

**Erratum: Strong-coupling expansions for the anharmonic Holstein model
and for the Holstein-Hubbard model**
[Phys. Rev. B 54, 9372 (1996)]

J. K. Freericks and G. D. Mahan

[S0163-1829(97)01941-3]

An error was discovered in the fourth-order expansions in the anharmonic case. The Hamiltonian actually does lose its electron-hole symmetry, because inequivalent virtual states are possible at fourth and higher order. This modifies all of the results for the anharmonic phonons. The changes occur in $H_4(c)$ and $H_4(d)$:

$$H_4(c) = \frac{1}{2} \sum_{i,j,k}' \left\{ j_{\parallel}'(-) \frac{1}{2} [J_i^z + J_k^z] - [j_{\parallel}'(-) + j_{\parallel}''(-)] \frac{1}{2} J_j^z + j_{\perp}'(+) \frac{1}{2} \sum_a [J_i^a J_j^{-a} + J_k^a J_j^{-a}] - j_{\parallel}'(+) \left[J_i^z J_j^z + J_k^z J_j^z - \frac{1}{2} \right] \right. \\ \left. + j_{\perp}''(+) \frac{1}{2} \sum_a J_i^a J_k^{-a} + [j_{\parallel}'(+) + j_{\parallel}''(+)] \left[J_i^z J_k^z - \frac{1}{4} \right] \right. \\ \left. - 2[j_{\parallel}'(-) - j_{\parallel}''(-)] J_i^z J_j^z J_k^z + j_{\perp}'(-) \sum_a [J_i^a J_j^{-a} J_k^z + J_k^a J_j^{-a} J_i^z] + j_{\perp}''(-) \sum_a J_i^a J_k^{-a} J_j^z \right\}, \quad (19)$$

$$H_4(d) = \frac{1}{8} \sum_{i,j,k,l}' \left\{ \frac{\alpha(+)}{2} + \frac{\delta}{4} + \frac{\nu}{8} + \frac{\alpha(-)}{2} [J_i^z + J_j^z + J_k^z + J_l^z] - \frac{\nu}{2} [J_i^z J_j^z + J_i^z J_l^z + J_k^z J_j^z + J_k^z J_l^z] \right. \\ \left. + \frac{\beta(+)+\epsilon}{2} \sum_a [J_i^a J_j^{-a} + J_i^a J_l^{-a} + J_k^a J_j^{-a} + J_k^a J_l^{-a}] - \left(\delta - \frac{\nu}{2} \right) [J_i^z J_k^z + J_j^z J_l^z] + \frac{\gamma(+)+\mu}{2} \sum_a [J_i^a J_k^{-a} + J_j^a J_l^{-a}] \right. \\ \left. - 2\alpha(-) [J_i^z J_j^z J_k^z + J_i^z J_j^z J_l^z + J_i^z J_k^z J_l^z + J_j^z J_k^z J_l^z] \right. \\ \left. + \beta(-) \sum_a [J_i^a J_j^{-a} (J_k^z + J_l^z) + J_k^a J_j^{-a} (J_i^z + J_l^z) + J_i^a J_l^{-a} (J_j^z + J_k^z) + J_k^a J_l^{-a} (J_i^z + J_j^z)] \right. \\ \left. + \gamma(-) \sum_a [J_i^a J_k^{-a} (J_j^z + J_l^z) + J_j^a J_l^{-a} (J_i^z + J_k^z)] \right. \\ \left. + 2(\beta(+)-\epsilon) \sum_a [J_i^z J_j^z J_k^a J_l^{-a} + J_k^z J_l^z J_i^a J_j^{-a} + J_i^z J_l^z J_k^a J_j^{-a} + J_k^z J_j^z J_i^a J_l^{-a}] \right. \\ \left. + 2(\gamma(+)-\mu) \sum_a [J_i^z J_k^z J_j^a J_l^{-a} + J_j^z J_l^z J_i^a J_k^{-a}] + [-8\alpha(+)+4\delta+2\nu] J_i^z J_j^z J_k^z J_l^z \right. \\ \left. + \frac{\rho}{2} \sum_a \sum_b [J_i^a J_j^{-a} J_k^b J_l^{-b} + J_i^a J_l^{-a} J_k^b J_j^{-b} - J_i^a J_k^{-a} J_j^b J_l^{-b}] \right\}. \quad (20)$$

In the harmonic limit ($\alpha_{an}=0$), we have all coefficients labeled with a minus sign ($-$) vanish, and $\beta(+)=\mu$, $\gamma(+)=\epsilon$, and $\delta=\nu$. In the anharmonic case, only the equality $\delta=\nu$ continues to hold. We have not been able to verify these identities, except by numerical calculation.

The self-consistent equation for the pseudospin magnetization is modified to

$$m = \tanh \frac{1}{2} \beta \left\{ 2\{\mu + d(2d-1)[j_{\parallel}'(-) - j_{\parallel}''(-)] + d(d-1)\alpha(-) - U\} \right. \\ \left. + md \left[-j_{\parallel}^{(2)} - j_{\parallel}^{(4)} + (2d-1)[j_{\parallel}'(+) - j_{\parallel}''(+)] + (d-1) \left(\delta + \frac{1}{2} \nu \right) \right] \right. \\ \left. + \frac{3}{2} m^2 \{ d(2d-1)[j_{\parallel}'(-) - j_{\parallel}''(-)] + 3d(d-1)\alpha(-) \} \right. \\ \left. + m^3 d(d-1) \left[2\alpha(+) - \delta - \frac{1}{2} \nu \right] \right\}. \quad (24)$$

The transition temperature for commensurate charge-density-wave (CDW) order becomes

$$T_c = \frac{1}{2} \rho_e (2 - \rho_e) \left\{ dj_{\parallel}^{(2)} - d^2 \left[6j_{\parallel}'(+)+2j_{\parallel}''(+)-\delta + \frac{3}{2} \nu \right. \right. \\ \left. \left. - 2[j_{\parallel}'(-)-j_{\parallel}''(-)+\alpha(-)](1-\rho_e) + \left(2\alpha(+)-\delta - \frac{1}{2} \nu \right) (1-\rho_e)^2 \right] \right. \\ \left. + d \left[j_{\parallel}^{(4)} + 3j_{\parallel}'(+)+j_{\parallel}''(+)-\delta + \frac{3}{2} \nu - [j_{\parallel}'(-)-j_{\parallel}''(-)+2\alpha(-)](1-\rho_e) + \left(2\alpha(+)-\delta - \frac{1}{2} \nu \right) (1-\rho_e)^2 \right] \right\}. \quad (26)$$

The superconducting (SC) transition temperature is changed to

$$T_c = \frac{\rho_e - 1}{\ln[\rho_e/(2-\rho_e)]} (dj_{\perp}^{(2)} + d^2 \{ 4j_{\perp}'(+)-2j_{\perp}''(+)+2\beta(+)-\gamma(+)+2\epsilon-\mu \\ - [4j_{\perp}'(-)-2j_{\perp}''(-)+4\beta(-)-2\gamma(-)](1-\rho_e) + [2\beta(+)-\gamma(+)-2\epsilon+\mu](1-\rho_e)^2 \} \\ + d \{ j_{\perp}^{(4)} - 2j_{\perp}'(+)+j_{\perp}''(+)-2\beta(+)+\gamma(+)-2\epsilon+\mu \\ - [-2j_{\perp}'(-)+j_{\perp}''(-)-4\beta(-)+2\gamma(-)](1-\rho_e) + [-2\beta(+)+\gamma(+)+2\epsilon-\mu](1-\rho_e)^2 \}). \quad (28)$$

Figure 3(a) is modified. Now the anharmonicity seems to indicate that there may be a small increase in the maximum CDW transition temperature at half filling, although quantum Monte Carlo results do not indicate that this is correct.

Figures 4(a) and 5(a) are modified. Note how the electron-hole asymmetry becomes more pronounced as the strength of the anharmonicity is increased. The enhancement of transition temperatures for electron densities less than half-filling is also seen in quantum Monte Carlo simulations.

Finally, the plot of the critical electron density, where the CDW-SC phase boundary lies, is also modified in Fig. 6(a).

The only conclusion that has been modified is that the strong-coupling perturbation theory preserves electron-hole symmetry. Otherwise, other conclusions remain the same.

ACKNOWLEDGMENT

We would like to acknowledge P. Grzybowski for pointing out how electron-hole symmetry is actually broken in fourth and higher orders.

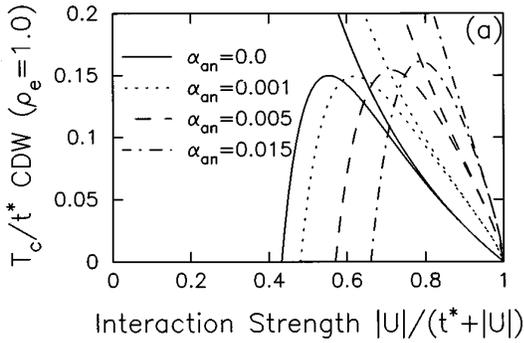


FIG. 3(a). Replacement for Fig. 3(a). Notice that the maximum T_c now increases with increasing anharmonicity.

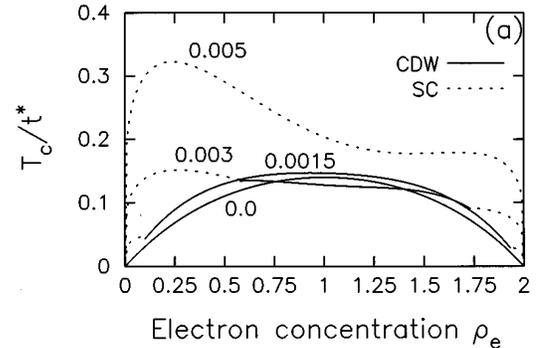


FIG. 4(a). Replacement for Fig. 4(a). Notice the electron-hole asymmetry as the anharmonicity is increased.

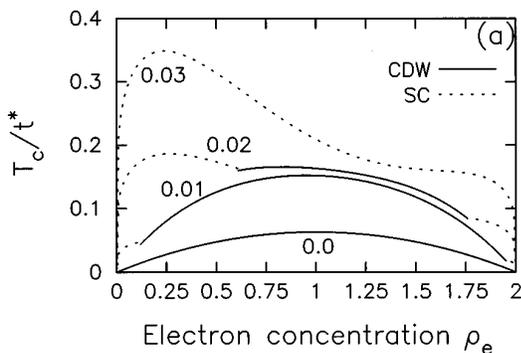


FIG. 5(a). Replacement for Fig. 5(a).

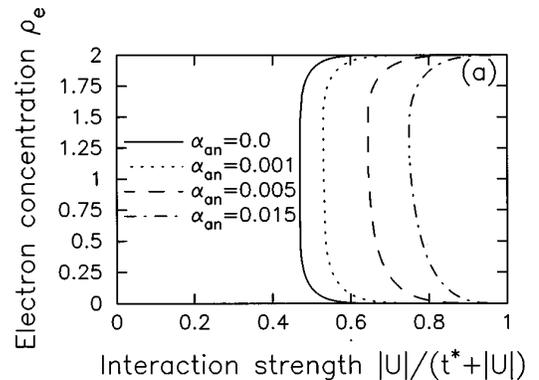


FIG. 6(a). Replacement for Fig. 6(a). Notice that the phase diagram is now no longer electron-hole symmetric.

APPENDIX A: PARAMETERS OF THE FOURTH-ORDER EFFECTIVE PSEUDOSPIN HAMILTONIAN

The parameters in Eq. (19) (an overall factor of $t_{ij}^2 t_{jk}^2$ is suppressed):

$$\begin{aligned}
 j_{\parallel}'(\pm) = & 2 \left\{ \sum_{l,l',m,n,n'=0}^{\infty} \frac{\langle +0|n\rangle\langle n|+0\rangle\langle -0|n'\rangle\langle n'|+m\rangle\langle +m|l'\rangle\langle l'|-0\rangle\langle +0|l\rangle\langle l|+0\rangle}{[E_0^+ + E_0^- - E_n - E_{n'}][2E_0^+ + E_0^- - E_m^+ - E_n - E_l]} \right. \\
 & \times \left[\frac{1}{E_0^+ + E_0^- - E_l - E_{l'}} + \frac{1}{E_0^+ + E_0^- - E_n - E_{l'}} \right] \\
 & + 2 \sum_{\substack{l,l',n,n'=0 \\ m \neq 0}}^{\infty} \frac{\langle +0|n\rangle\langle n|+0\rangle\langle -0|n'\rangle\langle n'|-m\rangle\langle -m|l'\rangle\langle l'|-0\rangle\langle +0|l\rangle\langle l|+0\rangle}{[E_0^+ + E_0^- - E_n - E_{n'}][E_0^- - E_m^-][E_0^+ + E_0^- - E_l - E_{l'}]} \\
 & \left. - 2 \sum_{l,l',n,n'=0}^{\infty} \frac{\langle +0|n\rangle\langle n|+0\rangle\langle -0|n'\rangle\langle n'|-0\rangle\langle -0|l'\rangle\langle l'|-0\rangle\langle +0|l\rangle\langle l|+0\rangle}{[E_0^+ + E_0^- - E_n - E_{n'}]^2[E_0^+ + E_0^- - E_l - E_{l'}]} \right\} \pm \{+\leftrightarrow-\}, \quad (\text{A3})
 \end{aligned}$$

$$j_{\parallel}''(\pm) = -2 \sum_{l,l',m,n,n'=0}^{\infty} \frac{\langle +0|n\rangle\langle n|+m\rangle\langle +m|l'\rangle\langle l'|+0\rangle\langle -0|n'\rangle\langle n'|-0\rangle\langle +0|l\rangle\langle l|+0\rangle}{[E_0^+ + E_0^- - E_n - E_{n'}][2E_0^+ + E_0^- - E_m^+ - E_l - E_{n'}][E_0^+ + E_0^- - E_{l'} - E_{n'}]} \pm \{+\leftrightarrow-\}, \quad (\text{A4})$$

$$\begin{aligned}
 j_{\perp}'(\pm) = & -2 \left\{ \sum_{l,l',m,n,n'=0}^{\infty} \frac{\langle +0|n\rangle\langle n|+0\rangle\langle -0|n'\rangle\langle n'|+m\rangle\langle +m|l'\rangle\langle l'|+0\rangle\langle +0|l\rangle\langle l|-0\rangle}{[E_0^+ + E_0^- - E_n - E_{n'}][2E_0^+ + E_0^- - E_m^+ - E_n - E_l]} \right. \\
 & \times \left[\frac{1}{E_0^+ + E_0^- - E_l - E_{l'}} + \frac{1}{E_0^+ + E_0^- - E_n - E_{l'}} \right] \\
 & + 2 \sum_{\substack{l,l',n,n'=0 \\ m \neq 0}}^{\infty} \frac{\langle +0|n\rangle\langle n|+0\rangle\langle -0|n'\rangle\langle n'|-m\rangle\langle -m|l'\rangle\langle l'|+0\rangle\langle +0|l\rangle\langle l|-0\rangle}{[E_0^+ + E_0^- - E_n - E_{n'}][E_0^- - E_m^-][E_0^+ + E_0^- - E_l - E_{l'}]} \\
 & - \sum_{l,l',n,n'=0}^{\infty} \frac{\langle +0|n\rangle\langle n|+0\rangle\langle -0|n'\rangle\langle n'|-0\rangle\langle -0|l'\rangle\langle l'|+0\rangle\langle +0|l\rangle\langle l|-0\rangle}{[E_0^+ + E_0^- - E_n - E_{n'}][E_0^+ + E_0^- - E_l - E_{l'}]} \\
 & \left. \times \left[\frac{1}{E_0^+ + E_0^- - E_n - E_{n'}} + \frac{1}{E_0^+ + E_0^- - E_l - E_{l'}} \right] \right\} \pm \{+\leftrightarrow-\}, \quad (\text{A5})
 \end{aligned}$$

$$\begin{aligned}
 j_{\perp}''(\pm) = & 2 \left\{ \sum_{l,l',m,n,n'=0}^{\infty} \frac{\langle +0|n\rangle\langle n|+m\rangle\langle +m|l'\rangle\langle l'|+0\rangle\langle -0|n'\rangle\langle n'|+0\rangle\langle +0|l\rangle\langle l|-0\rangle}{[E_0^+ + E_0^- - E_n - E_{n'}][2E_0^+ + E_0^- - E_m^+ - E_{n'} - E_l][E_0^+ + E_0^- - E_l - E_{l'}]} \right. \\
 & + 2 \sum_{\substack{l,l',n,n'=0 \\ m \neq 0}}^{\infty} \frac{\langle +0|n\rangle\langle n|-m\rangle\langle -m|l'\rangle\langle l'|+0\rangle\langle -0|n'\rangle\langle n'|+0\rangle\langle +0|l\rangle\langle l|-0\rangle}{[E_0^+ + E_0^- - E_n - E_{n'}][E_0^- - E_m^-][E_0^+ + E_0^- - E_l - E_{l'}]} \\
 & \left. - 2 \sum_{l,l',n,n'=0}^{\infty} \frac{\langle +0|n\rangle\langle n|-0\rangle\langle -0|n'\rangle\langle n'|+0\rangle\langle -0|l'\rangle\langle l'|+0\rangle\langle +0|l\rangle\langle l|-0\rangle}{[E_0^+ + E_0^- - E_n - E_{n'}]^2[E_0^+ + E_0^- - E_l - E_{l'}]} \right\} \pm \{+\leftrightarrow-\}, \quad (\text{A6})
 \end{aligned}$$

where the notation $\{+\leftrightarrow-\}$ denotes replacing $+$ by $-$ (and vice versa) in all of the matrix elements, and in all of the energy factors E_m^{\pm} .

Finally the parameters in Eq. (20) (an overall factor of $t_{ij}t_{jk}t_{kl}t_{ki}$ is suppressed):

$$\alpha(\pm) = 2 \sum_{l,l',n,n'=0}^{\infty} \frac{\langle +0|n\rangle\langle n|+0\rangle\langle -0|n'\rangle\langle n'|-0\rangle\langle +0|l\rangle\langle l|+0\rangle\langle +0|l'\rangle\langle l'|+0\rangle}{[E_0^+ + E_0^- - E_n - E_{n'}][E_0^+ + E_0^- - E_l - E_{n'}][E_0^+ + E_0^- - E_{l'} - E_{n'}]} \pm \{+\leftrightarrow-\}, \quad (\text{A7})$$

$$\begin{aligned}
\beta(\pm) = & - \sum_{l,l',n,n'=0}^{\infty} \left\{ \frac{\langle +0|n\rangle\langle n|-0\rangle\langle -0|n'\rangle\langle n'+0\rangle\langle +0|l\rangle\langle l+0\rangle\langle +0|l'\rangle\langle l'+0\rangle}{[E_0^+ + E_0^- - E_n - E_{n'}][E_0^+ + E_0^- - E_l - E_n][E_0^+ + E_0^- - E_{l'} - E_n]} \right. \\
& + \frac{\langle +0|n\rangle\langle n|+0\rangle\langle -0|n'\rangle\langle n'+0\rangle\langle +0|l\rangle\langle l+0\rangle\langle +0|l'\rangle\langle l'|-0\rangle}{E_0^+ + E_0^- - E_n - E_{n'}} \\
& \times \left[\frac{1}{[E_0^+ + E_0^- - E_{l'} - E_n][E_0^+ + E_0^- - E_l - E_{l'}]} \right. \\
& + \frac{1}{[E_0^+ + E_0^- - E_l - E_{n'}][E_0^+ + E_0^- - E_l - E_{l'}]} \\
& \left. \left. + \frac{1}{[E_0^+ + E_0^- - E_l - E_{n'}][E_0^+ + E_0^- - E_{l'} - E_{n'}]} \right] \right\} \pm \{+ \leftrightarrow -\}, \tag{A8}
\end{aligned}$$

$$\begin{aligned}
\gamma(\pm) = & 2 \sum_{l,l',n,n'=0}^{\infty} \left\{ \frac{\langle +0|n\rangle\langle n|+0\rangle\langle -0|n'\rangle\langle n'+0\rangle\langle +0|l\rangle\langle l+0\rangle\langle +0|l'\rangle\langle l'|-0\rangle}{[E_0^+ + E_0^- - E_n - E_{n'}][E_0^+ + E_0^- - E_{l'} - E_{n'}][E_0^+ + E_0^- - E_l - E_{l'}]} \right. \\
& + \frac{\langle +0|n\rangle\langle n|+0\rangle\langle -0|n'\rangle\langle n'+0\rangle\langle +0|l\rangle\langle l+0\rangle\langle +0|l'\rangle\langle l'|-0\rangle}{[E_0^+ + E_0^- - E_n - E_{n'}][E_0^+ + E_0^- - E_l - E_n]} \\
& \times \left[\frac{1}{E_0^+ + E_0^- - E_{l'} - E_n} + \frac{1}{E_0^+ + E_0^- - E_l - E_{l'}} \right] \right\} \pm \{+ \leftrightarrow -\}, \tag{A9}
\end{aligned}$$

$$\begin{aligned}
\epsilon = & 2 \sum_{l,l',n,n'=0}^{\infty} \left\{ \frac{\langle +0|n\rangle\langle n|-0\rangle\langle -0|n'\rangle\langle n'+0\rangle\langle +0|l\rangle\langle l+0\rangle\langle -0|l'\rangle\langle l'|-0\rangle}{[E_0^+ + E_0^- - E_n - E_{n'}][2E_0^+ + 2E_0^- - E_n - E_{n'} - E_l - E_{l'}]} \right. \\
& \times \left[\frac{1}{E_0^+ + E_0^- - E_{l'} - E_n} + \frac{1}{E_0^+ + E_0^- - E_l - E_n} \right] \\
& + \frac{\langle +0|n\rangle\langle n|-0\rangle\langle -0|n'\rangle\langle n'+0\rangle\langle +0|l\rangle\langle l+0\rangle\langle -0|l'\rangle\langle l'|-0\rangle}{[E_0^+ + E_0^- - E_l - E_{l'}][2E_0^+ + 2E_0^- - E_n - E_{n'} - E_l - E_{l'}]} \\
& \times \left[\frac{1}{E_0^+ + E_0^- - E_{l'} - E_{n'}} + \frac{1}{E_0^+ + E_0^- - E_l - E_n} \right] \\
& + \frac{\langle +0|n\rangle\langle n|+0\rangle\langle -0|n'\rangle\langle n'|-0\rangle\langle +0|l\rangle\langle l-0\rangle\langle -0|l'\rangle\langle l'+0\rangle}{[E_0^+ + E_0^- - E_n - E_{n'}][E_0^+ + E_0^- - E_l - E_{n'}]} \\
& \times \left[\frac{1}{E_0^+ + E_0^- - E_{l'} - E_{n'}} + \frac{1}{E_0^+ + E_0^- - E_l - E_{l'}} \right] \\
& + \frac{\langle +0|n\rangle\langle n|+0\rangle\langle -0|n'\rangle\langle n'|-0\rangle\langle -0|l\rangle\langle l+0\rangle\langle +0|l'\rangle\langle l'|-0\rangle}{[E_0^+ + E_0^- - E_n - E_{n'}][E_0^+ + E_0^- - E_l - E_n]} \\
& \times \left[\frac{1}{E_0^+ + E_0^- - E_{l'} - E_n} + \frac{1}{E_0^+ + E_0^- - E_l - E_{l'}} \right] \left. \right\}, \tag{A11}
\end{aligned}$$

$$\begin{aligned}
\mu = & -2 \sum_{l,l',n,n'=0}^{\infty} \left\{ \frac{\langle +0|n\rangle\langle n|-0\rangle\langle -0|n'\rangle\langle n'|-0\rangle\langle +0|l\rangle\langle l|+0\rangle\langle -0|l'\rangle\langle l'|+0\rangle}{[E_0^+ + E_0^- - E_n - E_{n'}][2E_0^+ + 2E_0^- - E_n - E_{n'} - E_l - E_{l'}]} \right. \\
& \times \left[\frac{1}{E_0^+ + E_0^- - E_{l'} - E_{n'}} + \frac{1}{E_0^+ + E_0^- - E_l - E_n} \right] \\
& + \frac{\langle +0|n\rangle\langle n|-0\rangle\langle -0|n'\rangle\langle n'|-0\rangle\langle +0|l\rangle\langle l|+0\rangle\langle -0|l'\rangle\langle l'|+0\rangle}{[E_0^+ + E_0^- - E_l - E_{l'}][2E_0^+ + 2E_0^- - E_n - E_{n'} - E_l - E_{l'}]} \\
& \times \left[\frac{1}{E_0^+ + E_0^- - E_{l'} - E_{n'}} + \frac{1}{E_0^+ + E_0^- - E_l - E_n} \right] \\
& + \frac{\langle +0|n\rangle\langle n|-0\rangle\langle -0|n'\rangle\langle n'|+0\rangle\langle -0|l\rangle\langle l|+0\rangle\langle +0|l'\rangle\langle l'|+0\rangle}{[E_0^+ + E_0^- - E_n - E_{n'}][E_0^+ + E_0^- - E_l - E_n][E_0^+ + E_0^- - E_{l'} - E_n]} \\
& \left. + \frac{\langle +0|n\rangle\langle n|+0\rangle\langle -0|n'\rangle\langle n'|+0\rangle\langle +0|l\rangle\langle l|-0\rangle\langle -0|l'\rangle\langle l'|-0\rangle}{[E_0^+ + E_0^- - E_n - E_{n'}][E_0^+ + E_0^- - E_l - E_{n'}][E_0^+ + E_0^- - E_{l'} - E_{n'}]} \right\}, \tag{A12}
\end{aligned}$$
