kk'}} v(\boldsymbol{k'}) \\ W_{(\boldsymbol{q}+\boldsymbol{G})(\boldsymbol{q'}+\boldsymbol{G'})} &= \epsilon^{-1}_{(\boldsymbol{q}+\boldsymbol{G})(\boldsymbol{q'}+\boldsymbol{G'})} v(\boldsymbol{q'}+\boldsymbol{G'}) \\ W_{\boldsymbol{GG'}}(\boldsymbol{q}) &= \epsilon^{-1}_{\boldsymbol{GG'}}(\boldsymbol{q}) v(\boldsymbol{q}+\boldsymbol{G'}) \end{aligned} \tag{10}$$

where in the second passage a generic vector $\boldsymbol{k}$ in reciprocal space has been written as the sum of a vector in the BZ $\boldsymbol{q}$ plus a reciprocal vector $\boldsymbol{G}$.

Distinguishing between resonant transitions $r : (v\boldsymbol{k}-\boldsymbol{q}) \rightarrow (c\boldsymbol{k})$ and anti-resonant transitions $a : (c\boldsymbol{k}) \rightarrow (v\boldsymbol{k}+\boldsymbol{q})$, the BSE hamiltonian can be written in the following block form (in the long-wavelength limit $\boldsymbol{q} \rightarrow 0$)

$$H_{BSE} = \begin{pmatrix} H_{rr} & H_{ra} \\ -(H_{ra})^{\dagger} & -(H_{rr})^* \end{pmatrix} \tag{11}$$

Writing the two main elements of the BSE hamiltonian in terms of the generalized dipole elements, we have for the resonant part $r = (\sigma_c c \sigma_v v\boldsymbol{k})$:

$$\begin{aligned} H_{rr'} &= E_r\delta_{rr'} + (\delta_M v_{rr'} - W_{rr'}) \\ v_{rr'} &= \frac{1}{N}\sum_{\boldsymbol{G}\neq\boldsymbol{0}} v(\boldsymbol{q}+\boldsymbol{G})(\rho_{\sigma_{c'}(c'\boldsymbol{k'})(v'\boldsymbol{k'}-\boldsymbol{q})}(\boldsymbol{G},\boldsymbol{q}))^*\rho_{\sigma_c(c\boldsymbol{k})(v\boldsymbol{k}-\boldsymbol{q})}(\boldsymbol{G},\boldsymbol{q})\delta_{\sigma_{c'}\sigma_{v'}}\delta_{\sigma_c\sigma_v} \\ W_{rr'} &= \frac{1}{N}\sum_{\boldsymbol{GG'}} W_{\boldsymbol{GG'}}(\boldsymbol{q})(\rho_{\sigma_v(v\boldsymbol{k}-\boldsymbol{q})(v'\boldsymbol{k'}-\boldsymbol{q})}(\boldsymbol{G'},\boldsymbol{q}))^*\rho_{\sigma_c(c\boldsymbol{k})(c'\boldsymbol{k'})}(\boldsymbol{G},\boldsymbol{q})\delta_{\sigma_c\sigma_{c'}}\delta_{\sigma_v\sigma_{v'}} \end{aligned} \tag{12}$$

while for the coupling part, considering $a = (\sigma_c c\sigma_v v\boldsymbol{k})$ (this is the ordering of the vectors and the indexing, it is not related to the proper anti-resonant transition, which is taken into account into building the terms):

$$
\begin{aligned}
H_{ra'} &= (\delta_M v_{ra'} - W_{ra'}) \\
v_{ra'} &= \frac{1}{N}\sum_{\boldsymbol{G}\neq\boldsymbol{0}} v(\boldsymbol{q}+\boldsymbol{G})(\rho_{\sigma_{v'}(v'\boldsymbol{k'}+\boldsymbol{q'})(c'\boldsymbol{k'})}(\boldsymbol{G},\boldsymbol{q}))^{*}\rho_{\sigma_c(c\boldsymbol{k})(v\boldsymbol{k}-\boldsymbol{q})}(\boldsymbol{G},\boldsymbol{q})\delta_{\sigma_{v'}\sigma_{c'}}\delta_{\sigma_c\sigma_v} \\
W_{ra'} &= \frac{1}{N}\sum_{\boldsymbol{G}\boldsymbol{G'}} W_{\boldsymbol{G}\boldsymbol{G'}}(\boldsymbol{q})(\rho_{\sigma_v(v\boldsymbol{k}-\boldsymbol{q})(c'\boldsymbol{k'})}(\boldsymbol{G'},\boldsymbol{q}))^{*}\rho_{\sigma_c(c\boldsymbol{k})(v'\boldsymbol{k'}+\boldsymbol{q})}(\boldsymbol{G},\boldsymbol{q})\delta_{\sigma_v\sigma_{c'}}\delta_{\sigma_c\sigma_{v'}}
\end{aligned}
\tag{13}
$$

Note that N is equal to the number of unit cells considered (i.e. the number of $\boldsymbol{k}$ vectors considered in the FBZ), while δ_M is equal to 2 in the case of non-magnetic calculations and to 1 in the case of magnetic calculations.

3 From BSE Hamiltonian to Optical Spectra

At this point, the BSE hamiltonian can be diagonalized, we have followed the usual procedure and a procedure passing through a Cholesky factorization (Structure preserving parallel algorithms for solving the Bethe–Salpeter eigenvalue problem Meiyue Shao, Felipe H. da Jornada, Chao Yang, Jack Deslippe, Steven G. Louie). From the excitonic eigenvalue E_λ and eigenvector A^λ (orthonormalized), we can build the oscilator force of the excitonic state λ:

$$
f_\alpha^\lambda = \sum_{\sigma c v \boldsymbol{k}} \rho_{\sigma(c\boldsymbol{k})(v\boldsymbol{k}-\boldsymbol{q}_\alpha)}(\boldsymbol{0},\boldsymbol{q}_\alpha)(A^\lambda_{\sigma c v \boldsymbol{k}})^{*} \tag{14}
$$

This allow us to express the macroscopic dielectric function as:

$$
(\epsilon_M)_\alpha(\omega) = 1 - \lim_{q_\alpha\to 0}\frac{8\pi}{|\boldsymbol{q}_\alpha|^2}\sum_\lambda \frac{f_\alpha^\lambda (f_\alpha^\lambda)^{*}}{\omega - E_\lambda} \tag{15}
$$

where Ω is the primitive cell volume and α the direction of the electric field.