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

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

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,

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

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:

$$\begin{aligned}
\mathbf{r}_{mn}(\mathbf{k})|_{-\mathbf{k}} &= \mathbf{r}_{nm}(\mathbf{k})|_{\mathbf{k}}, \\
(\mathbf{r}_{mn})_{;\mathbf{k}}(\mathbf{k})|_{-\mathbf{k}} &= (-\mathbf{r}_{nm})_{;\mathbf{k}}(\mathbf{k})|_{\mathbf{k}}, \\
\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}(\mathbf{k})|_{-\mathbf{k}} &= -\mathcal{V}^{\Sigma,\mathrm{a}}_{nm}(\mathbf{k})|_{\mathbf{k}}, \\
\omega^S_{mn}(\mathbf{k})|_{-\mathbf{k}} &= \omega^S_{mn}(\mathbf{k})|_{\mathbf{k}}, \\
\Delta^a_{nm}(\mathbf{k})|_{-\mathbf{k}} &= -\Delta^a_{nm}(\mathbf{k})|_{\mathbf{k}}.
\end{aligned} \tag{3} \qquad \boxed{\texttt{time_reversa}}$$

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

$$\begin{aligned}
C \to f_{mn}\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}|_{\mathbf{k}} + f_{mn}\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}|_{-\mathbf{k}}& \\
&= f_{mn}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}|_{\mathbf{k}} + \left(-\mathcal{V}^{\Sigma,\mathrm{a}}_{nm}\right)\left(-r^{\mathrm{LDA,b}}_{mn}\right)_{;k^{\mathrm{c}}}|_{\mathbf{k}}\right] \\
&= f_{mn}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}} + \mathcal{V}^{\Sigma,\mathrm{a}}_{nm}\left(r^{\mathrm{LDA,b}}_{mn}\right)_{;k^{\mathrm{c}}}\right] \\
&= f_{mn}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}} + \left(\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}\right)^*\right] \\
&= 2f_{mn}\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}\right],
\end{aligned} \tag{4} \qquad \boxed{\texttt{ct}}$$

and likewise,

$$
\begin{aligned}
D \to f_{mn}\mathcal{V}^{\Sigma,\mathrm{a}}_{mn} r^{\mathrm{b}}_{nm}\Delta^{\mathrm{c}}_{nm}|_{\mathbf{k}} + f_{mn}\mathcal{V}^{\Sigma,\mathrm{a}}_{mn} r^{\mathrm{b}}_{nm}\Delta^{\mathrm{c}}_{nm}|_{-\mathbf{k}} & \\
&= f_{mn}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn} r^{\mathrm{b}}_{nm}\Delta^{\mathrm{c}}_{nm}|_{\mathbf{k}} + \left(-\mathcal{V}^{\Sigma,\mathrm{a}}_{nm}\right) r^{\mathrm{b}}_{mn}\left(-\Delta^{\mathrm{c}}_{nm}\right)|_{\mathbf{k}}\right] \\
&= f_{mn}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn} r^{\mathrm{b}}_{nm} + \mathcal{V}^{\Sigma,\mathrm{a}}_{nm} r^{\mathrm{b}}_{mn}\right]\Delta^{\mathrm{c}}_{nm} \\
&= f_{mn}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn} r^{\mathrm{b}}_{nm} + \left(\mathcal{V}^{\Sigma,\mathrm{a}}_{mn} r^{\mathrm{b}}_{nm}\right)^{*}\right]\Delta^{\mathrm{c}}_{nm} \\
&= 2f_{mn}\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn} r^{\mathrm{b}}_{nm}\right]\Delta^{\mathrm{c}}_{nm}.
\end{aligned}
\tag{5}
$$

dt

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

$$
\begin{aligned}
\frac{D}{2(\omega^{S}_{nm})^2}\frac{1}{(\omega^{S}_{nm}-\omega)^2} &= \frac{f_{mn}}{2}\frac{\mathcal{V}^{\Sigma,\mathrm{a}}_{mn} r^{\mathrm{b}}_{nm}}{(\omega^{S}_{nm})^2}\frac{\Delta^{\mathrm{c}}_{nm}}{(\omega^{S}_{nm}-\omega)^2} = \frac{f_{mn}}{2}\frac{\mathcal{V}^{\Sigma,\mathrm{a}}_{mn} r^{\mathrm{b}}_{nm}}{(\omega^{S}_{nm})^2}\left(\frac{1}{\omega^{S}_{nm}-\omega}\right)_{;k^{\mathrm{c}}} \\
&= -\frac{f_{mn}}{2}\left(\frac{\mathcal{V}^{\Sigma,\mathrm{a}}_{mn} r^{\mathrm{b}}_{nm}}{(\omega^{S}_{nm})^2}\right)_{;k^{\mathrm{c}}}\frac{1}{\omega^{S}_{nm}-\omega}.
\end{aligned}
\tag{6}
$$

dresn

We use the fact that

$$
(\omega^{S}_{nm})_{;k^{\mathrm{c}}} = (\omega^{\mathrm{LDA}}_{nm})_{;k^{\mathrm{c}}} = \frac{p^{\mathrm{c}}_{nn}-p^{\mathrm{c}}_{mm}}{m_e} \equiv \Delta^{\mathrm{c}}_{nm},
\tag{7}
$$

wk

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

$$
\left(\frac{\mathcal{V}^{\Sigma,\mathrm{a}}_{mn} r^{\mathrm{b}}_{nm}}{(\omega^{S}_{nm})^2}\right)_{;k^{\mathrm{c}}} = \frac{r^{\mathrm{b}}_{nm}}{(\omega^{S}_{nm})^2}\left(\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\right)_{;k^{\mathrm{c}}} + \frac{\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}}{(\omega^{S}_{nm})^2}\left(r^{\mathrm{b}}_{nm}\right)_{;k^{\mathrm{c}}} - \frac{\mathcal{V}^{\Sigma,\mathrm{a}}_{mn} r^{\mathrm{b}}_{nm}}{2(\omega^{S}_{nm})^3}\left(\omega^{S}_{nm}\right)_{;k^{\mathrm{c}}}.
\tag{8}
$$

chr

We will check each term of (8) over $\mathbf{k}\to-\mathbf{k}$. The first term is reduced to

$$
\begin{aligned}
\frac{r^{\mathrm{b}}_{nm}}{(\omega^{S}_{nm})^2}\left(\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\right)_{;k^{\mathrm{c}}}|_{\mathbf{k}} + \frac{r^{\mathrm{b}}_{nm}}{(\omega^{S}_{nm})^2}\left(\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\right)_{;k^{\mathrm{c}}}|_{-\mathbf{k}} &= \frac{r^{\mathrm{b}}_{nm}}{(\omega^{S}_{nm})^2}\left(\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\right)_{;k^{\mathrm{c}}}|_{\mathbf{k}} - \frac{r^{\mathrm{b}}_{mn}}{(\omega^{S}_{nm})^2}\left(\mathcal{V}^{\Sigma,\mathrm{a}}_{nm}\right)_{;k^{\mathrm{c}}}|_{\mathbf{k}} \\
&= \frac{1}{(\omega^{S}_{nm})^2}\left[r^{\mathrm{b}}_{nm}\left(\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\right)_{;k^{\mathrm{c}}} - \left(r^{\mathrm{b}}_{nm}\left(\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\right)_{;k^{\mathrm{c}}}\right)^{*}\right] \\
&= \frac{2i}{(\omega^{S}_{nm})^2}\mathrm{Im}\left[r^{\mathrm{b}}_{nm}\left(\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\right)_{;k^{\mathrm{c}}}\right],
\end{aligned}
\tag{9}
$$

first_term_

the second term is reduced to

$$
\begin{aligned}
\frac{\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}}{(\omega^S_{nm})^2}\left(r^{\mathrm{b}}_{nm}\right)_{;k^{\mathrm{c}}}|_{\mathbf{k}} + \frac{\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}}{(\omega^S_{nm})^2}\left(r^{\mathrm{b}}_{nm}\right)_{;k^{\mathrm{c}}}|_{-\mathbf{k}} &= \frac{\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}}{(\omega^S_{nm})^2}\left(r^{\mathrm{b}}_{nm}\right)_{;k^{\mathrm{c}}}|_{\mathbf{k}} + \frac{\mathcal{V}^{\Sigma,\mathrm{a}}_{nm}}{(\omega^S_{nm})^2}\left(r^{\mathrm{b}}_{mn}\right)_{;k^{\mathrm{c}}}|_{\mathbf{k}} \\
&= \frac{1}{(\omega^S_{nm})^2}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\left(r^{\mathrm{b}}_{nm}\right)_{;k^{\mathrm{c}}} + \left(\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\left(r^{\mathrm{b}}_{nm}\right)_{;k^{\mathrm{c}}}\right)^*\right] \\
&= \frac{2}{(\omega^S_{nm})^2}\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\left(r^{\mathrm{b}}_{nm}\right)_{;k^{\mathrm{c}}}\right], \qquad (10)
\end{aligned}
$$

second_term_

and the third term is reduced to

$$
\frac{\mathcal{V}^{\Sigma,\mathrm{a}}_{mn} r^{\mathrm{b}}_{nm}}{2(\omega^S_{nm})^3}\left(\omega^S_{nm}\right)_{;k^{\mathrm{c}}}|_{\mathbf{k}} + \frac{\mathcal{V}^{\Sigma,\mathrm{a}}_{mn} r^{\mathrm{b}}_{nm}}{2(\omega^S_{nm})^3}\left(\omega^S_{nm}\right)_{;k^{\mathrm{c}}}|_{-\mathbf{k}} = \frac{\mathcal{V}^{\Sigma,\mathrm{a}}_{mn} r^{\mathrm{b}}_{nm}}{2(\omega^S_{nm})^3}\left(\omega^S_{nm}\right)_{;k^{\mathrm{c}}}|_{\mathbf{k}} - \frac{\mathcal{V}^{\Sigma,\mathrm{a}}_{nm} r^{\mathrm{b}}_{mn}}{2(\omega^S_{nm})^3}\left(\omega^S_{nm}\right)_{;k^{\mathrm{c}}}|_{\mathbf{k}} \qquad (11)
$$

third_term_