I. EXPRESSIONS FOR $\chi^{\rm abc}_{\rm surface}$ IN TERMS OF $\mathcal{V}^{\Sigma,\mathbf{a},\ell}_{mn}$

The prefactor of Eqs. (**??**) and (**??**) diverges as $\tilde\omega\to 0$. To remove this apparent divergence of $\boldsymbol{\chi}$, we perform a partial fraction expansion in $\tilde\omega$.

A. Intraband Contributions

For the intraband term of Eq. (**??**), we obtain

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

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

Time-reversal symmetry leads to the following relationships:

$$\begin{aligned}
\mathbf{r}_{mn}(\mathbf{k})|_{-\mathbf{k}} &= \mathbf{r}_{nm}(\mathbf{k})|_{\mathbf{k}},\\
(\mathbf{r}_{mn})_{;\mathbf{k}}(\mathbf{k})|_{-\mathbf{k}} &= (-\mathbf{r}_{nm})_{;\mathbf{k}}(\mathbf{k})|_{\mathbf{k}},\\
\mathcal{V}^{\Sigma,\rm a,\ell}_{mn}(\mathbf{k})|_{-\mathbf{k}} &= -\mathcal{V}^{\Sigma,\rm a,\ell}_{nm}(\mathbf{k})|_{\mathbf{k}},\\
(\mathcal{V}^{\Sigma,\rm a,\ell}_{mn})_{;\mathbf{k}}(\mathbf{k})|_{-\mathbf{k}} &= (\mathcal{V}^{\Sigma,\rm a,\ell}_{nm})_{;\mathbf{k}}(\mathbf{k})|_{\mathbf{k}},\\
\omega^\Sigma_{mn}(\mathbf{k})|_{-\mathbf{k}} &= \omega^\Sigma_{mn}(\mathbf{k})|_{\mathbf{k}},\\
\Delta^a_{nm}(\mathbf{k})|_{-\mathbf{k}} &= -\Delta^a_{nm}(\mathbf{k})|_{\mathbf{k}}.
\end{aligned}\tag{2}$$

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 $f_{nm}=-f_{mn}$. Using the relationships above, we can show that the $1/\omega$ terms cancel each other out. Therefore, all the remaining nonzero terms in expressions (1) are simple ω and 2ω resonant denominators that are well behaved at $\omega=0$.

To apply time-reversal invariance, we notice that the energy denominators are invariant under $\mathbf{k}\to-\mathbf{k}$, and then we only look at the numerators, then

$$\begin{aligned}
C\to f_{mn}\mathcal{V}^{\Sigma,\rm a,\ell}_{mn}\left(r^{\rm LDA,b}_{nm}\right)_{;k^{\rm c}}|_{\mathbf{k}}+f_{mn}\mathcal{V}^{\Sigma,\rm a,\ell}_{mn}\left(r^{\rm LDA,b}_{nm}\right)_{;k^{\rm c}}|_{-\mathbf{k}}&\\
=f_{mn}\left[\mathcal{V}^{\Sigma,\rm a,\ell}_{mn}\left(r^{\rm LDA,b}_{nm}\right)_{;k^{\rm c}}|_{\mathbf{k}}+\left(-\mathcal{V}^{\Sigma,\rm a,\ell}_{nm}\right)\left(-r^{\rm LDA,b}_{mn}\right)_{;k^{\rm c}}|_{\mathbf{k}}\right]&\\
=f_{mn}\left[\mathcal{V}^{\Sigma,\rm a,\ell}_{mn}\left(r^{\rm LDA,b}_{nm}\right)_{;k^{\rm c}}+\mathcal{V}^{\Sigma,\rm a,\ell}_{nm}\left(r^{\rm LDA,b}_{mn}\right)_{;k^{\rm c}}\right]&\\
=f_{mn}\left[\mathcal{V}^{\Sigma,\rm a,\ell}_{mn}\left(r^{\rm LDA,b}_{nm}\right)_{;k^{\rm c}}+\left(\mathcal{V}^{\Sigma,\rm a,\ell}_{mn}\left(r^{\rm LDA,b}_{nm}\right)_{;k^{\rm c}}\right)^*\right]&\\
=2f_{mn}\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\rm a,\ell}_{mn}\left(r^{\rm LDA,b}_{nm}\right)_{;k^{\rm c}}\right],&
\end{aligned}\tag{3}$$

and likewise,

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

The last term in the second line of Eq. (1) is dealt with as follows.

$$\begin{aligned}
\frac{D}{2(\omega^\Sigma_{nm})^2}\frac{1}{(\omega^\Sigma_{nm}-\tilde\omega)^2}&=\frac{f_{mn}}{2}\frac{\mathcal{V}^{\Sigma,\rm a}_{mn}r^{\rm b}_{nm}}{(\omega^\Sigma_{nm})^2}\frac{\Delta^{\rm c}_{nm}}{(\omega^\Sigma_{nm}-\tilde\omega)^2}=-\frac{f_{mn}}{2}\frac{\mathcal{V}^{\Sigma,\rm a}_{mn}r^{\rm b}_{nm}}{(\omega^\Sigma_{nm})^2}\left(\frac{1}{\omega^\Sigma_{nm}-\tilde\omega}\right)_{;k^{\rm c}}\\
&=\frac{f_{mn}}{2}\left(\frac{\mathcal{V}^{\Sigma,\rm a}_{mn}r^{\rm b}_{nm}}{(\omega^\Sigma_{nm})^2}\right)_{;k^{\rm c}}\frac{1}{\omega^\Sigma_{nm}-\tilde\omega},
\end{aligned}\tag{5}$$

where we used Eqs. (??) and for the last line, we performed an integration by parts over the Brillouin zone, where the contribution from the edges vanishes.[1] Now, we apply the chain rule, to get

$$\left(\frac{\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{LDA,b}}_{nm}}{(\omega^{\Sigma}_{nm})^2}\right)_{;k^{\mathrm{c}}} = \frac{r^{\mathrm{LDA,b}}_{nm}}{(\omega^{\Sigma}_{nm})^2}\left(\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}\right)_{;k^{\mathrm{c}}} + \frac{\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}}{(\omega^{\Sigma}_{nm})^2}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}} - \frac{2\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{LDA,b}}_{nm}}{(\omega^{\Sigma}_{nm})^3}\left(\omega^{\Sigma}_{nm}\right)_{;k^{\mathrm{c}}}, \tag{6}$$

and work the time-reversal on each term. The first term is reduced to

$$\begin{aligned}
\frac{r^{\mathrm{LDA,b}}_{nm}}{(\omega^{\Sigma}_{nm})^2}\left(\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}\right)_{;k^{\mathrm{c}}}|_{\mathbf{k}} + \frac{r^{\mathrm{LDA,b}}_{nm}}{(\omega^{\Sigma}_{nm})^2}\left(\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}\right)_{;k^{\mathrm{c}}}|_{-\mathbf{k}} &= \frac{r^{\mathrm{LDA,b}}_{nm}}{(\omega^{\Sigma}_{nm})^2}\left(\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}\right)_{;k^{\mathrm{c}}}|_{\mathbf{k}} + \frac{r^{\mathrm{LDA,b}}_{mn}}{(\omega^{\Sigma}_{nm})^2}\left(\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{nm}\right)_{;k^{\mathrm{c}}}|_{\mathbf{k}} \\
&= \frac{1}{(\omega^{\Sigma}_{nm})^2}\left[r^{\mathrm{LDA,b}}_{nm}\left(\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}\right)_{;k^{\mathrm{c}}} + \left(r^{\mathrm{LDA,b}}_{nm}\left(\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}\right)_{;k^{\mathrm{c}}}\right)^*\right] \\
&= \frac{2}{(\omega^{\Sigma}_{nm})^2}\mathrm{Re}\left[r^{\mathrm{LDA,b}}_{nm}\left(\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}\right)_{;k^{\mathrm{c}}}\right],
\end{aligned} \tag{7}$$

the second term is reduced to

$$\begin{aligned}
\frac{\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}}{(\omega^{\Sigma}_{nm})^2}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}|_{\mathbf{k}} + \frac{\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}}{(\omega^{\Sigma}_{nm})^2}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}|_{-\mathbf{k}} &= \frac{\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}}{(\omega^{\Sigma}_{nm})^2}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}|_{\mathbf{k}} + \frac{\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{nm}}{(\omega^{\Sigma}_{nm})^2}\left(r^{\mathrm{LDA,b}}_{mn}\right)_{;k^{\mathrm{c}}}|_{\mathbf{k}} \\
&= \frac{1}{(\omega^{\Sigma}_{nm})^2}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}} + \left(\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}\right)^*\right] \\
&= \frac{2}{(\omega^{\Sigma}_{nm})^2}\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}\right],
\end{aligned} \tag{8}$$

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

$$\begin{aligned}
\frac{2\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{LDA,b}}_{nm}}{(\omega^{\Sigma}_{nm})^3}\left(\omega^{\Sigma}_{nm}\right)_{;k^{\mathrm{c}}}|_{\mathbf{k}} + \frac{2\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{LDA,b}}_{nm}}{(\omega^{\Sigma}_{nm})^3}\left(\omega^{\Sigma}_{nm}\right)_{;k^{\mathrm{c}}}|_{-\mathbf{k}} &= \frac{2\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{LDA,b}}_{nm}}{(\omega^{\Sigma}_{nm})^3}\Delta^{\mathrm{c}}_{nm}|_{\mathbf{k}} + \frac{2\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{LDA,b}}_{nm}}{(\omega^{\Sigma}_{nm})^3}\Delta^{\mathrm{c}}_{nm}|_{-\mathbf{k}} \\
&= \frac{2\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{nm} r^{\mathrm{LDA,b}}_{mn}}{(\omega^{\Sigma}_{nm})^3}\Delta^{\mathrm{c}}_{nm}|_{\mathbf{k}} + \frac{2\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{LDA,b}}_{nm}}{(\omega^{\Sigma}_{nm})^3}\Delta^{\mathrm{c}}_{nm}|_{\mathbf{k}} \\
&= \frac{2}{(\omega^{\Sigma}_{nm})^3}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{nm} r^{\mathrm{LDA,b}}_{mn} + \left(\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{nm} r^{\mathrm{LDA,b}}_{mn}\right)^*\right]\Delta^{\mathrm{c}}_{nm} \\
&= \frac{4}{(\omega^{\Sigma}_{nm})^3}\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{nm} r^{\mathrm{LDA,b}}_{mn}\right]\Delta^{\mathrm{c}}_{nm}.
\end{aligned} \tag{9}$$

Combining the results from (7), (8), and (9) into (6),

$$\begin{aligned}
&\frac{f_{mn}}{2}\left[\left(\frac{\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{LDA,b}}_{nm}}{(\omega^{\Sigma}_{nm})^2}\right)_{;k^{\mathrm{c}}}|_{\mathbf{k}} + \left(\frac{\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{LDA,b}}_{nm}}{(\omega^{\Sigma}_{nm})^2}\right)_{;k^{\mathrm{c}}}|_{-\mathbf{k}}\right]\frac{1}{\omega^{\Sigma}_{nm} - \tilde{\omega}} = \\
&\left(2\,\mathrm{Re}\left[r^{\mathrm{LDA,b}}_{nm}\left(\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}\right)_{;k^{\mathrm{c}}}\right] + 2\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}\right] - \frac{4}{\omega^{\Sigma}_{nm}}\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{nm} r^{\mathrm{LDA,b}}_{mn}\right]\Delta^{\mathrm{c}}_{nm}\right)\frac{f_{mn}}{2(\omega^{\Sigma}_{nm})^2}\frac{1}{\omega^{\Sigma}_{nm} - \tilde{\omega}}.
\end{aligned} \tag{10}$$

We substitute (3), (4), and (10) in (1),

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

If we simplify,

$$
\begin{aligned}
I = &-\frac{2f_{mn}\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}\right]}{2(\omega^{\Sigma}_{nm})^2}\frac{1}{\omega^{\Sigma}_{nm}-\tilde{\omega}} + \frac{4f_{mn}\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}\right]}{(\omega^{\Sigma}_{nm})^2}\frac{1}{\omega^{\Sigma}_{nm}-2\tilde{\omega}}\\
&+\frac{6f_{mn}\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}r^{\mathrm{LDA,b}}_{nm}\right]\Delta^{\mathrm{c}}_{nm}}{2(\omega^{\Sigma}_{nm})^3}\frac{1}{\omega^{\Sigma}_{nm}-\tilde{\omega}} - \frac{8f_{mn}\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}r^{\mathrm{LDA,b}}_{nm}\right]\Delta^{\mathrm{c}}_{nm}}{(\omega^{\Sigma}_{nm})^3}\frac{1}{\omega^{\Sigma}_{nm}-2\tilde{\omega}}\\
&+\frac{2f_{mn}\,\mathrm{Re}\left[r^{\mathrm{LDA,b}}_{nm}\left(\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}\right)_{;k^{\mathrm{c}}}\right]}{2(\omega^{\Sigma}_{nm})^2}\frac{1}{\omega^{\Sigma}_{nm}-\tilde{\omega}}\\
&+\frac{2f_{mn}\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}\right]}{2(\omega^{\Sigma}_{nm})^2}\frac{1}{\omega^{\Sigma}_{nm}-\tilde{\omega}}\\
&-\frac{4f_{mn}\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{nm}r^{\mathrm{LDA,b}}_{mn}\right]\Delta^{\mathrm{c}}_{nm}}{2(\omega^{\Sigma}_{nm})^3}\frac{1}{\omega^{\Sigma}_{nm}-\tilde{\omega}},
\end{aligned}
\tag{11}
$$

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 above equation

$$
\begin{aligned}
I_{2\omega} &= -\frac{e^3}{\hbar^2}\sum_{mn\mathbf{k}}\left[\frac{4f_{mn}\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}\right]}{(\omega^{\Sigma}_{nm})^2} - \frac{8f_{mn}\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}r^{\mathrm{LDA,b}}_{nm}\right]\Delta^{\mathrm{c}}_{nm}}{(\omega^{\Sigma}_{nm})^3}\right]\frac{1}{\omega^{\Sigma}_{nm}-2\tilde{\omega}}\\
&= -\frac{e^3}{\hbar^2}\sum_{mn\mathbf{k}}\frac{4f_{mn}}{(\omega^{\Sigma}_{nm})^2}\left[\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}\right] - \frac{2\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}r^{\mathrm{LDA,b}}_{nm}\right]\Delta^{\mathrm{c}}_{nm}}{\omega^{\Sigma}_{nm}}\right]\frac{1}{\omega^{\Sigma}_{nm}-2\tilde{\omega}}.
\end{aligned}
\tag{12}
$$

We can express the energies in terms of transitions between bands. Therefore, $\omega^{\Sigma}_{nm}=\omega^{\Sigma}_{cv}$ for transitions between conduction and valence bands. To take the limit $\eta\to 0$, we use

$$
\lim_{\eta\to 0}\frac{1}{x\pm i\eta} = P\frac{1}{x}\mp i\pi\delta(x),
\tag{13}
$$

and can finally rewrite (12) in the desired form,

$$
\mathrm{Im}[\chi^{s,\ell}_{i,\mathrm{a},\ell\mathrm{bc},2\omega}] = -\frac{\pi|e|^3}{2\hbar^2}\sum_{vc\mathbf{k}}\frac{4}{(\omega^{\Sigma}_{cv})^2}\left(\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{vc}\left(r^{\mathrm{LDA,b}}_{cv}\right)_{;k^{\mathrm{c}}}\right] - \frac{2\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{vc}r^{\mathrm{LDA,b}}_{cv}\right]\Delta^{\mathrm{c}}_{cv}}{\omega^{\Sigma}_{cv}}\right)\delta(\omega^{\Sigma}_{cv}-2\omega).
\tag{14}
$$

where we added a $1/2$ from the sum over $\mathbf{k}\to-\mathbf{k}$. We do the same for the $\tilde{\omega}$ terms in (11) to obtain

$$
\begin{aligned}
I_{\omega} = -\frac{e^3}{2\hbar^2}\sum_{nm\mathbf{k}}\Bigg[&-\frac{2f_{mn}\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}\right]}{(\omega^{\Sigma}_{nm})^2} + \frac{6f_{mn}\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}r^{\mathrm{LDA,b}}_{nm}\right]\Delta^{\mathrm{c}}_{nm}}{(\omega^{\Sigma}_{nm})^3}\\
&+\frac{2f_{mn}\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}\left(r^{\mathrm{LDA,b}}_{nm}\right)_{;k^{\mathrm{c}}}\right]}{(\omega^{\Sigma}_{nm})^2} - \frac{4f_{mn}\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{nm}r^{\mathrm{LDA,b}}_{mn}\right]\Delta^{\mathrm{c}}_{nm}}{(\omega^{\Sigma}_{nm})^3}\\
&+\frac{2f_{mn}\,\mathrm{Re}\left[r^{\mathrm{LDA,b}}_{nm}\left(\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}\right)_{;k^{\mathrm{c}}}\right]}{(\omega^{\Sigma}_{nm})^2}\Bigg]\frac{1}{\omega^{\Sigma}_{nm}-\tilde{\omega}}.
\end{aligned}
\tag{15}
$$

We reduce in the same way as (12),

$$
I_{\omega} = -\frac{e^3}{2\hbar^2}\sum_{nm\mathbf{k}}\frac{f_{mn}}{(\omega^{\Sigma}_{nm})^2}\left[2\,\mathrm{Re}\left[r^{\mathrm{LDA,b}}_{nm}\left(\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}\right)_{;k^{\mathrm{c}}}\right] + \frac{2\,\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}r^{\mathrm{LDA,b}}_{nm}\right]\Delta^{\mathrm{c}}_{nm}}{\omega^{\Sigma}_{nm}}\right]\frac{1}{\omega^{\Sigma}_{nm}-\tilde{\omega}},
\tag{16}
$$

and using (13) we obtain our final form,

$$
\mathrm{Im}[\chi^{s,\ell}_{i,\mathrm{a},\ell\mathrm{bc},\omega}] = -\frac{\pi|e|^3}{2\hbar^2}\sum_{cv}\frac{1}{(\omega^{\Sigma}_{cv})^2}\left(\mathrm{Re}\left[r^{\mathrm{LDA,b}}_{cv}\left(\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{vc}\right)_{;k^{\mathrm{c}}}\right] + \frac{\mathrm{Re}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{vc}r^{\mathrm{LDA,b}}_{cv}\right]\Delta^{\mathrm{c}}_{cv}}{\omega^{\Sigma}_{cv}}\right)\delta(\omega^{\Sigma}_{cv}-\omega),
\tag{17}
$$

where again we added a $1/2$ from the sum over $\mathbf{k}\to-\mathbf{k}$.

B. Interband Contributions

We follow an equivalent procedure for the interband contribution. From Eq. (**??**) we have

$$\begin{aligned} E = A &\left[-\frac{1}{2\omega^\Sigma_{lm}(2\omega^\Sigma_{lm}-\omega^\Sigma_{nm})}\frac{1}{\omega^\Sigma_{lm}-\tilde\omega}+\frac{2}{\omega^\Sigma_{nm}(2\omega^\Sigma_{lm}-\omega^\Sigma_{nm})}\frac{1}{\omega^\Sigma_{nm}-2\tilde\omega}+\frac{1}{2\omega^\Sigma_{lm}\omega^\Sigma_{nm}}\frac{1}{\tilde\omega}\right] \\ - B &\left[-\frac{1}{2\omega^\Sigma_{nl}(2\omega^\Sigma_{nl}-\omega^\Sigma_{nm})}\frac{1}{\omega^\Sigma_{nl}-\tilde\omega}+\frac{2}{\omega^\Sigma_{nm}(2\omega^\Sigma_{nl}-\omega^\Sigma_{nm})}\frac{1}{\omega^\Sigma_{nm}-2\tilde\omega}+\frac{1}{2\omega^\Sigma_{nl}\omega^\Sigma_{nm}}\frac{1}{\tilde\omega}\right], \end{aligned} \tag{18}$$

where $A = f_{ml}\mathcal{V}^{\Sigma,\mathrm{a}}_{mn} r^{\mathrm{c}}_{nl} r^{\mathrm{b}}_{lm}$ and $B = f_{ln}\mathcal{V}^{\Sigma,\mathrm{a}}_{mn} r^{\mathrm{b}}_{nl} r^{\mathrm{c}}_{lm}$.

Just as above, the $\frac{1}{\tilde\omega}$ terms cancel out. We multiply out the A and B terms,

$$\begin{aligned} E = &\left[-\frac{A}{2\omega^\Sigma_{lm}(2\omega^\Sigma_{lm}-\omega^\Sigma_{nm})}\frac{1}{\omega^\Sigma_{lm}-\tilde\omega}+\frac{2A}{\omega^\Sigma_{nm}(2\omega^\Sigma_{lm}-\omega^\Sigma_{nm})}\frac{1}{\omega^\Sigma_{nm}-2\tilde\omega}\right] \\ + &\left[\frac{B}{2\omega^\Sigma_{nl}(2\omega^\Sigma_{nl}-\omega^\Sigma_{nm})}\frac{1}{\omega^\Sigma_{nl}-\tilde\omega}-\frac{2B}{\omega^\Sigma_{nm}(2\omega^\Sigma_{nl}-\omega^\Sigma_{nm})}\frac{1}{\omega^\Sigma_{nm}-2\tilde\omega}\right]. \end{aligned} \tag{19}$$

As before, we notice that the energy denominators are invariant under $\mathbf{k}\to-\mathbf{k}$ so we need only look at the numerators. Starting with A,

$$\begin{aligned} A \to f_{ml}\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{c}}_{nl} r^{\mathrm{b}}_{lm}|_{\mathbf{k}} &+ f_{ml}\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{c}}_{nl} r^{\mathrm{b}}_{lm}|_{-\mathbf{k}} \\ &= f_{ml}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{c}}_{nl} r^{\mathrm{b}}_{lm}|_{\mathbf{k}} + \left(-\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{nm}\right) r^{\mathrm{c}}_{ln} r^{\mathrm{b}}_{ml}|_{\mathbf{k}}\right] \\ &= f_{ml}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{c}}_{nl} r^{\mathrm{b}}_{lm} - \mathcal{V}^{\Sigma,\mathrm{a},\ell}_{nm} r^{\mathrm{c}}_{ln} r^{\mathrm{b}}_{ml}\right] \\ &= f_{ml}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{c}}_{nl} r^{\mathrm{b}}_{lm} - \left(\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{c}}_{nl} r^{\mathrm{b}}_{lm}\right)^*\right] \\ &= -2f_{ml}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{c}}_{nl} r^{\mathrm{b}}_{lm}\right], \end{aligned}$$

then B,

$$\begin{aligned} B \to f_{ln}\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{b}}_{nl} r^{\mathrm{c}}_{lm}|_{\mathbf{k}} &+ f_{ln}\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{b}}_{nl} r^{\mathrm{c}}_{lm}|_{-\mathbf{k}} \\ &= f_{ln}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{b}}_{nl} r^{\mathrm{c}}_{lm}|_{\mathbf{k}} + \left(-\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{nm}\right) r^{\mathrm{b}}_{ln} r^{\mathrm{c}}_{ml}|_{\mathbf{k}}\right] \\ &= f_{ln}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{b}}_{nl} r^{\mathrm{c}}_{lm} - \mathcal{V}^{\Sigma,\mathrm{a},\ell}_{nm} r^{\mathrm{b}}_{ln} r^{\mathrm{c}}_{ml}\right] \\ &= f_{ln}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{b}}_{nl} r^{\mathrm{c}}_{lm} - \left(\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{b}}_{nl} r^{\mathrm{c}}_{lm}\right)^*\right] \\ &= -2f_{ln}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{b}}_{nl} r^{\mathrm{c}}_{lm}\right]. \end{aligned}$$

We then substitute in (19),

$$\begin{aligned} E = \Bigg[&\frac{2f_{ml}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{c}}_{nl} r^{\mathrm{b}}_{lm}\right]}{2\omega^\Sigma_{lm}(2\omega^\Sigma_{lm}-\omega^\Sigma_{nm})}\frac{1}{\omega^\Sigma_{lm}-\tilde\omega}-\frac{4f_{ml}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{c}}_{nl} r^{\mathrm{b}}_{lm}\right]}{\omega^\Sigma_{nm}(2\omega^\Sigma_{lm}-\omega^\Sigma_{nm})}\frac{1}{\omega^\Sigma_{nm}-2\tilde\omega} \\ &-\frac{2f_{ln}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{b}}_{nl} r^{\mathrm{c}}_{lm}\right]}{2\omega^\Sigma_{nl}(2\omega^\Sigma_{nl}-\omega^\Sigma_{nm})}\frac{1}{\omega^\Sigma_{nl}-\tilde\omega}+\frac{4f_{ln}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{b}}_{nl} r^{\mathrm{c}}_{lm}\right]}{\omega^\Sigma_{nm}(2\omega^\Sigma_{nl}-\omega^\Sigma_{nm})}\frac{1}{\omega^\Sigma_{nm}-2\tilde\omega}\Bigg]. \end{aligned}$$

We manipulate indices and simplify,

$$\begin{aligned} E &= \left[\frac{f_{ml}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{c}}_{nl} r^{\mathrm{b}}_{lm}\right]}{\omega^\Sigma_{lm}(2\omega^\Sigma_{lm}-\omega^\Sigma_{nm})}\frac{1}{\omega^\Sigma_{lm}-\tilde\omega}-\frac{f_{ln}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{b}}_{nl} r^{\mathrm{c}}_{lm}\right]}{\omega^\Sigma_{nl}(2\omega^\Sigma_{nl}-\omega^\Sigma_{nm})}\frac{1}{\omega^\Sigma_{nl}-\tilde\omega}\right] \\ &\quad+\left[\frac{f_{ln}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{b}}_{nl} r^{\mathrm{c}}_{lm}\right]}{2\omega^\Sigma_{nl}-\omega^\Sigma_{nm}}-\frac{f_{ml}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{c}}_{nl} r^{\mathrm{b}}_{lm}\right]}{2\omega^\Sigma_{lm}-\omega^\Sigma_{nm}}\right]\frac{4}{\omega^\Sigma_{nm}}\frac{1}{\omega^\Sigma_{nm}-2\tilde\omega} \\ &= \left[\frac{f_{mn}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{ml} r^{\mathrm{c}}_{ln} r^{\mathrm{b}}_{nm}\right]}{2\omega^\Sigma_{nm}-\omega^\Sigma_{lm}}-\frac{f_{mn}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{ln} r^{\mathrm{b}}_{nm} r^{\mathrm{c}}_{ml}\right]}{2\omega^\Sigma_{nm}-\omega^\Sigma_{nl}}\right]\frac{1}{\omega^\Sigma_{nm}}\frac{1}{\omega^\Sigma_{nm}-\tilde\omega} \\ &\quad+\left[\frac{f_{ln}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{b}}_{nl} r^{\mathrm{c}}_{lm}\right]}{2\omega^\Sigma_{nl}-\omega^\Sigma_{nm}}-\frac{f_{ml}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn} r^{\mathrm{c}}_{nl} r^{\mathrm{b}}_{lm}\right]}{2\omega^\Sigma_{lm}-\omega^\Sigma_{nm}}\right]\frac{4}{\omega^\Sigma_{nm}}\frac{1}{\omega^\Sigma_{nm}-2\tilde\omega}, \end{aligned}$$

and substitute in (??),

$$I=-\frac{e^3}{2\hbar^2}\sum_{nm}\frac{1}{\omega^\Sigma_{nm}}\left[\frac{f_{mn}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{ml}\{r^{\mathrm{c}}_{ln}r^{\mathrm{b}}_{nm}\}\right]}{2\omega^\Sigma_{nm}-\omega^\Sigma_{lm}}-\frac{f_{mn}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{ln}\{r^{\mathrm{b}}_{nm}r^{\mathrm{c}}_{ml}\}\right]}{2\omega^\Sigma_{nm}-\omega^\Sigma_{nl}}\right]\frac{1}{\omega^\Sigma_{nm}-\tilde\omega}$$
$$+4\left[\frac{f_{ln}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}\{r^{\mathrm{b}}_{nl}r^{\mathrm{c}}_{lm}\}\right]}{2\omega^\Sigma_{nl}-\omega^\Sigma_{nm}}-\frac{f_{ml}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{mn}\{r^{\mathrm{c}}_{nl}r^{\mathrm{b}}_{lm}\}\right]}{2\omega^\Sigma_{lm}-\omega^\Sigma_{nm}}\right]\frac{1}{\omega^\Sigma_{nm}-2\tilde\omega}.$$

Finally, we take $n=c$, $m=v$, and $l=q$ and substitute,

$$\begin{aligned}I=&-\frac{e^3}{2\hbar^2}\sum_{cv}\frac{1}{\omega^\Sigma_{cv}}\left(\left[\frac{f_{vc}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{vq}\{r^{\mathrm{c}}_{qc}r^{\mathrm{b}}_{cv}\}\right]}{2\omega^\Sigma_{cv}-\omega^\Sigma_{qv}}-\frac{f_{vc}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{qc}\{r^{\mathrm{b}}_{cv}r^{\mathrm{c}}_{vq}\}\right]}{2\omega^\Sigma_{cv}-\omega^\Sigma_{cq}}\right]\frac{1}{\omega^\Sigma_{cv}-\tilde\omega}\right.\\&\left.+4\left[\frac{f_{qc}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{vc}\{r^{\mathrm{b}}_{cq}r^{\mathrm{c}}_{qv}\}\right]}{2\omega^\Sigma_{cq}-\omega^\Sigma_{cv}}-\frac{f_{vq}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{vc}\{r^{\mathrm{c}}_{cq}r^{\mathrm{b}}_{qv}\}\right]}{2\omega^\Sigma_{qv}-\omega^\Sigma_{cv}}\right]\frac{1}{\omega^\Sigma_{cv}-2\tilde\omega}\right)\\=&\frac{e^3}{2\hbar^2}\sum_{cv}\frac{1}{\omega^\Sigma_{cv}}\left(\left[\frac{\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{qc}\{r^{\mathrm{b}}_{cv}r^{\mathrm{c}}_{vq}\}\right]}{2\omega^\Sigma_{cv}-\omega^\Sigma_{cq}}-\frac{\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{vq}\{r^{\mathrm{c}}_{qc}r^{\mathrm{b}}_{cv}\}\right]}{2\omega^\Sigma_{cv}-\omega^\Sigma_{qv}}\right]\frac{1}{\omega^\Sigma_{cv}-\tilde\omega}\right.\\&\left.-4\left[\frac{f_{qc}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{vc}\{r^{\mathrm{b}}_{cq}r^{\mathrm{c}}_{qv}\}\right]}{2\omega^\Sigma_{cq}-\omega^\Sigma_{cv}}-\frac{f_{vq}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{vc}\{r^{\mathrm{c}}_{cq}r^{\mathrm{b}}_{qv}\}\right]}{2\omega^\Sigma_{qv}-\omega^\Sigma_{cv}}\right]\frac{1}{\omega^\Sigma_{cv}-2\tilde\omega}\right).\end{aligned}$$

We use (13),

$$\begin{aligned}I=&\frac{\pi|e^3|}{2\hbar^2}\sum_{cv}\frac{1}{\omega^\Sigma_{cv}}\left(\left[\frac{\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{qc}\{r^{\mathrm{b}}_{cv}r^{\mathrm{c}}_{vq}\}\right]}{2\omega^\Sigma_{cv}-\omega^\Sigma_{cq}}-\frac{\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{vq}\{r^{\mathrm{c}}_{qc}r^{\mathrm{b}}_{cv}\}\right]}{2\omega^\Sigma_{cv}-\omega^\Sigma_{qv}}\right]\delta(\omega^\Sigma_{cv}-\omega)\right.\\&\left.-4\left[\frac{f_{qc}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{vc}\{r^{\mathrm{b}}_{cq}r^{\mathrm{c}}_{qv}\}\right]}{2\omega^\Sigma_{cq}-\omega^\Sigma_{cv}}-\frac{f_{vq}\,\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{vc}\{r^{\mathrm{c}}_{cq}r^{\mathrm{b}}_{qv}\}\right]}{2\omega^\Sigma_{qv}-\omega^\Sigma_{cv}}\right]\delta(\omega^\Sigma_{cv}-2\omega)\right),\end{aligned}$$

and recognize that for the 1ω terms, $q\neq(v,c)$, and for the 2ω q can have two distinct values such that,

$$\begin{aligned}I=&\frac{\pi|e^3|}{2\hbar^2}\sum_{cv}\frac{1}{\omega^\Sigma_{cv}}\left(\sum_{q\neq(v,c)}\left[\frac{\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{qc}\{r^{\mathrm{b}}_{cv}r^{\mathrm{c}}_{vq}\}\right]}{2\omega^\Sigma_{cv}-\omega^\Sigma_{cq}}-\frac{\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{vq}\{r^{\mathrm{c}}_{qc}r^{\mathrm{b}}_{cv}\}\right]}{2\omega^\Sigma_{cv}-\omega^\Sigma_{qv}}\right]\delta(\omega^\Sigma_{cv}-\omega)\right.\\&\left.-4\left[\sum_{v'\neq v}\frac{\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{vc}\{r^{\mathrm{b}}_{cv'}r^{\mathrm{c}}_{v'v}\}\right]}{2\omega^\Sigma_{cv'}-\omega^\Sigma_{cv}}-\sum_{c'\neq c}\frac{\mathrm{Im}\left[\mathcal{V}^{\Sigma,\mathrm{a},\ell}_{vc}\{r^{\mathrm{c}}_{cc'}r^{\mathrm{b}}_{c'v}\}\right]}{2\omega^\Sigma_{c'v}-\omega^\Sigma_{cv}}\right]\delta(\omega^\Sigma_{cv}-2\omega)\right).\end{aligned}$$

[1] N. W. Ashcroft and N. D. Mermin. *Solid State Physics*. Brooks Cole, Saunders College, Philadelphia, 1976.