We start with the expression for the susceptibility for the intraband transtitions,

$$\chi^{s,\ell}_{i,\mathrm{abc}} = -\frac{e^3}{\Omega\hbar^2\omega_3}\sum_{mn\mathbf{k}}\frac{\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}}{\omega^S_{nm}-\omega_3}\left(\frac{f_{mn}r^{\mathrm{b}}_{nm}}{\omega^S_{nm}-\omega_\beta}\right)_{;k^{\mathrm{c}}}, \tag{1}$$

chii

where s denotes *surface* and S refers to the *scissors* correction. This expression diverges as $\omega_3 \to 0$. To eliminate this divergence we take the partial fraction expansion,

$$\begin{aligned} I &= C\left[-\frac{1}{2(\omega^S_{nm})^2}\frac{1}{\omega^S_{nm}-\omega}+\frac{2}{(\omega^S_{nm})^2}\frac{1}{\omega^S_{nm}-2\omega}+\frac{1}{2(\omega^S_{nm})^2}\frac{1}{\omega}\right] \\ &- D\left[-\frac{3}{2(\omega^S_{nm})^2}\frac{1}{\omega^S_{nm}-\omega}+\frac{4}{(\omega^S_{nm})^3}\frac{1}{\omega^S_{nm}-2\omega}+\frac{1}{2(\omega^S_{nm})^3}\frac{1}{\omega}-\frac{1}{2(\omega^S_{nm})^2}\frac{1}{(\omega^S_{nm}-\omega)^2}\right], \end{aligned} \tag{2}$$

where $C = f_{mn}\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}(r^{\mathrm{LDA,b}}_{nm})_{;k^{\mathrm{c}}}$, and $D = f_{mn}\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}r^{\mathrm{b}}_{nm}\Delta^{\mathrm{c}}_{nm}$.

Time-reversal symmetry leads to the following relationships:

$$\begin{aligned} \mathbf{r}_{mn}(\mathbf{k}) &= \mathbf{r}_{nm}(-\mathbf{k}), \\ \mathbf{r}_{mn;\mathbf{k}}(\mathbf{k}) &= -\mathbf{r}_{nm;\mathbf{k}}(-\mathbf{k}), \\ \mathcal{V}^{\Sigma,\mathrm{a}}_{mn}(-\mathbf{k}) &= -\mathcal{V}^{\Sigma,\mathrm{a}}_{nm}(\mathbf{k}), \\ \omega^S_{mn}(-\mathbf{k}) &= \omega^S_{mn}(\mathbf{k}), \\ \Delta^a_{nm}(-\mathbf{k}) &= -\Delta^a_{nm}(\mathbf{k}). \end{aligned}$$

For a clean cold semiconductor, $f_n = 1$ for an occupied or valence ($n = v$) band, and $f_n = 0$ for an empty or conduction ($n = c$) band independent of $\mathbf{k}$, and $f_{nm} = -f_{mn}$.

The $\frac{1}{\omega}$ terms cancel each other out. We notice that the energy denominators are invariant under $\mathbf{k} \to -\mathbf{k}$, and then we only look at the numerators, then

$$\begin{aligned} C \to f_{mn}\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}(r^{\mathrm{b}}_{nm})_{;k^{\mathrm{c}}}|_{\mathbf{k}} + f_{mn}\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}(r^{\mathrm{b}}_{nm})_{;k^{\mathrm{c}}}|_{-\mathbf{k}} &= f_{mn}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}(r^{\mathrm{b}}_{nm})_{;k^{\mathrm{c}}}|_{\mathbf{k}} + (-\mathcal{V}^{\Sigma,\mathrm{a}}_{nm})(-(r^{\mathrm{b}}_{mn})_{;k^{\mathrm{c}}})|_{\mathbf{k}}\right] \\ &= f_{mn}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}(r^{\mathrm{b}}_{nm})_{;k^{\mathrm{c}}} + \mathcal{V}^{\Sigma,\mathrm{a}}_{nm}(r^{\mathrm{b}}_{mn})_{;k^{\mathrm{c}}}\right] \\ &= f_{mn}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}(r^{\mathrm{b}}_{nm})_{;k^{\mathrm{c}}} + (\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}(r^{\mathrm{b}}_{nm})_{;k^{\mathrm{c}}})^*\right] \end{aligned} \tag{3}$$

The last term in the second line of (2) is dealt with as follows,

$$\begin{aligned} \frac{D}{2(\omega^S_{nm})^2}\frac{1}{(\omega^S_{nm}-\omega)^2} &= \frac{f_{mn}}{2}\frac{\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}r^{\mathrm{b}}_{nm}}{(\omega^S_{nm})^2}\frac{\Delta^{\mathrm{c}}_{nm}}{(\omega^S_{nm}-\omega)^2} = \frac{f_{mn}}{2}\frac{\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}r^{\mathrm{b}}_{nm}}{(\omega^S_{nm})^2}\left(\frac{1}{\omega^S_{nm}-\omega}\right)_{;k^{\mathrm{c}}} \\ &= -\frac{f_{mn}}{2}\left(\frac{\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}r^{\mathrm{b}}_{nm}}{(\omega^S_{nm})^2}\right)_{;k^{\mathrm{c}}}\frac{1}{\omega^S_{nm}-\omega}. \end{aligned} \tag{4}$$

We use the fact that

$$(\omega^S_{nm})_{;k^{\rm c}} = (\omega^{\rm LDA}_{nm})_{;k^{\rm c}} = \frac{p^{\rm c}_{nn} - p^{\rm c}_{mm}}{m_e} \equiv \Delta^{\rm c}_{nm}, \tag{5}$$ `wk`

and for the last line, we performed an integration by parts over the Brillouin zone, where the contribution from the edges vanishes.

1 Generalized Derivative

Using the chain rule we obtain

$$\left(\frac{\mathcal{V}^{\Sigma,{\rm a}}_{mn} r^{\rm b}_{nm}}{(\omega^S_{nm})^2}\right)_{;k^{\rm c}} = \frac{r^{\rm b}_{nm}}{(\omega^S_{nm})^2}\left(\mathcal{V}^{\Sigma,{\rm a}}_{mn}\right)_{;k^{\rm c}} + \frac{\mathcal{V}^{\Sigma,{\rm a}}_{mn}}{(\omega^S_{nm})^2}\left(r^{\rm b}_{nm}\right)_{;k^{\rm c}} - \frac{\mathcal{V}^{\Sigma,{\rm a}}_{mn} r^{\rm b}_{nm}}{2(\omega^S_{nm})^3}\left(\omega^S_{nm}\right)_{;k^{\rm c}}. \tag{6}$$ `chrn`

The individual terms for this expression can be expanded as follows. First,

$$\left(\omega^S_{nm}\right)_{;k^{\rm c}} = \Delta^{\rm LDA,c}_{nm}, \tag{7}$$ `eli.1`

and,

$$(r^{\rm b}_{nm})_{;k^{\rm a}} \approx \frac{r^{\rm a}_{nm}\Delta^{\rm LDA,b}_{mn} + r^{\rm b}_{nm}\Delta^{\rm LDA,a}_{mn}}{\omega^{\rm LDA}_{nm}} + \frac{i}{\omega^{\rm LDA}_{nm}}\sum_\ell\left(\omega^{\rm LDA}_{\ell m} r^{\rm a}_{n\ell} r^{\rm b}_{\ell m} - \omega^{\rm LDA}_{n\ell} r^{\rm b}_{n\ell} r^{\rm a}_{\ell m}\right). \tag{8}$$ `eli.2`

1.1 Generalized derivative for $\mathcal{V}^{\Sigma,\mathbf{a},\ell}_{nm}$

We must include the generalized derivative for $\mathcal{V}^{\Sigma,{\rm a},\ell}_{nm}$. We can seperate the expression into its components,

$$\left(\mathcal{V}^{\Sigma,{\rm a},\ell}_{nm}\right)_{;k^{\rm b}} = \left(\mathcal{V}^{{\rm LDA,a},\ell}_{nm}\right)_{;k^{\rm b}} + \left(\mathcal{V}^{S,{\rm a},\ell}_{nm}\right)_{;k^{\rm b}}, \tag{9}$$

where,

$$(\mathcal{V}^{\rm LDA,a}_{nm})_{;k^{\rm b}} = \frac{1}{2}\sum_q\left((v^{\rm LDA,a}_{nq})_{;k^{\rm b}}\mathcal{F}^\ell_{qm} + v^{\rm LDA,a}_{nq}(\mathcal{F}^\ell_{qm})_{;k^{\rm b}} + (\mathcal{F}^\ell_{nq})_{;k^{\rm b}} v^{\rm LDA,a}_{qm} + \mathcal{F}^\ell_{nq}(v^{\rm LDA,a}_{qm})_{;k^{\rm b}}\right), \tag{10}$$ `a.2`

and $\left(v^{\rm LDA,a}_{nn}\right)_{;k^{\rm b}}$ is given by

$$\left(v_{nn}^{\mathrm{LDA,a}}\right)_{;k^{\mathrm{b}}} = \frac{\hbar}{m_e}\delta_{\mathrm{ab}} - \sum_{\ell \neq n} \omega_{\ell n}^{\mathrm{LDA}} \left(r_{n\ell}^{\mathrm{a}} r_{\ell n}^{\mathrm{b}} + r_{n\ell}^{\mathrm{b}} r_{\ell n}^{\mathrm{a}} \right). \tag{11}$$

Lastly,

$$\mathcal{V}_{nm}^{S,\mathrm{a},\ell} = \frac{1}{2} \sum_{q} \left((v_{nq}^{S,\mathrm{a}})_{;k^{\mathrm{b}}} \mathcal{F}_{qm} + v_{nq}^{S,\mathrm{a}} (\mathcal{F}_{qm})_{;k^{\mathrm{b}}} + (\mathcal{F}_{nq})_{;k^{\mathrm{b}}} v_{qm}^{S,\mathrm{a}} + \mathcal{F}_{nq} (v_{qm}^{S,\mathrm{a}})_{;k^{\mathrm{b}}} \right), \tag{12} \quad \boxed{\texttt{a.3b}}$$

where $\left(v_{nm}^{S,\mathrm{a}}\right)_{;k^{\mathrm{b}}}$ is given by

$$\left(v_{nm}^{S,\mathrm{a}}\right)_{;k^{\mathrm{b}}} = i \Delta f_{mn} (r_{nm}^{\mathrm{a}})_{;k^{\mathrm{b}}}. \tag{13}$$