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

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

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,

$$I = C \left[-\frac{1}{2(\omega_{nm}^S)^2} \frac{1}{\omega_{nm}^S - \omega} + \frac{2}{(\omega_{nm}^S)^2} \frac{1}{\omega_{nm}^S - 2\omega} + \frac{1}{2(\omega_{nm}^S)^2} \frac{1}{\omega} \right] - D \left[-\frac{3}{2(\omega_{nm}^S)^3} \frac{1}{\omega_{nm}^S - \omega} + \frac{4}{(\omega_{nm}^S)^3} \frac{1}{\omega_{nm}^S - 2\omega} + \frac{1}{2(\omega_{nm}^S)^3} \frac{1}{\omega} - \frac{1}{2(\omega_{nm}^S)^2} \frac{1}{(\omega_{nm}^S)^2} \frac{1}{(\omega_{nm}^S - \omega)^2} \right],$$
 (2)

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

Time-reversal symmetry leads to the following relationships:

$$\mathbf{r}_{mn}(\mathbf{k})|_{-\mathbf{k}} = \mathbf{r}_{nm}(\mathbf{k})|_{\mathbf{k}},$$

$$(\mathbf{r}_{mn})_{;\mathbf{k}}(\mathbf{k})|_{-\mathbf{k}} = (-\mathbf{r}_{nm})_{;\mathbf{k}}(\mathbf{k})|_{\mathbf{k}},$$

$$\mathcal{V}_{mn}^{\Sigma,\mathbf{a}}(\mathbf{k})|_{-\mathbf{k}} = -\mathcal{V}_{nm}^{\Sigma,\mathbf{a}}(\mathbf{k})|_{\mathbf{k}},$$

$$(\mathcal{V}_{mn}^{\Sigma,\mathbf{a}})_{;\mathbf{k}}(\mathbf{k})|_{-\mathbf{k}} = (\mathcal{V}_{nm}^{\Sigma,\mathbf{a}})_{;\mathbf{k}}(\mathbf{k})|_{\mathbf{k}},$$

$$\omega_{mn}^{S}(\mathbf{k})|_{-\mathbf{k}} = \omega_{mn}^{S}(\mathbf{k})|_{\mathbf{k}},$$

$$\Delta_{nm}^{a}(\mathbf{k})|_{-\mathbf{k}} = -\Delta_{nm}^{a}(\mathbf{k})|_{\mathbf{k}}.$$
(3)

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

$$C \to f_{mn} \mathcal{V}_{mn}^{\Sigma,a} \left(r_{nm}^{\text{LDA,b}} \right)_{;k^{c}} |_{\mathbf{k}} + f_{mn} \mathcal{V}_{mn}^{\Sigma,a} \left(r_{nm}^{\text{LDA,b}} \right)_{;k^{c}} |_{-\mathbf{k}}$$

$$= f_{mn} \left[\mathcal{V}_{mn}^{\Sigma,a} \left(r_{nm}^{\text{LDA,b}} \right)_{;k^{c}} |_{\mathbf{k}} + \left(-\mathcal{V}_{nm}^{\Sigma,a} \right) \left(-r_{mn}^{\text{LDA,b}} \right)_{;k^{c}} |_{\mathbf{k}} \right]$$

$$= f_{mn} \left[\mathcal{V}_{mn}^{\Sigma,a} \left(r_{nm}^{\text{LDA,b}} \right)_{;k^{c}} + \mathcal{V}_{nm}^{\Sigma,a} \left(r_{mn}^{\text{LDA,b}} \right)_{;k^{c}} \right]$$

$$= f_{mn} \left[\mathcal{V}_{mn}^{\Sigma,a} \left(r_{nm}^{\text{LDA,b}} \right)_{;k^{c}} + \left(\mathcal{V}_{mn}^{\Sigma,a} \left(r_{nm}^{\text{LDA,b}} \right)_{;k^{c}} \right)^{*} \right]$$

$$= 2f_{mn} \operatorname{Re} \left[\mathcal{V}_{mn}^{\Sigma,a} \left(r_{nm}^{\text{LDA,b}} \right)_{;k^{c}} \right], \tag{4}$$

and likewise,

$$D \to f_{mn} \mathcal{V}_{mn}^{\Sigma, \mathbf{a}} r_{nm}^{\mathrm{LDA}, \mathbf{b}} \Delta_{nm}^{\mathbf{c}}|_{\mathbf{k}} + f_{mn} \mathcal{V}_{mn}^{\Sigma, \mathbf{a}} r_{nm}^{\mathrm{LDA}, \mathbf{b}} \Delta_{nm}^{\mathbf{c}}|_{-\mathbf{k}}$$

$$= f_{mn} \left[\mathcal{V}_{mn}^{\Sigma, \mathbf{a}} r_{nm}^{\mathrm{LDA}, \mathbf{b}} \Delta_{nm}^{\mathbf{c}}|_{\mathbf{k}} + \left(-\mathcal{V}_{nm}^{\Sigma, \mathbf{a}} \right) r_{mn}^{\mathrm{LDA}, \mathbf{b}} \left(-\Delta_{nm}^{\mathbf{c}} \right) |_{\mathbf{k}} \right]$$

$$= f_{mn} \left[\mathcal{V}_{mn}^{\Sigma, \mathbf{a}} r_{nm}^{\mathrm{LDA}, \mathbf{b}} + \mathcal{V}_{nm}^{\Sigma, \mathbf{a}} r_{mn}^{\mathrm{LDA}, \mathbf{b}} \right] \Delta_{nm}^{\mathbf{c}}$$

$$= f_{mn} \left[\mathcal{V}_{mn}^{\Sigma, \mathbf{a}} r_{nm}^{\mathrm{LDA}, \mathbf{b}} + \left(\mathcal{V}_{mn}^{\Sigma, \mathbf{a}} r_{nm}^{\mathrm{LDA}, \mathbf{b}} \right)^* \right] \Delta_{nm}^{\mathbf{c}}$$

$$= 2 f_{mn} \operatorname{Re} \left[\mathcal{V}_{mn}^{\Sigma, \mathbf{a}} r_{nm}^{\mathrm{LDA}, \mathbf{b}} \right] \Delta_{nm}^{\mathbf{c}}. \tag{5}$$

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

$$\frac{D}{2(\omega_{nm}^S)^2} \frac{1}{(\omega_{nm}^S - \omega)^2} = \frac{f_{mn}}{2} \frac{\mathcal{V}_{mn}^{\Sigma,a} r_{nm}^{\text{LDA,b}}}{(\omega_{nm}^S)^2} \frac{\Delta_{nm}^c}{(\omega_{nm}^S - \omega)^2} = \frac{f_{mn}}{2} \frac{\mathcal{V}_{mn}^{\Sigma,a} r_{nm}^{\text{LDA,b}}}{(\omega_{nm}^S)^2} \left(\frac{1}{\omega_{nm}^S - \omega}\right)_{;k^c} \\
= -\frac{f_{mn}}{2} \left(\frac{\mathcal{V}_{mn}^{\Sigma,a} r_{nm}^{\text{LDA,b}}}{(\omega_{nm}^S)^2}\right)_{:k^c} \frac{1}{\omega_{nm}^S - \omega}.$$
(6)

We use the fact that

$$(\omega_{nm}^S)_{;k^c} = (\omega_{nm}^{LDA})_{;k^c} = \frac{p_{nn}^c - p_{mm}^c}{m_e} \equiv \Delta_{nm}^c,$$
 (7)

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

$$\left(\frac{\mathcal{V}_{mn}^{\Sigma, \mathbf{a}} r_{nm}^{\text{LDA,b}}}{(\omega_{nm}^{S})^{2}}\right)_{.k^{c}} = \frac{r_{nm}^{\text{LDA,b}}}{(\omega_{nm}^{S})^{2}} \left(\mathcal{V}_{mn}^{\Sigma, \mathbf{a}}\right)_{;k^{c}} + \frac{\mathcal{V}_{mn}^{\Sigma, \mathbf{a}}}{(\omega_{nm}^{S})^{2}} \left(r_{nm}^{\text{LDA,b}}\right)_{;k^{c}} - \frac{\mathcal{V}_{mn}^{\Sigma, \mathbf{a}} r_{nm}^{\text{LDA,b}}}{2(\omega_{nm}^{S})^{3}} \left(\omega_{nm}^{S}\right)_{;k^{c}}.$$
(8)

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

$$\frac{r_{nm}^{\text{LDA,b}}}{(\omega_{nm}^{S})^{2}} \left(\mathcal{V}_{mn}^{\Sigma,a} \right)_{;k^{c}} |_{\mathbf{k}} + \frac{r_{nm}^{\text{LDA,b}}}{(\omega_{nm}^{S})^{2}} \left(\mathcal{V}_{mn}^{\Sigma,a} \right)_{;k^{c}} |_{-\mathbf{k}} = \frac{r_{nm}^{\text{LDA,b}}}{(\omega_{nm}^{S})^{2}} \left(\mathcal{V}_{mn}^{\Sigma,a} \right)_{;k^{c}} |_{\mathbf{k}} + \frac{r_{mn}^{\text{LDA,b}}}{(\omega_{nm}^{S})^{2}} \left(\mathcal{V}_{nm}^{\Sigma,a} \right)_{;k^{c}} |_{\mathbf{k}}$$

$$= \frac{1}{(\omega_{nm}^{S})^{2}} \left[r_{nm}^{\text{LDA,b}} \left(\mathcal{V}_{mn}^{\Sigma,a} \right)_{;k^{c}} + \left(r_{nm}^{\text{LDA,b}} \left(\mathcal{V}_{mn}^{\Sigma,a} \right)_{;k^{c}} \right)^{*} \right]$$

$$= \frac{2}{(\omega_{nm}^{S})^{2}} \text{Re} \left[r_{nm}^{\text{LDA,b}} \left(\mathcal{V}_{mn}^{\Sigma,a} \right)_{;k^{c}} \right], \tag{9}$$

the second term is reduced to

$$\frac{\mathcal{V}_{mn}^{\Sigma,a}}{(\omega_{nm}^{S})^{2}} \left(r_{nm}^{\text{LDA,b}}\right)_{;k^{c}} |_{\mathbf{k}} + \frac{\mathcal{V}_{mn}^{\Sigma,a}}{(\omega_{nm}^{S})^{2}} \left(r_{nm}^{\text{LDA,b}}\right)_{;k^{c}} |_{-\mathbf{k}} = \frac{\mathcal{V}_{mn}^{\Sigma,a}}{(\omega_{nm}^{S})^{2}} \left(r_{nm}^{\text{LDA,b}}\right)_{;k^{c}} |_{\mathbf{k}} + \frac{\mathcal{V}_{nm}^{\Sigma,a}}{(\omega_{nm}^{S})^{2}} \left(r_{mn}^{\text{LDA,b}}\right)_{;k^{c}} |_{\mathbf{k}} \\
= \frac{1}{(\omega_{nm}^{S})^{2}} \left[\mathcal{V}_{mn}^{\Sigma,a} \left(r_{nm}^{\text{LDA,b}}\right)_{;k^{c}} + \left(\mathcal{V}_{mn}^{\Sigma,a} \left(r_{nm}^{\text{LDA,b}}\right)_{;k^{c}}\right)^{*} \right] \\
= \frac{2}{(\omega_{nm}^{S})^{2}} \text{Re} \left[\mathcal{V}_{mn}^{\Sigma,a} \left(r_{nm}^{\text{LDA,b}}\right)_{;k^{c}} \right], \tag{10}$$

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

$$\frac{\mathcal{V}_{mn}^{\Sigma,a}r_{nm}^{\text{LDA},b}}{2(\omega_{nm}^{S})^{3}} \left(\omega_{nm}^{S}\right)_{;k^{c}}|_{\mathbf{k}} + \frac{\mathcal{V}_{mn}^{\Sigma,a}r_{nm}^{\text{LDA},b}}{2(\omega_{nm}^{S})^{3}} \left(\omega_{nm}^{S}\right)_{;k^{c}}|_{-\mathbf{k}} = \frac{\mathcal{V}_{mn}^{\Sigma,a}r_{nm}^{\text{LDA},b}}{2(\omega_{nm}^{S})^{3}} \Delta_{nm}^{c}|_{\mathbf{k}} + \frac{\mathcal{V}_{mn}^{\Sigma,a}r_{nm}^{\text{LDA},b}}{2(\omega_{nm}^{S})^{3}} \Delta_{nm}^{c}|_{-\mathbf{k}}$$

$$= \frac{\mathcal{V}_{nm}^{\Sigma,a}r_{mn}^{\text{LDA},b}}{2(\omega_{nm}^{S})^{3}} \Delta_{nm}^{c}|_{\mathbf{k}} + \frac{\mathcal{V}_{mn}^{\Sigma,a}r_{nm}^{\text{LDA},b}}{2(\omega_{nm}^{S})^{3}} \Delta_{nm}^{c}|_{\mathbf{k}}$$

$$= \frac{1}{2(\omega_{nm}^{S})^{3}} \left[\mathcal{V}_{nm}^{\Sigma,a}r_{mn}^{\text{LDA},b} + \left(\mathcal{V}_{nm}^{\Sigma,a}r_{mn}^{\text{LDA},b} \right)^{*} \right] \Delta_{nm}^{c}$$

$$= \frac{1}{(\omega_{nm}^{S})^{3}} \operatorname{Re} \left[\mathcal{V}_{nm}^{\Sigma,a}r_{mn}^{\text{LDA},b} \right] \Delta_{nm}^{c}.$$
(11)

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

$$-\frac{f_{mn}}{2} \left[\left(\frac{\mathcal{V}_{mn}^{\Sigma,a} r_{nm}^{\text{LDA,b}}}{(\omega_{nm}^{S})^{2}} \right)_{;k^{c}} |_{\mathbf{k}} + \left(\frac{\mathcal{V}_{mn}^{\Sigma,a} r_{nm}^{\text{LDA,b}}}{(\omega_{nm}^{S})^{2}} \right)_{;k^{c}} |_{-\mathbf{k}} \right] \frac{1}{\omega_{nm}^{S} - \omega} =$$

$$-f_{mn} \left(2\text{Re} \left[r_{nm}^{\text{LDA,b}} \left(\mathcal{V}_{mn}^{\Sigma,a} \right)_{;k^{c}} \right] + 2\text{Re} \left[\mathcal{V}_{mn}^{\Sigma,a} \left(r_{nm}^{\text{LDA,b}} \right)_{;k^{c}} \right] - \frac{1}{\omega_{nm}^{S}} \text{Re} \left[\mathcal{V}_{nm}^{\Sigma,a} r_{mn}^{\text{LDA,b}} \right] \Delta_{nm}^{c} \right) \frac{1}{2(\omega_{nm}^{S})^{2}} \frac{1}{\omega_{nm}^{S} - \omega}.$$

$$(12)$$

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

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

If we simplify and homogenize,

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

$$(13)$$

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),

$$I_{2\omega} = -\frac{e^3}{\hbar^2} \sum_{mn\mathbf{k}} \left[\frac{4f_{mn} \operatorname{Re} \left[\mathcal{V}_{mn}^{\Sigma,a} \left(r_{nm}^{\mathrm{LDA,b}} \right)_{;k^{\mathrm{c}}} \right]}{(\omega_{nm}^S)^2} - \frac{8f_{mn} \operatorname{Re} \left[\mathcal{V}_{mn}^{\Sigma,a} r_{nm}^{\mathrm{LDA,b}} \right] \Delta_{nm}^{\mathrm{c}}}{(\omega_{nm}^S)^3} \right] \frac{1}{\omega_{nm}^S - 2\omega}$$

$$= -\frac{e^3}{\hbar^2} \sum_{mn\mathbf{k}} \frac{4f_{mn}}{(\omega_{nm}^S)^2} \left[\operatorname{Re} \left[\mathcal{V}_{mn}^{\Sigma,a} \left(r_{nm}^{\mathrm{LDA,b}} \right)_{;k^{\mathrm{c}}} \right] - \frac{2 \operatorname{Re} \left[\mathcal{V}_{mn}^{\Sigma,a} r_{nm}^{\mathrm{LDA,b}} \right] \Delta_{nm}^{\mathrm{c}}}{\omega_{nm}^S} \right] \frac{1}{\omega_{nm}^S - 2\omega}. \tag{14}$$

We can express the energies in terms of transitions between bands. Therefore, $\omega_{nm}^S = \omega_{cv}^S$ 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,

$$\operatorname{Im}\left[\chi_{i,\mathrm{abc},2\omega}^{s,\ell}\right] = -\frac{\pi e^{3}}{\hbar^{2}} \sum_{mn\mathbf{k}} \frac{4}{(\omega_{nm}^{S})^{2}} \left(\operatorname{Re}\left[\mathcal{V}_{mn}^{\Sigma,a}\left(r_{nm}^{\mathrm{LDA,b}}\right)_{;k^{c}}\right] - \frac{2\operatorname{Re}\left[\mathcal{V}_{mn}^{\Sigma,a}r_{nm}^{\mathrm{LDA,b}}\right]\Delta_{nm}^{c}}{\omega_{nm}^{S}}\right) \delta(\omega_{nm}^{S} - 2\omega). \quad (16)$$

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

$$I_{\omega} = -\frac{e^{3}}{2\hbar^{2}} \sum_{mn\mathbf{k}} \left[-\frac{2f_{mn} \operatorname{Re} \left[\mathcal{V}_{mn}^{\Sigma,a} \left(r_{nm}^{\operatorname{LDA,b}} \right)_{;k^{c}} \right]}{(\omega_{nm}^{S})^{2}} + \frac{6f_{mn} \operatorname{Re} \left[\mathcal{V}_{mn}^{\Sigma,a} r_{nm}^{\operatorname{LDA,b}} \right] \Delta_{nm}^{c}}{(\omega_{nm}^{S})^{2}} \right.$$

$$\left. -\frac{2f_{mn} \operatorname{Re} \left[r_{nm}^{\operatorname{LDA,b}} \left(\mathcal{V}_{mn}^{\Sigma,a} \right)_{;k^{c}} \right]}{(\omega_{nm}^{S})^{2}} - \frac{2f_{mn} \operatorname{Re} \left[\mathcal{V}_{mn}^{\Sigma,a} \left(r_{nm}^{\operatorname{LDA,b}} \right)_{;k^{c}} \right]}{(\omega_{nm}^{S})^{2}} \right.$$

$$\left. + \frac{f_{mn} \operatorname{Re} \left[\mathcal{V}_{nm}^{\Sigma,a} r_{mn}^{\operatorname{LDA,b}} \right] \Delta_{nm}^{c}}{(\omega_{nm}^{S})^{3}} \right] \frac{1}{\omega_{nm}^{S} - \omega}, \tag{17}$$

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

I can't seem to reduce this any further. When using $\mathcal{R}_{nm}^{\mathbf{a},\ell}$ there are *i*'s that allow two terms to cancel out leaving only three. See (A17) and (A18).

$$I_{\omega} = \frac{e^{3}}{2\hbar^{2}} \sum_{mn\mathbf{k}} \frac{f_{mn}}{(\omega_{nm}^{S})^{2}} \left[2 \operatorname{Re} \left[\mathcal{V}_{mn}^{\Sigma,a} \left(r_{nm}^{\mathrm{LDA,b}} \right)_{;k^{c}} \right] \right.$$

$$\left. - 6 \operatorname{Re} \left[\mathcal{V}_{mn}^{\Sigma,a} r_{nm}^{\mathrm{LDA,b}} \right] \Delta_{nm}^{c} + 2 \operatorname{Re} \left[r_{nm}^{\mathrm{LDA,b}} \left(\mathcal{V}_{mn}^{\Sigma,a} \right)_{;k^{c}} \right] \right.$$

$$\left. + 2 \operatorname{Re} \left[\mathcal{V}_{mn}^{\Sigma,a} \left(r_{nm}^{\mathrm{LDA,b}} \right)_{;k^{c}} \right] - \frac{\operatorname{Re} \left[\mathcal{V}_{nm}^{\Sigma,a} r_{mn}^{\mathrm{LDA,b}} \right] \Delta_{nm}^{c}}{(\omega_{nm}^{S})} \right] \frac{1}{\omega_{nm}^{S} - \omega}$$

$$= \frac{e^{3}}{2\hbar^{2}} \sum_{mn\mathbf{k}} \frac{f_{mn}}{(\omega_{nm}^{S})^{2}} \left[4 \operatorname{Re} \left[\mathcal{V}_{mn}^{\Sigma,a} \left(r_{nm}^{\mathrm{LDA,b}} \right)_{;k^{c}} \right] + 2 \operatorname{Re} \left[r_{nm}^{\mathrm{LDA,b}} \left(\mathcal{V}_{mn}^{\Sigma,a} \right)_{;k^{c}} \right] \right.$$

$$\left. - 6 \operatorname{Re} \left[\mathcal{V}_{mn}^{\Sigma,a} r_{nm}^{\mathrm{LDA,b}} \right] \Delta_{nm}^{c} - \frac{\operatorname{Re} \left[\mathcal{V}_{nm}^{\Sigma,a} r_{mn}^{\mathrm{LDA,b}} \right] \Delta_{nm}^{c}}{(\omega_{nm}^{S})} \right] \frac{1}{\omega_{nm}^{S} - \omega}$$

$$(18)$$