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

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

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

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

Time-reversal symmetry leads to the following relationships:

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

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

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

and likewise,

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

The last term in the second line of ($\overset{\texttt{pfi}}{2}$) is dealt with as follows,

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

We use the fact that

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

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

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

We will check each term of ($\overset{\texttt{chr}}{8}$) over $\mathbf{k}\to-\mathbf{k}$ using the relations in ($\overset{\texttt{time\_reversal}}{3}$). The first term is reduced to

$$
\begin{aligned}
\frac{r^{\mathrm{LDA,b}}_{nm}}{(\omega^{S}_{nm})^2}\left(\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\right)_{;k^{\mathrm{c}}}|_{\mathbf{k}} + \frac{r^{\mathrm{LDA,b}}_{nm}}{(\omega^{S}_{nm})^2}\left(\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\right)_{;k^{\mathrm{c}}}|_{-\mathbf{k}} &= \frac{r^{\mathrm{LDA,b}}_{nm}}{(\omega^{S}_{nm})^2}\left(\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\right)_{;k^{\mathrm{c}}}|_{\mathbf{k}} + \frac{r^{\mathrm{LDA,b}}_{mn}}{(\omega^{S}_{nm})^2}\left(\mathcal{V}^{\Sigma,\mathrm{a}}_{nm}\right)_{;k^{\mathrm{c}}}|_{\mathbf{k}}\\
&= \frac{1}{(\omega^{S}_{nm})^2}\left[r^{\mathrm{LDA,b}}_{nm}\left(\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\right)_{;k^{\mathrm{c}}} + \left(r^{\mathrm{LDA,b}}_{nm}\left(\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\right)_{;k^{\mathrm{c}}}\right)^{*}\right]\\
&= \frac{2}{(\omega^{S}_{nm})^2}\mathrm{Re}\left[r^{\mathrm{LDA,b}}_{nm}\left(\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\right)_{;k^{\mathrm{c}}}\right], \qquad (9) \quad \boxed{\texttt{first\_term\_g}}
\end{aligned}
$$

the second term is reduced to

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

and by using (7), the third term is reduced to

$$
\begin{aligned}
\frac{\mathcal{V}_{mn}^{\Sigma,\mathrm{a}} r_{nm}^{\mathrm{LDA,b}}}{2(\omega_{nm}^S)^3}\left(\omega_{nm}^S\right)_{;k^{\mathrm{c}}}|_{\mathbf{k}} + \frac{\mathcal{V}_{mn}^{\Sigma,\mathrm{a}} r_{nm}^{\mathrm{LDA,b}}}{2(\omega_{nm}^S)^3}\left(\omega_{nm}^S\right)_{;k^{\mathrm{c}}}|_{-\mathbf{k}} &= \frac{\mathcal{V}_{mn}^{\Sigma,\mathrm{a}} r_{nm}^{\mathrm{LDA,b}}}{2(\omega_{nm}^S)^3}\Delta_{nm}^{\mathrm{c}}|_{\mathbf{k}} + \frac{\mathcal{V}_{mn}^{\Sigma,\mathrm{a}} r_{nm}^{\mathrm{LDA,b}}}{2(\omega_{nm}^S)^3}\Delta_{nm}^{\mathrm{c}}|_{-\mathbf{k}} \\
&= \frac{\mathcal{V}_{nm}^{\Sigma,\mathrm{a}} r_{mn}^{\mathrm{LDA,b}}}{2(\omega_{nm}^S)^3}\Delta_{nm}^{\mathrm{c}}|_{\mathbf{k}} + \frac{\mathcal{V}_{mn}^{\Sigma,\mathrm{a}} r_{nm}^{\mathrm{LDA,b}}}{2(\omega_{nm}^S)^3}\Delta_{nm}^{\mathrm{c}}|_{\mathbf{k}} \\
&= \frac{1}{2(\omega_{nm}^S)^3}\left[\mathcal{V}_{nm}^{\Sigma,\mathrm{a}} r_{mn}^{\mathrm{LDA,b}} + \left(\mathcal{V}_{nm}^{\Sigma,\mathrm{a}} r_{mn}^{\mathrm{LDA,b}}\right)^*\right]\Delta_{nm}^{\mathrm{c}} \\
&= \frac{1}{(\omega_{nm}^S)^3}\mathrm{Re}\left[\mathcal{V}_{nm}^{\Sigma,\mathrm{a}} r_{mn}^{\mathrm{LDA,b}}\right]\Delta_{nm}^{\mathrm{c}}. \qquad (11)
\end{aligned}
$$

Combining the results from (9), (10), and (11) into (8),

$$
\begin{aligned}
&-\frac{f_{mn}}{2}\left[\left(\frac{\mathcal{V}_{mn}^{\Sigma,\mathrm{a}} r_{nm}^{\mathrm{LDA,b}}}{(\omega_{nm}^S)^2}\right)_{;k^{\mathrm{c}}}|_{\mathbf{k}} + \left(\frac{\mathcal{V}_{mn}^{\Sigma,\mathrm{a}} r_{nm}^{\mathrm{LDA,b}}}{(\omega_{nm}^S)^2}\right)_{;k^{\mathrm{c}}}|_{-\mathbf{k}}\right]\frac{1}{\omega_{nm}^S-\omega} = \\
&-f_{mn}\left(2\mathrm{Re}\left[r_{nm}^{\mathrm{LDA,b}}\left(\mathcal{V}_{mn}^{\Sigma,\mathrm{a}}\right)_{;k^{\mathrm{c}}}\right] + 2\mathrm{Re}\left[\mathcal{V}_{mn}^{\Sigma,\mathrm{a}}\left(r_{nm}^{\mathrm{LDA,b}}\right)_{;k^{\mathrm{c}}}\right] - \frac{1}{\omega_{nm}^S}\mathrm{Re}\left[\mathcal{V}_{nm}^{\Sigma,\mathrm{a}} r_{mn}^{\mathrm{LDA,b}}\right]\Delta_{nm}^{\mathrm{c}}\right)\frac{1}{2(\omega_{nm}^S)^2}\frac{1}{\omega_{nm}^S-\omega}. \qquad (12)
\end{aligned}
$$

We have all the elements to be substituted in (2). We substitute (4), (5), and (12) in (2),

$$
\begin{aligned}
I = &\left[-\frac{2f_{mn}\,\mathrm{Re}\left[\mathcal{V}_{mn}^{\Sigma,\mathrm{a}}\left(r_{nm}^{\mathrm{LDA,b}}\right)_{;k^{\mathrm{c}}}\right]}{2(\omega_{nm}^S)^2}\frac{1}{\omega_{nm}^S-\omega} + \frac{4f_{mn}\,\mathrm{Re}\left[\mathcal{V}_{mn}^{\Sigma,\mathrm{a}}\left(r_{nm}^{\mathrm{LDA,b}}\right)_{;k^{\mathrm{c}}}\right]}{(\omega_{nm}^S)^2}\frac{1}{\omega_{nm}^S-2\omega}\right] \\
&-\left[-\frac{6f_{mn}\,\mathrm{Re}\left[\mathcal{V}_{mn}^{\Sigma,\mathrm{a}} r_{nm}^{\mathrm{LDA,b}}\right]\Delta_{nm}^{\mathrm{c}}}{2(\omega_{nm}^S)^2}\frac{1}{\omega_{nm}^S-\omega} + \frac{8f_{mn}\,\mathrm{Re}\left[\mathcal{V}_{mn}^{\Sigma,\mathrm{a}} r_{nm}^{\mathrm{LDA,b}}\right]\Delta_{nm}^{\mathrm{c}}}{(\omega_{nm}^S)^3}\frac{1}{\omega_{nm}^S-2\omega}\right. \\
&\left. + \frac{f_{mn}\left(2\,\mathrm{Re}\left[r_{nm}^{\mathrm{LDA,b}}\left(\mathcal{V}_{mn}^{\Sigma,\mathrm{a}}\right)_{;k^{\mathrm{c}}}\right] + 2\,\mathrm{Re}\left[\mathcal{V}_{mn}^{\Sigma,\mathrm{a}}\left(r_{nm}^{\mathrm{LDA,b}}\right)_{;k^{\mathrm{c}}}\right] - \frac{1}{\omega_{nm}^S}\mathrm{Re}\left[\mathcal{V}_{nm}^{\Sigma,\mathrm{a}} r_{mn}^{\mathrm{LDA,b}}\right]\Delta_{nm}^{\mathrm{c}}\right)}{2(\omega_{nm}^S)^2}\frac{1}{\omega_{nm}^S-\omega}\right].
\end{aligned}
$$

If we simplify and homogenize,

$$
\begin{aligned}
I = &-\frac{2f_{mn}\,\mathrm{Re}\left[\mathcal{V}_{mn}^{\Sigma,\mathrm{a}}\left(r_{nm}^{\mathrm{LDA,b}}\right)_{;k^{\mathrm{c}}}\right]}{2(\omega_{nm}^S)^2}\frac{1}{\omega_{nm}^S-\omega} + \frac{4f_{mn}\,\mathrm{Re}\left[\mathcal{V}_{mn}^{\Sigma,\mathrm{a}}\left(r_{nm}^{\mathrm{LDA,b}}\right)_{;k^{\mathrm{c}}}\right]}{(\omega_{nm}^S)^2}\frac{1}{\omega_{nm}^S-2\omega} \\
&+\frac{6f_{mn}\,\mathrm{Re}\left[\mathcal{V}_{mn}^{\Sigma,\mathrm{a}} r_{nm}^{\mathrm{LDA,b}}\right]\Delta_{nm}^{\mathrm{c}}}{2(\omega_{nm}^S)^2}\frac{1}{\omega_{nm}^S-\omega} - \frac{8f_{mn}\,\mathrm{Re}\left[\mathcal{V}_{mn}^{\Sigma,\mathrm{a}} r_{nm}^{\mathrm{LDA,b}}\right]\Delta_{nm}^{\mathrm{c}}}{(\omega_{nm}^S)^3}\frac{1}{\omega_{nm}^S-2\omega} \\
&-\frac{2f_{mn}\,\mathrm{Re}\left[r_{nm}^{\mathrm{LDA,b}}\left(\mathcal{V}_{mn}^{\Sigma,\mathrm{a}}\right)_{;k^{\mathrm{c}}}\right]}{2(\omega_{nm}^S)^2}\frac{1}{\omega_{nm}^S-\omega} \\
&-\frac{2f_{mn}\,\mathrm{Re}\left[\mathcal{V}_{mn}^{\Sigma,\mathrm{a}}\left(r_{nm}^{\mathrm{LDA,b}}\right)_{;k^{\mathrm{c}}}\right]}{2(\omega_{nm}^S)^2}\frac{1}{\omega_{nm}^S-\omega} \\
&+\frac{f_{mn}\mathrm{Re}\left[\mathcal{V}_{nm}^{\Sigma,\mathrm{a}} r_{mn}^{\mathrm{LDA,b}}\right]\Delta_{nm}^{\mathrm{c}}}{2(\omega_{nm}^S)^3}\frac{1}{\omega_{nm}^S-\omega}, \qquad (13)
\end{aligned}
$$

we conveniently collect the terms in columns of ω and 2ω. We can now express the susceptibility in terms of ω and 2ω. Separating the 2ω terms and substituting in (1),

$$
\begin{aligned}
I_{2\omega} &= -\frac{e^3}{\hbar^2}\sum_{mn\mathbf{k}}\left[\frac{4f_{mn}\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}\right]}{(\omega^S_{nm})^2}-\frac{8f_{mn}\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}r^{\mathrm{LDA,b}}_{nm}\right]\Delta^{\mathrm{c}}_{nm}}{(\omega^S_{nm})^3}\right]\frac{1}{\omega^S_{nm}-2\omega}\\
&= -\frac{e^3}{\hbar^2}\sum_{mn\mathbf{k}}\frac{4f_{mn}}{(\omega^S_{nm})^2}\left[\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}\right]-\frac{2\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}r^{\mathrm{LDA,b}}_{nm}\right]\Delta^{\mathrm{c}}_{nm}}{\omega^S_{nm}}\right]\frac{1}{\omega^S_{nm}-2\omega}.
\end{aligned}
\tag{14}
$$

2wchii

We can express the energies in terms of transitions between bands. Therefore, $\omega^S_{nm}=\omega^S_{cv}$ for transitions between conduction and valence bands. We analyze the limit,

$$
\lim_{\eta\to 0}\frac{1}{x\pm i\eta}=P\frac{1}{x}\mp i\pi\delta(x),
\tag{15}
$$

and can finally rewrite (14) in the desired form,

$$
\mathrm{Im}[\chi^{s,\ell}_{i,\mathrm{abc},2\omega}]=-\frac{\pi e^3}{\hbar^2}\sum_{mn\mathbf{k}}\frac{4}{(\omega^S_{nm})^2}\left(\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}\right]-\frac{2\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}r^{\mathrm{LDA,b}}_{nm}\right]\Delta^{\mathrm{c}}_{nm}}{\omega^S_{nm}}\right)\delta(\omega^S_{nm}-2\omega).
\tag{16}
$$

imchi2w

We do the same for the ω terms in (13) and substitute in (1),

$$
\begin{aligned}
I_{\omega} = -\frac{e^3}{2\hbar^2}\sum_{mn\mathbf{k}}\Bigg[&-\frac{2f_{mn}\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}\right]}{(\omega^S_{nm})^2}+\frac{6f_{mn}\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}r^{\mathrm{LDA,b}}_{nm}\right]\Delta^{\mathrm{c}}_{nm}}{(\omega^S_{nm})^2}\\
&-\frac{2f_{mn}\,\mathrm{Re}\left[r^{\mathrm{LDA,b}}_{nm}\left(\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\right)_{;k^{\mathrm{c}}}\right]}{(\omega^S_{nm})^2}-\frac{2f_{mn}\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}\right]}{(\omega^S_{nm})^2}\\
&+\frac{f_{mn}\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{nm}r^{\mathrm{LDA,b}}_{mn}\right]\Delta^{\mathrm{c}}_{nm}}{(\omega^S_{nm})^3}\Bigg]\frac{1}{\omega^S_{nm}-\omega},
\end{aligned}
\tag{17}
$$

wchii

and we reduce in the same way as (14),

$$
\begin{aligned}
I_{\omega} &= \frac{e^3}{2\hbar^2}\sum_{mn\mathbf{k}}\frac{f_{mn}}{(\omega^S_{nm})^2}\Bigg[2\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}\right]\\
&\qquad -6\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}r^{\mathrm{LDA,b}}_{nm}\right]\Delta^{\mathrm{c}}_{nm}+2\,\mathrm{Re}\left[r^{\mathrm{LDA,b}}_{nm}\left(\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\right)_{;k^{\mathrm{c}}}\right]\\
&\qquad +2\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}\right]-\frac{\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{nm}r^{\mathrm{LDA,b}}_{mn}\right]\Delta^{\mathrm{c}}_{nm}}{(\omega^S_{nm})}\Bigg]\frac{1}{\omega^S_{nm}-\omega}\\
&= \frac{e^3}{2\hbar^2}\sum_{mn\mathbf{k}}\frac{f_{mn}}{(\omega^S_{nm})^2}\Bigg[4\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}\right]\\
&\qquad -6\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}r^{\mathrm{LDA,b}}_{nm}\right]\Delta^{\mathrm{c}}_{nm}+2\,\mathrm{Re}\left[r^{\mathrm{LDA,b}}_{nm}\left(\mathcal{V}^{\Sigma,\mathrm{a}}_{mn}\right)_{;k^{\mathrm{c}}}\right]\\
&\qquad -\frac{\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a}}_{nm}r^{\mathrm{LDA,b}}_{mn}\right]\Delta^{\mathrm{c}}_{nm}}{(\omega^S_{nm})}\Bigg]\frac{1}{\omega^S_{nm}-\omega}
\end{aligned}
\tag{18}
$$

wchii_simpli