contribution can in general be written as:

$$(C_{(2)})^{aa}_{bb} = \sum_{m,m'} \sum_{pp'} \left(\sum_{\sigma\sigma'} T^{p}_{\sigma}(b,m)\, T^{p'}_{\sigma'}(m,a) T^{\bar{p}'}_{\sigma'}(a,m')\, T^{\bar{p}}_{\sigma}(m',b) \right) \times \left(\sum_{ll'} \tilde{C}_{(2)}(E_{mb} + peV_l, E_{am'} + p'eV_{l'}, E_{ab'} + peV_l + p'eV_{l'}) \right).$$

Here, $p, p' \in \{+,-\}$. As we stated before, the contribution is split into a part containing merely the tunnelling matrix elements and an energy dependent function $\tilde{C}_{(2)}$ specific for the diagram group. This function distinguishes the two cases of secular ($E_m = E_{m'}$) and non-secular ($E_m \neq E_{m'}$) intermediate states,

$$\tilde{C}_{(2)}(\mu,\mu',\Delta) = \frac{\beta}{\mathrm{i}\hbar} \int \mathrm{d}\omega \int \mathrm{d}\omega'\, f^{-}(\omega)\, f^{-}(\omega') \times \begin{cases} \lim_{\eta\to 0} \frac{1}{\omega-\beta\mu+\mathrm{i}\eta} \frac{1}{\omega'-\beta\mu'+\mathrm{i}\eta} \frac{1}{\omega+\omega'-\beta\Delta+\mathrm{i}\eta} & \mu+\mu' = \Delta, \\ -\lim_{\eta\to 0} \frac{1}{\omega-\beta\mu'+\mathrm{i}\eta} \frac{1}{\omega+\beta(\Delta-\mu)-\mathrm{i}\eta} \frac{1}{\omega+\omega'-\beta\Delta+\mathrm{i}\eta} & \mu+\mu' \neq \Delta. \end{cases} \tag{39}$$

Here, as usual, $\beta = (k_B T)^{-1}$. We remark that the second expression is one commonly encountered in T-matrix based rate approach calculations and diverges in the limit $\mu + \mu' \to \Delta$ (which is equivalent to $E_m \to E_{m'}$). We investigate it in more detail in Sect. 2.4, where we show in particular that the typical regularisation *cannot* recover the solution for $E_m = E_{m'}$ exactly.

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