

$$\begin{aligned}
\text{Im}[\chi_v^{abc}(-2\omega; \omega, \omega)] &= \frac{\pi|e|^3}{2\hbar^2} \int \frac{d^3k}{8\pi^3} \left[\sum_{vc} \frac{16}{(\omega_{cv}^S)^3} \left(\sum_{c'} \frac{\text{Im}[v_{vc}^{\Sigma,a} \{v_{cc'}^{\Sigma,b} v_{c'v}^{\Sigma,c}\}]}{\omega_{cv}^S - 2\omega_{c'v}^S} \right. \right. \\
&\quad \left. \left. - \sum_{v'} \frac{\text{Im}[v_{vc}^{\Sigma,a} \{v_{cv'}^{\Sigma,b} v_{v'v}^{\Sigma,c}\}]}{\omega_{cv}^S - 2\omega_{cv'}^S} \right) \delta(\omega_{cv}^S - 2\omega) \right. \\
&\quad \left. + \sum_{(vc) \neq \ell} \frac{1}{(\omega_{cv}^S)^3} \left(\frac{\text{Im}[v_{\ell c}^{\Sigma,a} \{v_{cv}^{\Sigma,b} v_{v\ell}^{\Sigma,c}\}]}{\omega_{c\ell}^S - 2\omega_{cv}^S} - \frac{\text{Im}[v_{v\ell}^{\Sigma,a} \{v_{\ell c}^{\Sigma,b} v_{cv}^{\Sigma,c}\}]}{\omega_{\ell v}^S - 2\omega_{cv}^S} \right) \delta(\omega_{cv}^S - \omega) \right. \\
&\quad \left. - \sum_{vc} \frac{1}{(\omega_{cv}^S)^3} \left(4\text{Re}[v_{vc}^{\Sigma,a} \{\mathcal{F}_{cv}^{bc}\}] \delta(\omega_{cv}^S - 2\omega) + \text{Re}[\{\mathcal{F}_{vc}^{ab} v_{cv}^{\Sigma,c}\}] \delta(\omega_{cv}^S - \omega) \right) \right]. \quad (1)
\end{aligned}$$

Let's take $\omega_n \rightarrow \omega_n + \Delta_n$ that implies $\omega_n^S \rightarrow \omega_n^S + \Delta_n$, with Δ_n the energy difference of two calculations. Then, $\omega_{nm} \rightarrow \omega_{nm} + \Delta_{nm}$ and $\omega_{nm}^S \rightarrow \omega_{nm}^S + \Delta_{nm}$, with $\Delta_{nm} = \Delta_n - \Delta_m$. Then, $\omega_{nm}^S \rightarrow \omega_{nm}^S(1 + \Delta_{nm}/\omega_{nm}^S) = \omega_{nm}^S(1 + \delta_{nm}^S)$, with $\delta_{nm}^S = \Delta_{nm}/\omega_{nm}^S$. Likewise $\omega_{nm} \rightarrow \omega_{nm}(1 + \delta_{nm})$, with $\delta_{nm} = \Delta_{nm}/\omega_{nm}$. Also, $\delta(\omega_{cv} - \omega) \rightarrow \delta(\omega_{cv} + \Delta_{cv} - \omega) \sim \delta(\omega_{cv} - \omega)$, since the difference Δ_{cv} is very small.

We expand to first order in δ_{nm} . The ω terms are

$$\begin{aligned}
\frac{1}{(\omega_{cv}^S)^3} \frac{1}{\omega_{c\ell}^S - 2\omega_{cv}^S} &\rightarrow \frac{1}{(\omega_{cv}^S(1 + \delta_{cv}^S))^3} \frac{1}{\omega_{c\ell}^S(1 + \delta_{c\ell}^S) - 2\omega_{cv}^S(1 + \delta_{cv}^S)} \\
&= \frac{1}{(\omega_{cv}^S)^3} (1 + \delta_{cv}^S)^{-3} \frac{1}{\omega_{c\ell}^S - 2\omega_{cv}^S + \Delta_{c\ell} - 2\Delta_{cv}} \\
&= \frac{1}{(\omega_{cv}^S)^3} (1 - 3\delta_{cv}^S) \frac{(1 + (\Delta_{c\ell} - 2\Delta_{cv})/(\omega_{c\ell}^S - 2\omega_{cv}^S))^{-1}}{\omega_{c\ell}^S - 2\omega_{cv}^S} \\
&= \frac{1}{(\omega_{cv}^S)^3} \frac{1}{\omega_{c\ell}^S - 2\omega_{cv}^S} (1 - 3\delta_{cv}^S) \left(1 - \frac{\Delta_{c\ell} - 2\Delta_{cv}}{\omega_{c\ell}^S - 2\omega_{cv}^S}\right) \\
&= \frac{1}{(\omega_{cv}^S)^3} \frac{1}{\omega_{c\ell}^S - 2\omega_{cv}^S} \left(1 - 3\delta_{cv}^S - \frac{\Delta_{c\ell} - 2\Delta_{cv}}{\omega_{c\ell}^S - 2\omega_{cv}^S}\right), \quad (2)
\end{aligned}$$

and

$$\frac{1}{(\omega_{cv}^S)^3} \frac{1}{\omega_{\ell v}^S - 2\omega_{cv}^S} \rightarrow \frac{1}{(\omega_{cv}^S)^3} \frac{1}{\omega_{\ell v}^S - 2\omega_{cv}^S} \left(1 - 3\frac{\Delta_{cv}}{\omega_{cv}^S} - \frac{\Delta_{\ell v} - 2\Delta_{cv}}{\omega_{\ell v}^S - 2\omega_{cv}^S}\right). \quad (3)$$

$$\begin{aligned}
\mathbf{v}_{nm}^\Sigma &= \frac{\omega_{nm}^S}{\omega_{nm}} \mathbf{v}_{nm} \\
&\rightarrow \frac{\omega_{nm}^S(1 + \delta_{nm}^S)}{\omega_{nm}(1 + \delta_{nm})} \mathbf{v}_{nm} \\
&= \frac{\omega_{nm}^S}{\omega_{nm}} \mathbf{v}_{nm} (1 + \delta_{nm}^S)(1 - \delta_{nm}) \\
&= \frac{\omega_{nm}^S}{\omega_{nm}} \mathbf{v}_{nm} (1 + \delta_{nm}^S - \delta_{nm}) \\
\mathbf{v}_{nm}^\Sigma &\rightarrow \mathbf{v}_{nm}^\Sigma (1 + \delta_{nm}^S - \delta_{nm}), \quad (4)
\end{aligned}$$

then

$$\begin{aligned} v_{\ell c}^{\Sigma,a} \{v_{cv}^{\Sigma,b} v_{v\ell}^{\Sigma,c}\} &\rightarrow v_{\ell c}^{\Sigma,a} \{v_{cv}^{\Sigma,b} v_{v\ell}^{\Sigma,c}\} (1 + \delta_{\ell c}^S - \delta_{\ell c}) (1 + \delta_{cv}^S - \delta_{cv}) (1 + \delta_{v\ell}^S - \delta_{v\ell}) \\ &\rightarrow v_{\ell c}^{\Sigma,a} \{v_{cv}^{\Sigma,b} v_{v\ell}^{\Sigma,c}\} (1 + \delta_{\ell c}^S + \delta_{cv}^S + \delta_{v\ell}^S - \delta_{\ell c} - \delta_{cv} - \delta_{v\ell}). \end{aligned} \quad (5)$$

Then,

$$\begin{aligned} \frac{1}{(\omega_{cv}^S)^3} \frac{\text{Im}[v_{\ell c}^{\Sigma,a} \{v_{cv}^{\Sigma,b} v_{v\ell}^{\Sigma,c}\}]}{\omega_{\ell c}^S - 2\omega_{cv}^S} &\rightarrow \frac{1}{(\omega_{cv}^S)^3} \frac{\text{Im}[v_{\ell c}^{\Sigma,a} \{v_{cv}^{\Sigma,b} v_{v\ell}^{\Sigma,c}\}]}{\omega_{\ell c}^S - 2\omega_{cv}^S} \left(1 - 3\delta_{cv}^S - \frac{\Delta_{\ell c} - 2\Delta_{cv}}{\omega_{\ell c}^S - 2\omega_{cv}^S}\right) \\ &\times (1 + \delta_{\ell c}^S + \delta_{cv}^S + \delta_{v\ell}^S - \delta_{\ell c} - \delta_{cv} - \delta_{v\ell}) \\ &\rightarrow \frac{1}{(\omega_{cv}^S)^3} \frac{\text{Im}[v_{\ell c}^{\Sigma,a} \{v_{cv}^{\Sigma,b} v_{v\ell}^{\Sigma,c}\}]}{\omega_{\ell c}^S - 2\omega_{cv}^S} \left(1 - 3\delta_{cv}^S - \frac{\Delta_{\ell c} - 2\Delta_{cv}}{\omega_{\ell c}^S - 2\omega_{cv}^S}\right. \\ &\left.+ \delta_{\ell c}^S + \delta_{cv}^S + \delta_{v\ell}^S - \delta_{\ell c} - \delta_{cv} - \delta_{v\ell}\right), \end{aligned} \quad (6)$$

and

$$\begin{aligned} \frac{1}{(\omega_{cv}^S)^3} \frac{\text{Im}[v_{v\ell}^{\Sigma,a} \{v_{\ell c}^{\Sigma,b} v_{cv}^{\Sigma,c}\}]}{\omega_{\ell v}^S - 2\omega_{cv}^S} &\rightarrow \frac{1}{(\omega_{cv}^S)^3} \frac{\text{Im}[v_{v\ell}^{\Sigma,a} \{v_{\ell c}^{\Sigma,b} v_{cv}^{\Sigma,c}\}]}{\omega_{\ell v}^S - 2\omega_{cv}^S} \left(1 - 3\delta_{cv}^S - \frac{\Delta_{\ell v} - 2\Delta_{cv}}{\omega_{\ell v}^S - 2\omega_{cv}^S}\right) \\ &+ \delta_{v\ell}^S + \delta_{\ell c}^S + \delta_{cv}^S - \delta_{v\ell} - \delta_{\ell c} - \delta_{cv}, \end{aligned} \quad (7)$$

For the matrix elements of the position operator we have that

$$\begin{aligned} \mathbf{r}_{nm} &= \frac{\mathbf{P}_{nm}}{im_e \omega_{nm}} \rightarrow \frac{\mathbf{P}_{nm}}{im_e \omega_{nm} (1 + \delta_{nm})} = \mathbf{r}_{nm} (1 - \delta_{nm}) \\ \mathbf{r}_{nm} &\rightarrow \mathbf{r}_{nm} (1 - \delta_{nm}). \end{aligned} \quad (8)$$

where we recall that $\mathbf{r}_{nm}^S = \mathbf{r}_{nm}$, and $\omega_{nm} \mathbf{r}_{nm}$ is invariant under the energy differences.

$$\begin{aligned} r_{nm;k^a}^b &= \frac{r_{nm}^a \mathcal{V}_{mn}^b + r_{nm}^b \mathcal{V}_{mn}^a}{\omega_{nm}} + \frac{i}{\omega_{nm}} \sum_{\ell} (\omega_{\ell m} r_{n\ell}^a r_{\ell m}^b - \omega_{n\ell} r_{n\ell}^b r_{\ell m}^a) \\ &\rightarrow \frac{r_{nm}^a \mathcal{V}_{mn}^b + r_{nm}^b \mathcal{V}_{mn}^a}{\omega_{nm} (1 + \delta_{nm})} (1 - \delta_{nm}) \\ &+ \frac{i}{\omega_{nm} (1 + \delta_{nm})} \sum_{\ell} (\omega_{\ell m} r_{\ell m}^b r_{n\ell}^a (1 - \delta_{n\ell}) - \omega_{n\ell} r_{n\ell}^b r_{\ell m}^a (1 - \delta_{\ell m})) \\ r_{nm;k^a}^b \rightarrow \tilde{r}_{nm;k^a}^b &= \left[\frac{r_{nm}^a \mathcal{V}_{mn}^b + r_{nm}^b \mathcal{V}_{mn}^a}{\omega_{nm}} (1 - \delta_{nm}) \right. \\ &\left. + \frac{i}{\omega_{nm}} \sum_{\ell} (\omega_{\ell m} r_{\ell m}^b r_{n\ell}^a (1 - \delta_{n\ell}) - \omega_{n\ell} r_{n\ell}^b r_{\ell m}^a (1 - \delta_{\ell m})) \right] (1 - \delta_{nm}) \\ \tilde{r}_{nm;k^a}^b &= \tilde{r}_{nm;k^a}^b (1 - \delta_{nm}). \end{aligned} \quad (9)$$

Then, $\mathcal{F}_{vc}^{\text{ab}}$ is given by

$$\begin{aligned}
\mathcal{F}_{vc}^{\text{ab}} &= -i\Delta \sum_{\ell \neq (vc)} \left(r_{v\ell}^{\text{a}} r_{\ell c}^{\text{b}} - r_{v\ell}^{\text{b}} r_{\ell c}^{\text{a}} \right) (1 - \delta_{v\ell} - \delta_{\ell c}) + \Delta \tilde{r}_{vc;k^{\text{a}}}^{\text{b}} (1 - \delta_{vc}) \\
&= \left[-i\Delta \sum_{\ell \neq (vc)} \left(r_{v\ell}^{\text{a}} r_{\ell c}^{\text{b}} - r_{v\ell}^{\text{b}} r_{\ell c}^{\text{a}} \right) (1 - \delta_{v\ell} - \delta_{\ell c} + \delta_{vc}) + \Delta \tilde{r}_{vc;k^{\text{a}}}^{\text{b}} \right] (1 - \delta_{vc}) \\
&= \tilde{\mathcal{F}}_{vc}^{\text{ab}} (1 - \delta_{vc}),
\end{aligned} \tag{10}$$

and

$$\frac{1}{(\omega_{cv}^S)^3} \mathcal{F}_{vc}^{\text{ab}} v_{cv}^{\Sigma, c} \rightarrow \frac{1}{(\omega_{cv}^S)^3} (1 - 3\delta_{cv}^S) \tilde{\mathcal{F}}_{vc}^{\text{ab}} v_{cv}^{\Sigma, c} (1 + \delta_{cv}^S) = \frac{1}{(\omega_{cv}^S)^3} \tilde{\mathcal{F}}_{vc}^{\text{ab}} v_{cv}^{\Sigma, c} (1 - 2\delta_{cv}^S), \tag{11}$$

since $\delta_{cv} - \delta_{vc} = \Delta_{cv}/\omega_{cv} - \Delta_{vc}/\omega_{vc} = \Delta_{cv}/\omega_{cv} - (-\Delta_{cv})/(-\omega_{cv}) = 0$.