Electron-phonon interaction enhanced by antiferromagnetic and superconducting fluctuations in cuprate oxide superconductors

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An electron-phonon interaction arising from the modulation of the superexchange interaction by phonons is studied within the theoretical framework of Kondo lattices. It is relevant in strongly correlated electron liquids in cuprate oxide superconductors, which lie in the vicinity of the Mott-Hubbard metal-insulator transition. It is enhanced by antiferromagnetic and superconducting fluctuations, which are developed mainly because of the superexchange interaction. When the enhancement of the electron-phonon interaction is large enough, it can explain the softening of phonons and kinks in the quasiparticle dispersion in cuprate oxide superconductors. However, the superexchange interaction itself must be mainly responsible for the formation of Cooper pairs.

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I. INTRODUCTION

It is an important issue to elucidate the mechanism of high-$T_c$ superconductivity occurring in cuprate oxides. It was shown in previous papers published in 1987 that the condensation of $d_\gamma$-wave Cooper pair bound by the superexchange interaction can explain observed $T_c$; $T_c$ for $d_\gamma$ wave are definitely much higher than those of other waves, as long as the on-site repulsion is so strong that cuprate oxides with no dopings might be Mott-Hubbard insulators. On the other hand, two observations, the softening of phonons and kinks in the quasiparticle dispersion imply the relevance of an electron-phonon interaction. In particular, the softening of phonons is evidence that an electron-phonon interaction is strong in cuprate oxides. One may argue that it must be responsible for high-$T_c$ superconductivity or, at least, it must play some role in the realization of high-$T_c$ superconductivity.

Various experiments imply or show the opening of anisotropic pseudogaps at temperatures above $T_c$ in quasiparticle spectra of the so called optimal and under-doped cuprate oxide superconductors. One may argue that kinks are caused by or are closely related with what cause pseudogaps, rather than phonons. Antiferromagnetic (AF) and superconducting (SC) fluctuations are developed in cuprate oxide superconductors; not only antiferromagnetism and superconductivity themselves but also the development of their fluctuations are mainly caused by the superexchange interaction. It was shown in a previous paper that large lifetime widths, which are mainly caused by well developed $d_\gamma$-wave SC fluctuations so that they are anisotropic or wave-number dependent, are responsible for anisotropic pseudogaps; spectral weights around the chemical potential are swept away because of large life-time widths. Small kinks appear in calculated spectra but they are too small to explain observed kinks. It is difficult to explain kinks by AF or SC fluctuations. It is reasonable that not only the softening of phonons but also kinks are caused by an electron-phonon interaction.

Doped holes mainly go into O ions. This implies that the local charge susceptibility of 3$d$ electrons on Cu ions is much smaller than that of 2$p$ electrons on O ions and charge fluctuation of 3$d$ electrons can never be developed. It is quite unlikely that the conventional electron-phonon interaction, which directly couples with charge fluctuations, plays a crucial role in cuprate oxide superconductors.

A necessary condition for a relevant electron-phonon interaction is that it can work even in strongly correlated electron liquids in the vicinity of the Mott-Hubbard metal-insulator transition or even when charge fluctuations are significantly suppressed. One of the most plausible ones is an electron-phonon interaction arising from the modulation of the superexchange interaction by phonons. It was pointed out that it plays a role in phonon-assisted multi-magnon optical absorption. It can couple directly with AF and SC fluctuations, so that it can be substantially enhanced by AF and SC fluctuations. One of the purposes of this paper is to show that the electron-phonon interaction arising from the modulation of the superexchange interaction by phonons is relevant, at least, in cuprate oxide superconductors where AF and SC fluctuations are substantially developed.

II. FORMULATION

A. Electron-phonon interaction

It was shown in a previous paper that Gutzwiller’s quasiparticle band lies between the lower and upper Hubbard bands in metallic phases in the vicinity of the Mott-Hubbard transition. Gutzwiller’s quasiparticles are responsible for metallic properties. The superexchange interaction arises from the virtual exchange of pair excitations of electrons across the lower and upper Hubbard bands. As long as the Hubbard splitting is significant, therefore, it works between Gutzwiller’s quasiparticles.

When we follow previous papers and we ignore nonzero bandwidths of the lower and upper Hubbard
bands, it is straightforward to show that the virtual exchange process gives the following exchange constant between nearest-neighbor \(i\)th and \(j\)th Cu ions:

\[
J_{ij} = -4V_{i,j}^2 V^2_{j,i} \left\{ \frac{2}{\epsilon_{dj} - \epsilon_{di}} \times \left[ \frac{1}{(\epsilon_{di} + U - \epsilon_{p_{ij}})^2} - \frac{1}{(\epsilon_{dj} + U - \epsilon_{p_{ij}})^2} \right] + \frac{2}{(\epsilon_{di} + U - \epsilon_{p_{ij}})^2} \frac{1}{\epsilon_{dj} + U - \epsilon_{di}} \right\},
\]  

(2.1)

where the 3d levels of the \(i\)th and \(j\)th Cu ions are denoted by \(\epsilon_{di}\) and \(\epsilon_{dj}\), the 2p level of the \(i\)th O ion between the two Cu ions by \(\epsilon_{p_{ij}}\), and the hybridization energies between the Cu ions and the O ion by \(V_{i,j}\) and \(V_{j,i}\), respectively. When we put \(\epsilon_{di} \rightarrow \epsilon_{d}, \epsilon_{dj} \rightarrow \epsilon_{d}, \) and \(V_{i,j} = V_{j,i,j} = V\), we obtain a well-known one:

\[
J = -\frac{4V^4}{(\epsilon_{d} + U - \epsilon_{p})^2} \left[ \frac{1}{\epsilon_{d} + U - \epsilon_{p}} + \frac{1}{U} \right].
\]  

(2.2)

The variation of \(J_{ij}\) is given by

\[
\Delta J_{ij} = \frac{2V^4}{(\epsilon_{d} + U - \epsilon_{p})^3} \left[ \frac{3}{\epsilon_{d} + U - \epsilon_{p}} + \frac{2}{U} \right] \times (\Delta \epsilon_{di} + \Delta \epsilon_{dj} - 2\Delta \epsilon_{p_{ij}}) + 2J \left( \Delta V_{i,j} + \Delta V_{j,i,j} \right).
\]  

(2.3)

When we take the \(x\)- and \(y\)-axes along Cu-O-Cu bonds, variations of \(\epsilon_{di}, \epsilon_{p_{ij}}\) and \(V_{i,j}\) are given by

\[
\Delta \epsilon_{di} = A_d \left[ \epsilon_x \cdot (u_{i,x} + u_{i,x}) + \epsilon_y \cdot (u_{i,y} + u_{i,y}) \right],
\]  

(2.4)

\[
\Delta \epsilon_{p_{ij}} = A_p \left[ \epsilon_y \cdot (u_{i} - u_{j}) \right],
\]  

(2.5)

\[
\Delta V_{i,j} + \Delta V_{j,i,j} = A_V \left[ \epsilon_x \cdot (u_{i} - u_{j}) \right],
\]  

(2.6)

to linear order in displacement of ions, with \(A_d, A_p\) and \(A_V\) being constants, \(u_{i,j}\) the displacement of the \(i\)th Cu ion, \(u_{i,j}\), that of an O ion on the adjacent \(s = +\) or \(s = -\) side along the \(\xi\)-axis of the \(i\)th Cu ion, \(\epsilon_x = (1,0), \epsilon_y = (0,1), \epsilon_{ij} = (R_i - R_j)/|R_i - R_j|, \) with \(R_i\) the position of the \(i\)th Cu ion.

Displacements of the \(i\)th Cu and the \([i,j]\)th O ions are given by

\[
\begin{align*}
u_{i} & = \sum_{\lambda_{q}} \frac{h_{\nu_{i},\lambda_{q}}}{\sqrt{2NM_{\nu_{i}}} \omega_{\lambda_{q}}} e^{iq R_{i} \varepsilon_{\lambda_{q}}} b_{\lambda_{q}}^{\dagger} + b_{\lambda_{q}} \
u_{i,j} & = \sum_{\lambda_{q}} \frac{h_{\nu_{i,j},\lambda_{q}}}{\sqrt{2NM_{\nu_{i,j}}} \omega_{\lambda_{q}}} e^{iq R_{i,j} \varepsilon_{\lambda_{q}}} b_{\lambda_{q}}^{\dagger} + b_{\lambda_{q}}
\end{align*}
\]  

(2.7)

(2.8)

with \(R_{i,j} = (1/2)(R_i + R_j)\), \(M_{\nu_{i}}\) the mass of Cu ions, \(M_{\nu_{i,j}}\) the mass of O ions, \(b_{\lambda_{q}}\) and \(b_{\lambda_{q}}^{\dagger}\) annihilation and creation operators of phonons with polarization \(\lambda\) and wave vector \(q\). \(\omega_{\lambda_{q}}\) energies of phonons, \(\varepsilon_{\lambda_{q}}\) unit polarization vectors, and \(N\) the number of unit cells. The \(q\) dependence of \(\varepsilon_{\nu_{i,j},\lambda_{q}}\) and \(\omega_{\lambda_{q}}\) can play a crucial role. For example, \(\varepsilon_{\nu_{i,j},\lambda_{q}} = 0\) and \(\omega_{\lambda_{q}} = O(1)\) for breathing modes that bring no changes in adjacent Cu-Cu distances.

The electronic part can be well described by the \(t-J\) model on a square lattice:

\[
H = \sum_{\langle ij \rangle} \sum_{\sigma} t_{ij} d_{i\sigma}^{\dagger} d_{j\sigma} - \frac{1}{2} J \sum_{\langle ij \rangle} \left( S_i \cdot S_j \right) + U \sum_{\langle ii \rangle} n_{i\uparrow} n_{i\downarrow},
\]  

(2.9)

with the summation over \(\langle ij \rangle\) restricted to nearest neighbors.

\[
S_i = \frac{1}{2} \sum_{\alpha\beta} \left( \sigma_{\alpha}^{\beta} \sigma_{\beta}^{\alpha} \right) d_{i\alpha}^{\dagger} d_{i\beta},
\]  

(2.10)

with \(\sigma_{\alpha}, \sigma_{\beta}\) the Pauli matrices, and \(n_{i\sigma} = d_{i\sigma}^{\dagger} d_{i\sigma}\). An infinitely large on-site repulsion, \(U_{\infty}/|t_{ij}| \rightarrow +\infty\), is introduced to exclude any doubly occupied sites.

According to Eq. (2.4), there are two types of electron-phonon interactions. Define an operator by

\[
P_{\Gamma}(q) = \frac{1}{2} \sum_{\alpha\beta} \eta_{\Gamma}(q) \left[ S(q + \frac{1}{2}q) \cdot S(-q + \frac{1}{2}q) \right].
\]  

(2.11)

with

\[
S(q) = \frac{1}{\sqrt{N}} \sum_{k_{\alpha\beta}} \frac{1}{\sqrt{2NM_{\nu}} \omega_{\lambda_{q}}} \left( b_{\lambda_{q}}^{\dagger} + b_{\lambda_{q}} \right),
\]  

(2.12)

with \(\sigma = (\sigma_{x}, \sigma_{y}, \sigma_{z})\). They are given by

\[
H_{p} = iC_p \sum_{q} \frac{h_{\nu_{p},\lambda_{q}}}{\sqrt{2NM_{\nu_{p}}} \omega_{\lambda_{q}}} \left( b_{\lambda_{q}}^{\dagger} - b_{\lambda_{q}} \right) \times \eta_{\Gamma}(q) \sum_{\Gamma = s,d} \eta_{\Gamma}(\frac{1}{2}q) P_{\Gamma}(q),
\]  

(2.13)

\[
H_{d} = iC_d \sum_{q} \frac{h_{\nu_{d},\lambda_{q}}}{\sqrt{2NM_{\nu_{d}}} \omega_{\lambda_{q}}} \left( b_{\lambda_{q}}^{\dagger} - b_{\lambda_{q}} \right) \times \sum_{\Gamma = s,d} \eta_{\Gamma}(q) P_{\Gamma}(q),
\]  

(2.14)

with

\[
C_{p} = \frac{8A_{p}V^{4}}{(\epsilon_{d} + U - \epsilon_{p})^3} \frac{3}{\epsilon_{d} + U - \epsilon_{p} + \frac{2}{U}},
\]  

(2.15)

\[
C_{d} = -\frac{4A_{p}V^{4}}{(\epsilon_{d} + U - \epsilon_{p})^3} \frac{3}{\epsilon_{d} + U - \epsilon_{p} + \frac{2}{U}} + \frac{2A_{V}J}{V},
\]  

(2.16)

\[
\eta_{\Gamma}(q) = 2 \left[ \frac{q_{x}}{q} \sin \left( \frac{q_{x}q_{a}}{2} \right) + \frac{q_{y}}{q} \sin \left( \frac{q_{y}q_{a}}{2} \right) \right],
\]  

(2.17)
\[ \tilde{\eta}_d(q) = 2 \left[ \frac{g_s}{q} \sin \left( \frac{g_s a}{2} \right) - \frac{g_d}{q} \sin \left( \frac{g_d a}{2} \right) \right], \quad (2.18) \]

\[ \eta_s(k) = \cos(k_x a) + \cos(k_y a), \quad (2.19) \]

\[ \eta_d(k) = \cos(k_x a) - \cos(k_y a), \quad (2.20) \]

with \( a \) the lattice constant. Here, we consider only longitudinal phonons or \( \epsilon_{Aq} = (q_x, q_y, q_z)/q \) is assumed.

### B. Theory of Kondo lattices

We follow the previous paper\(^{23}\) to treat the infinitely large \( U_\infty \), where a theory of Kondo lattice is developed. A renormalized single-site approximation (SSA), which includes not only all the single-site terms but also the Fock term \( \Delta \Sigma(k) \) due to the superexchange interaction, is reduced to solving the Anderson model with the infinitely large on-site repulsion \( U_\infty \). The self-energy of the Anderson model is expanded as

\[ \tilde{\Sigma}_{\sigma}(\epsilon_n) = \tilde{\Sigma}(0) + (1 - \tilde{\phi}_\gamma)\epsilon_n \quad + \sum_{\sigma'} (1 - \tilde{\phi}_{\sigma\sigma'}) \Delta \mu_{\sigma'} + \cdots, \quad (2.21) \]

with \( \Delta \mu_{\sigma} \) infinitesimally small spin-dependent chemical potential shifts. Note that \( \phi_\gamma = \phi_{\sigma\sigma} \). The Wilson ratio \( \tilde{\phi}_\gamma \) is defined by \( \tilde{W}_\gamma = \tilde{\phi}_\gamma / \tilde{\phi}_\gamma \), with \( \tilde{\phi}_\gamma = \phi_{\sigma\sigma} - \phi_{\sigma\sigma} \). For almost half filling, charge fluctuations are suppressed so that \( \tilde{\phi}_\gamma \equiv \phi_{\sigma\sigma} + \phi_{\sigma\sigma} \ll 1 \). For such filling, \( \tilde{\phi}_\gamma \gg 1 \) so that \( \tilde{\phi}_\gamma \approx 2\tilde{\phi}_\gamma \) or \( \tilde{W}_\gamma \approx 2 \). The dispersion relation of quasiparticles is given by

\[ \xi(k) = \frac{1}{\tilde{\phi}_\gamma} \left[ d - \sum_{ij} t_{ij} e^{ik(R_i - R_j)} + \tilde{\Sigma}(0) + \Delta \Sigma(k) - \mu \right], \quad (2.22) \]

with \( \mu \) the chemical potential.

The spin susceptibility is given by

\[ \chi_s(\omega_n, q) = \frac{2\pi_s(\omega_n, q)}{1 - \frac{2}{J(q) + U_\infty} \pi_s(\omega_n, q)}, \quad (2.23) \]

with \( \pi_s(\omega_n, q) \) the irreducible polarization function in spin channels and

\[ J(q) = 2J\eta_d(q). \quad (2.24) \]

The function \( \pi_s(\omega_n, q) \) is divided into single-site \( \tilde{\pi}_s(\omega_n) \) and multi-site \( \Delta \pi_s(\omega_n, q) \) in such a way that \( \pi_s(\omega_n, q) = \tilde{\pi}_s(\omega_n) + \Delta \pi_s(\omega_n, q) \). In Kondo lattices, local spin fluctuations at different sites interact with each other by an exchange interaction. Following this physical picture, we define an exchange interaction \( I_s(\omega_n, q) \) by

\[ \chi_s(\omega_n, q) = \frac{\tilde{\chi}_s(\omega_n)}{1 - \frac{2I_s(\omega_n, q)\tilde{\chi}_s(\omega_n)}{1 - \frac{2\pi_s(\omega_n, q)}{1 - \frac{2}{J(q) + U_\infty} \pi_s(\omega_n, q)}}}, \quad (2.25) \]

with

\[ \tilde{\chi}_s(\omega_n) = \frac{2\pi_s(\omega_n)}{1 - \frac{2}{J(q) + U_\infty} \pi_s(\omega_n)} \quad (2.26) \]

the susceptibility for the mapped Anderson model. Then, we obtain

\[ I_s(\omega_n, q) = J(q) + 2U_\infty^2 \Delta \pi_s(\omega_n, q). \quad (2.27) \]

The main part of \( 2U_\infty^2 \Delta \pi_s(\omega_n, q) \) is an exchange interaction arising from the virtual exchange of pair excitations of quasiparticles.

When the Ward relation\(^{23}\) is made use of, the irreducible single-site three-point vertex function in spin channels, \( \chi_s(\omega_n, \omega_n + \omega_l; \omega_l) \), is given by

\[ U_\infty \chi_s(\omega_n, \omega_n + \omega_l; \omega_l) = 2\tilde{\phi}_s / \tilde{\chi}_s(\omega_n), \quad (2.28) \]

for \( |\epsilon_n| \to +0 \) and \( |\omega_l| \to +0 \). We approximately use Eq. (2.28) for \( |\epsilon_n| \lesssim k_B T_K \) and \( |\omega_l| \lesssim k_B T_K \), with \( T_K \) the Kondo temperature defined by

\[ k_B T_K = |1/\tilde{\chi}_s(0)|_{T \to 0}. \quad (2.29) \]

The so called spin-fluctuation mediated interaction, whose single-site term should be subtracted because it is considered in SSA, is given by

\[ \frac{1}{4} \left[ 2\tilde{\phi}_s / \tilde{\chi}_s(\omega_n) \right]^2 F(\omega_n, q) = \frac{1}{4} I_s(\omega_n, q), \quad (2.30) \]

with

\[ F(\omega_n, q) = \chi_s(\omega_n, q) - \tilde{\chi}_s(\omega_n), \quad (2.31) \]

and

\[ \frac{1}{4} I_s(\omega_n, q) = \frac{1}{1 - \frac{2}{J(q) + U_\infty} \pi_s(\omega_n, q)} \quad (2.32) \]

Because of these equations, we call \( I_s(\omega_n, q) \) a bare exchange interaction. \( I_s(\omega_n, q) \) an enhanced one, and \( \tilde{\phi}_s \) an effective three-point vertex function in spin channels. Intricate effects can be perturbatively considered in terms of \( F(\omega_n, q) \), \( I_s(\omega_n, q) \) or \( I_s(\omega_n, q) \) depending on each situation.

The enhanced one is expanded as

\[ I_s(\omega_n, q) = I_0 + 2I_2 \eta_2(q) + 2I_2 \eta_2(q) + \cdots, \quad (2.33) \]

with

\[ \eta_2(q) = \cos [(k_x + k_y) a] + \cos [(k_x - k_y) a]. \quad (2.34) \]

The nearest-neighbor \( I_0 \) is mainly responsible for the development of SC and charge bond-order (CBO) fluctuations\(^{23}\). Because contributions from \( |\omega_l| \lesssim k_B T_K \) are the most effective, we ignore its energy dependence. An effective SC susceptibility is calculated in the ladder approximation:

\[ \chi_{\text{SC}}(\omega_n, q) = \frac{\pi_{d}(\omega_n, q)}{1 + \frac{2I_2}{W_s^2 \pi_{d}(\omega_n, q)}}, \quad (2.35) \]
for $\Gamma = d$ wave or $d\gamma$ wave, with

$$
\pi_\Gamma^{(SC)}(i\omega_l, \mathbf{q}) = \frac{k_BT}{N} \sum_{nk} \eta_\Gamma^2(k) \frac{1}{i\varepsilon_n - \xi(k + \frac{1}{2}q)} \times \frac{1}{-i\varepsilon_n - i\omega_l - \xi(-k + \frac{1}{2}q)}, 
$$

(2.36)

Only $d\gamma$-wave SC fluctuation are considered in this paper because $T_c$ of $d\gamma$ wave are definitely much higher than $T_c$ of other waves. An effective CBO susceptibility is similarly given by

$$
\chi_\Gamma^{(CBO)}(i\omega_l, \mathbf{q}) = \frac{\pi_\Gamma^{(CBO)}(i\omega_l, \mathbf{q})}{1 + \frac{4}{3}I_1^*W_s^2\pi_\Gamma^{(CBO)}(i\omega_l, \mathbf{q})}, 
$$

(2.37)

for $\Gamma = s, p$ and $d\gamma$ waves, with

$$
\pi_\Gamma^{(CBO)}(i\omega_l, \mathbf{q}) = -\frac{k_BT}{N} \sum_{nk} \eta_\Gamma^2(k) \frac{1}{i\varepsilon_n - \xi(k - \frac{1}{2}q)} \times \frac{1}{i\varepsilon_n + i\omega_l - \xi(k + \frac{1}{2}q)}. 
$$

(2.38)

The form factors of $p$ waves are defined by

$$
\eta_x(k) = \sqrt{2}\sin(k_x a), \quad \eta_y(k) = \sqrt{2}\sin(k_y a). 
$$

(2.39)

According to Eq. 2.25, $T_c$ of $d\gamma$ wave superconductivity are given by

$$
1 + \frac{4}{3}I_1^*W_s^2\pi_d(0, 0) = 0. 
$$

(2.40)

It was shown in the previous papers that

$$
\frac{4}{3}I_1^*W_s^2 \simeq 100 \text{ meV} 
$$

(2.41)

is needed in order to explain observed $T_c$. The Wilson ratio is as large as $W_s \simeq 2$ in SSA, and the superexchange interaction is as strong as $J = -(100-150) \text{ meV}$ in actual cuprate oxide superconductors. Then, it follows that $\frac{4}{3}I_1^*W_s^2 \gtrsim 400 \text{ meV}; |I_1^*| > |J|$. The theory published in 1987 has a drawback that it gives too high theoretical $T_c$ to explain observed $T_c$. The mass enhancement factor and the effective three-point vertex function are renormalized by AF, SC and CBO fluctuations, so that $\tilde{W}_s$ that is the effective three-point vertex function divided by the mass enhancement factor is also renormalized by the fluctuations. We argued in the previous paper that the renormalization of $\tilde{W}_s$ is substantial so that $\tilde{W}_s \lesssim 1$ or $W_s \lesssim 1$; a phenomenological argument also implies that $\tilde{W}_s = 0.7-1$ had better been used in order to explain quantitatively $T_c$ and $T$-linear resistivities. For example, Eq. (2.41) can only be satisfied for such small $\tilde{W}_s$. We follow this argument. Taking the renormalization into account, we regard $W_s$ as a phenomenological parameter; we assume

$$
\tilde{W}_s = 1 
$$

(2.42)

in this paper.

### C. Renormalization of phonons

The Green function for phonons is given by

$$
D_\lambda(i\omega_l, \mathbf{q}) = \frac{2\omega_{\lambda q}}{(i\omega_l)^2 - \omega_{\lambda q}^2 + 2\omega_{\lambda q}\Delta\omega_\lambda(i\omega_l, \mathbf{q})}, 
$$

(2.43)

with

$$
\Delta\omega_\lambda(i\omega_l, \mathbf{q}) = -\frac{\hbar^2}{2M_{\lambda q}^2} S(i\omega_l, \mathbf{q}). 
$$

(2.44)

Because phonons are renormalized by AF, SC and CBO fluctuations as well as charge density fluctuations, we consider four processes shown in Fig. 2. If $S(i\omega_l, \mathbf{q}) = S_s(i\omega_l, \mathbf{q}) + S_{sc}(i\omega_l, \mathbf{q}) + S_{cbo}(i\omega_l, \mathbf{q}) + S_t(i\omega_l, \mathbf{q})$. The expression for $\Delta\omega_\lambda$ in Eq. (2.44) is convenient in treating couplings with AF fluctuations. Other expressions, which are convenient in treating couplings with SC and CBO fluctuations, are shown in Appendix. When Eqs. (A1), (A3), and (A6) are made use of and only the parts of $\Gamma = s$ in Eqs. (2.13) and (2.14) are considered, it follows that

$$
S_s(i\omega_l, \mathbf{q}) = \frac{3}{4\lambda}Y_s^2(i\omega_l, \mathbf{q}) \frac{k_BT}{N} \sum_{k_1} \eta_s^2(k_1) \chi_s(i\omega_l + i\omega_{\lambda q}, \mathbf{q}' + \frac{1}{2}\mathbf{q}) \chi_s(-i\omega_{\lambda q}, -\mathbf{q}' + \frac{1}{2}\mathbf{q}), 
$$

(2.45)

$$
S_{sc}(i\omega_l, \mathbf{q}) = \frac{3}{4\lambda}Y_s^2(i\omega_l, \mathbf{q}) \frac{k_BT}{N} \sum_{k_1} \chi_d^{sc}(i\omega_l + i\omega_{\lambda q}, \mathbf{q}' + \frac{1}{2}\mathbf{q}) \chi_d^{sc}(-i\omega_{\lambda q}, -\mathbf{q}' + \frac{1}{2}\mathbf{q}) 
$$

$$
-\pi_d^{sc}(i\omega_l + i\omega_{\lambda q}, \mathbf{q}' + \frac{1}{2}\mathbf{q}) \pi_d^{sc}(-i\omega_{\lambda q}, -\mathbf{q}' + \frac{1}{2}\mathbf{q}), 
$$

(2.46)
FIG. 1: Four processes of the renormalization of phonons. A solid line stands for an electron, a broken line for a phonon, a wavy line for the superexchange interaction \( J \), and a solid circle for the effective vertex function \( \phi_s \). Hatched parts in Figs. (a), (b) and (c) stand for AF (spin), SC and CBO fluctuations, respectively, and a hatched part, including an internal electron line, in Figs. (d) for the vertex function \( Z(i\varepsilon_n, i\omega_l; k, q) \). The contribution from Figs. (d) is larger than those of Figs. (a), (b) and (c): two fluctuation-lines with different \( q \) or two susceptibilities of different \( q \) appear in the convolution form in Figs. (a), (b) and (c) so that their contributions can be large only when fluctuations are developed in a wide region of the momentum space.

\[
S_{CBO}(i\omega_l, q) = \frac{3^2}{4^2} \tilde{W}_s^4 Y_s^2(q) \sum_{\Gamma} \frac{k_B T}{N} \sum_{\nu' q'} \left[ \chi_{\Gamma}^{CBO}(i\omega_l + i\omega_{l'}, q' + \frac{1}{2} q) \chi_{\Gamma}^{CBO}(-i\omega_{l'}, -q' + \frac{1}{2} q) \right. \\
- \pi_d^{CBO}(i\omega_l + i\omega_{l'}, q' + \frac{1}{2} q) \pi_d^{CBO}(-i\omega_{l'}, -q' + \frac{1}{2} q) \right],
\]

\[
S_c(i\omega_l, q) = \frac{3^2}{4^2} \tilde{W}_s^4 Y_s^2(q) \frac{k_B T}{N} \sum_{\nu k \sigma} Z^2(i\varepsilon_n, i\omega_l; k, q) \frac{1}{i\varepsilon_n - \xi(k)} \frac{1}{i\varepsilon_n + i\omega_l - \xi(k + q)},
\]

with

\[
Y_s(q) = \tilde{\eta}_s(q) \left[ C_{\nu p, \lambda} \eta_s \left( \frac{1}{2} q \right) + C_{d\nu d, \lambda} \sqrt{M_p/M_d} \right].
\]

In Eq. (2.48), \( Z(i\varepsilon_n, i\omega_l; k, q) \) is the vertex function in the charge channel. It is also enhanced by AF, SC and CBO fluctuations; \( Z(i\varepsilon_n, i\omega_l; k, q) = Z_s(i\varepsilon_n, i\omega_l; k, q) + Z_{SC}(i\varepsilon_n, i\omega_l; k, q) + Z_{CBO}(i\varepsilon_n, i\omega_l; k, q) + \cdots \), with

\[
Z_s(i\varepsilon_n, i\omega_l; k, q) = \frac{k_B T}{N} \sum_{\nu' q'} \eta_s(q') K_s(i\omega_{l'}, q' + \frac{1}{2} q) K_s(-i\omega_{l'} + i\omega_l, -q' + \frac{1}{2} q) \frac{1}{i\varepsilon_n + i\omega_l - \xi(k + q' + \frac{1}{2} q)},
\]

\[
Z_{SC}(i\varepsilon_n, i\omega_l; k, q) = \frac{k_B T}{2} \sum_{\nu' q'} \eta_d(q') K_d(i\omega_{l'}, q' - \frac{1}{2} q) K_d^SC(i\omega_{l'} + i\omega_l, q' + \frac{1}{2} q) \frac{1}{-i\varepsilon_n + i\omega_l' - \xi(-k + q' - \frac{1}{2} q)},
\]

\[
Z_{CBO}(i\varepsilon_n, i\omega_l; k, q) = \frac{k_B T}{2} \sum_{\nu' q'} \sum_{\Gamma} \eta_r(q' + \frac{1}{2} q) K_r^CBO(i\omega_{l'}, q' + \frac{1}{2} q) K_r^CBO(-i\omega_{l'} + i\omega_l, -q' + \frac{1}{2} q) \frac{1}{i\varepsilon_n + i\omega_l - \xi(k + q' + \frac{1}{2} q)},
\]

with

\[
K_s(i\omega_l, q) = \frac{1}{1 - \frac{3}{4} I(i\omega_l, q) \tilde{\chi}_s(i\omega_l)},
\]

\[
K_d^SC(i\omega_l, q) = \frac{1}{1 + \frac{3}{4} I^2 W_s^2 \pi_d^{SC}(i\omega_l, q)} - 1,
\]

\[
K_r^CBO(i\omega_l, q) = \frac{1}{1 + \frac{3}{2} I^2 W_s^{CBO}(i\omega_l, q)} - 1.
\]

Here, Eqs. (A1), (A3), and (A6) are also made use of; zero-th order terms in \( I_1 \) are subtracted in Eqs. (2.49),
to avoid any double counting.

III. APPLICATION TO CUPRATE OXIDE SUPERCONDUCTORS

A. Softening of phonons

Because it is not a purpose of this paper to study phonon modes themselves, we study only issues that can be clarified without calculating them. First, we consider the softening of the so-called half breathing mode of O ions with \( Q_X = (\pm \pi/a, 0) \) or \((0, \pm \pi/a)\). Because

\[
v_{d,\lambda Q_X} = 0, \quad v_{p,\lambda Q_X} = 1, \tag{3.1}
\]

we have to consider only the electron-phonon interaction given by Eq. \( (2.14)\).

Because doped holes mainly go into O ions, one may argue that 3d levels of Cu ions are deeper than 2p levels of O ions, \( \epsilon_d < \epsilon_p \). However, this argument disagrees with what band calculations predict. When we use \( d \), the softening of the so-called half breathing mode of O ions, \( \epsilon_d < \epsilon_p \), but it simply means that the local charge susceptibility of 3d electrons is much smaller than that of 2p electrons, as is discussed in Introduction. Because it is unlikely that band calculations give such a bad prediction on relative positions between the 3d and 2p levels, we follow what band calculations predict. When we use

\[
V = 1.6 \text{ eV}, \quad \epsilon_d - \epsilon_p = 1 \text{ eV}, \quad U = 5 \text{ eV}, \tag{3.2}
\]

following the previous paper\( ^{29}\), Eq. \( (2.2)\) gives \( J = -0.27 \text{ eV} \). This is about twice as large as the experimental one of \( J = -(0.10-0.15) \text{ eV} \). This discrepancy is resolved when nonzero bandwidths of the lower and upper Hubbard band are considered.\(^{29}\) Because of this, we assume a half of \( C_p \) given by Eq. \( (2.14)\): \( C_p = 0.1 \times A_d \) instead of \( C_p = 0.22 \times A_d \). When we take \( A_d \approx 5 \text{ eV/Å} \), it follows that

\[
C_p \approx 0.5 \text{ eV/ Å}, \quad Y_\lambda(Q_X) \approx 1 \text{ eV/Å}. \tag{3.3}
\]

Two susceptibilities appear in the convolution form in Eqs. \( (2.45)\), \( (2.46)\) and \( (2.47)\). Unless AF, SC and CBO fluctuations are developed in a wide region of the momentum space, the convolutions cannot be large. We assume that \( S_c(\delta \omega l, \mathbf{q}) \) given by Eq. \( (2.48)\) is dominant in \( S(\delta \omega l, \mathbf{q}) \). When only \( S_c(\delta \omega l, \mathbf{q}) \) is considered,

\[
S(\delta \omega l, \mathbf{q}) \approx \frac{3 \hbar^2}{4} \mathbf{W}_s^4 \langle Z^2 \rangle \frac{Y_\lambda(Q_X)}{2k_BT_K}, \tag{3.4}
\]

with \( \langle Z^2 \rangle \) an average of \( Z^2(\delta \omega n, \delta \omega l; \mathbf{k}, \mathbf{q}) \). When we assume \( \mathbf{W}_s = 1 \), the softening at X point is given by

\[
\Delta \omega_\lambda(\omega_{\lambda Q_X}, Q_X) \approx -0.01 \langle Z^2 \rangle \left( \frac{10^3 \text{ meV}^2}{\omega_{\lambda Q_X} k_BT_K} \right) \text{ meV}. \tag{3.5}
\]

When we put

\[
\omega_{\lambda Q_X} \approx k_BT_K \approx 10^2 \text{ meV}, \tag{3.6}
\]

it follows that

\[
\Delta \omega_\lambda(\omega_{\lambda Q_X}, Q_X) \approx \langle Z^2 \rangle \text{ meV}. \tag{3.7}
\]

When AF, SC and CBO fluctuations are not developed, \( \langle Z^2 \rangle \lesssim 1 \) and the softening must be very small. When AF, SC and CBO fluctuations are well developed, \( \langle Z^2 \rangle \) might be as large as \( \langle Z^2 \rangle \approx 10 \), we can explain the observed softening as large as

\[
\Delta \omega_\lambda(\omega_{\lambda Q_X}, Q_X) \approx 10 \text{ meV}. \tag{3.8}
\]

When other contributions are considered in addition to \( S_c(\delta \omega l, \mathbf{q}) \), \( \langle Z^2 \rangle \) can be smaller than 10 to explain the observed softening.

No softening occurs for \( q = 0 \) because \( \eta_\lambda(0) = 0 \). When \( q \) goes from \( \Gamma \) point to X point, the softening must increase first but it is unlikely that the softening is the largest at X point. Because \( v_{d,\lambda Q_X} = 0 \), the electron-phonon interaction described by Eq. \( (2.14)\) vanishes. This implies that the softening cannot be the largest at X point along \( \Gamma-X \) line. In actual, several experimental data imply that the softening is the largest for \( q \) a little different from \( Q_X \) along \( \Gamma-X \) line.

No softening cannot occur either at M point or for the breathing mode of O ions with \( Q_M = (\pm \pi/a, \pm \pi/a) \) because \( v_{d,\lambda Q_M} = 0 \) and \( \eta_\lambda(\pm Q_M) = 0 \). It is interesting to confirm this prediction.

B. Kinks in the quasiparticle dispersion

A process corresponding to Fig. 1(d) renormalizes quasiparticles. The self-energy correction is given by

\[
\frac{1}{\phi_\gamma} \Delta \Sigma(\delta \varepsilon_n, \mathbf{k}) = -\frac{k_BT}{N} \sum_{\lambda \mathbf{q}} g_\lambda^2(\delta \varepsilon_n, \delta \omega_l; \mathbf{k}, \mathbf{q}) D_\lambda(\delta \omega_l, \mathbf{q}) \times \sum_{\delta \varepsilon_n + i\delta \omega_l - \xi(\mathbf{k} + \mathbf{q})} \frac{1}{\delta \varepsilon_n + i\delta \omega_l - \xi(\mathbf{k} + \mathbf{q})}. \tag{3.9}
\]

with

\[
g_\lambda(\delta \varepsilon_n, \delta \omega_l; \mathbf{k}, \mathbf{q}) = \frac{\hbar}{2M_p \delta \varepsilon_n \delta \omega_l} \frac{3}{4} \mathbf{W}_s \mathbf{Y}_\lambda(q) \times Z(\delta \varepsilon_n, \delta \omega_l; \mathbf{k}, \mathbf{q}). \tag{3.10}
\]

It is likely that the contribution of Fig. 2(d) dominate those of the other three, Figs. 2(a)–(c). In such a case,

\[
g_\lambda(\delta \varepsilon_n, \delta \omega_l; \mathbf{k}, Q_X) \approx \sqrt{2k_BT_K} |\Delta \omega_\lambda(\omega_{\lambda Q_X}, Q_X)|. \tag{3.11}
\]

Here, Eqs. \( (2.43)\) and \( (3.3)\) are made use of. When the experimental value \( 3.5\) is used, we obtain

\[
g_\lambda(\delta \varepsilon_n, \delta \omega_l; \mathbf{k}, Q_X) \approx 45 \text{ meV}. \tag{3.12}
\]
This is large enough for optical phonons to cause kinks in the quasiparticle dispersion.

Two types of kinks are observed. The renormalization by phonons can explain one type of kinks observed in both normal and SC phases. However, it is difficult to explain the other type of kinks observed only in SC phases; low-energy AF and SC fluctuations are suppressed when SC gaps open.

C. Cooper-pair interaction

The phonon-mediated pairing interaction is given by

\[ V_{ph}(q; k) = -2g_3^2(0, 0; k, q) / \omega_{\lambda q}. \]  (3.13)

Its average over \( k \) on the Fermi surface is expanded in such a way that

\[ \langle V_{ph}(q; k) \rangle = V_0 + 2V_1 \eta_0(q) + 2V_2 \eta_{q^2}(q) + \cdots. \]  (3.14)

No softening at \( \Gamma \) and \( M \) points implies \( \langle V_{ph}(0; k) \rangle = 0 \) and \( \langle V_{ph}(Q_M; k) \rangle = 0 \), so that

\[ V_0 + 2V_1 + 2V_2 \simeq 0, \quad V_0 - 2V_1 + 2V_2 \simeq 0. \]  (3.15)

Because of Eq. (3.12), \( \langle V_{ph}(Q_X; k) \rangle \simeq -40 \text{ meV} \) or

\[ V_0 - 2V_2 \simeq -40 \text{ meV}. \]  (3.16)

Then, we obtain

\[ V_0 \simeq -20 \text{ meV}, \quad V_1 \simeq 0 \text{ meV}, \quad V_2 \simeq 10 \text{ meV}. \]  (3.17)

The interaction \( V_1 \) between nearest neighbors should be included in addition to \( \frac{3}{4}J I_t^3 W_s^2 \) in the theory of \( d^- \) wave high-\( T_c \) superconductivity. When Eq. (4.1) is extended to include \( V_1, T_c \) are determined by

\[ 1 + \left( \frac{3}{4}J I_t^3 W_s^2 + V_1 \right) \tau_d^{(SC)}(0, 0) = 0. \]  (3.18)

Although the \( q \) dependence of \( \langle V_{ph}(q; k) \rangle \) in the whole Brillouin zone is necessary to estimate \( V_1 \) accurately, we can conclude that \( |V_1| \) must be much smaller than \( \frac{3}{4}J I_t^3 W_s^2 \simeq 100 \text{ meV} \), which is needed in order to explain observed \( T_c \).

There are various branches of phonon modes beside the mode discussed above. The virtual exchange of phonons that do not become soft cannot give a significant pairing interaction.

IV. DISCUSSION

Following Barnes, we can map the \( t-J \) model to the so called auxiliary-particle \( t-J \) model: \( \hat{H}_{t-J} = \mathcal{P}^{-1} \hat{H} \mathcal{P} \), with

\[ \hat{H} = \delta \sum_i \left( c_i^\dagger c_i + c_{i\uparrow}^\dagger c_{i\downarrow} + c_i^\dagger c_i - 1 \right) + \epsilon_d \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} \]
\[ - \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma}^{\dagger} - \frac{1}{2} J \sum_{ij} \langle \hat{S}_i \cdot \hat{S}_j \rangle, \]  (4.1)

with \( \delta \) being an arbitrary constant and

\[ \hat{S}_i = \frac{1}{2} \sum_{\alpha\beta} \left( \sigma_{\alpha\beta}^x \sigma_{\alpha\beta}^y + \sigma_{\alpha\beta}^z \right) \]  (4.2)

Two kinds of auxiliary particles, which correspond to empty and occupied sites in the original \( t-J \) model, are introduced: \( e_i^\dagger \) and \( c_i^\dagger \) are their creation operators. We call them \( e \) and \( c \) particles in this paper. The projection operator \( \mathcal{P} \) restricts the Hilbert space within

\[ Q_i = e_i^\dagger e_i + c_i^\dagger c_i + c_i^\dagger c_i = 1 \]  (4.3)

for any \( i \), if empty or multiply occupied sites are allowed. This restriction is guaranteed by the conservation of the number of auxiliary particles such as

\[ [\hat{H}, Q_i] = 0 \]  (4.4)

for any \( i \), or local gauge symmetry. This symmetry is inherent in the auxiliary-particle model. Local gauge symmetry can never be broken. Therefore, no single auxiliary particle can be added or removed, or no single-particle excitation of auxiliary particles is allowed. Auxiliary particles themselves are never itinerant but are localized; pair excitations of auxiliary particles are itinerant. Fermionic pair excitations of auxiliary particles correspond to electrons in \( t-J \) model. Two ways of statistics are possible: fermionic \( e \) and bosonic \( c \) particles, and fermionic \( e \) and bosonic \( e \) particles. The model with bosonic \( e \) and fermionic \( c \) particles is often called the slave-boson \( t-J \) model. The mean-field (MF) theory for \( \hat{H} \), instead of \( \mathcal{P}^{-1} \hat{H} \mathcal{P} \), and its more or less improved theories, which include gauge fluctuations, assume the breaking of local gauge symmetry, and they treat single-particle excitations of itinerant auxiliary particles. Such theories are never relevant to study dynamics of electrons in the original \( t-J \) model; condensation energies derived in these treatments are consistent with Gutzwiller’s theory and are reliable. A more precise discussion on this issue can be found in Appendix of Ref. 29. Although an apparently similar theoretical development to that of this paper is possible when one starts from the MF approximation for the slave-boson \( t-J \) model, it is physically and essentially different from the theory of Kondo lattices: states considered in the two theories are of totally different symmetry from each other. Therefore, we should abstain from comparing results based on the theory of Kondo lattices with those of the MF theory of the slave-boson \( t-J \) model. Note that \( \hat{\phi}_c \) and \( 1/\hat{\phi}_c \) are small parameters in the vicinity of the Mott-Hubbard transition. What are considered in this paper are of leading order in both \( \hat{\phi}_c \) and \( 1/\hat{\phi}_c \), that is, order of \( (\hat{\phi}_c)^0 (1/\hat{\phi}_c)^0 \).

There are two other types of electron-phonon interactions: the modulation of 3d-electron levels, \( \epsilon_d \), and that of the transfer integrals, \( t_{ij} \). The conventional one arising from the modulation of \( \epsilon_d \), which can directly couples with charge fluctuations, gives renormalization effects higher order in \( \hat{\phi}_c \) and \( 1/\hat{\phi}_c \), so that its effects must
be very small. The electron-phonon interaction arising from the modulation of \( t_{ij} \) gives renormalization effects higher order in \( 1/\phi_n \), so that their effects of the electron-phonon interaction must be \( 1/\phi_n^2 \) times as small as those studied in this paper; we expect that coupling constants for \( t_{ij} \), which correspond to \( A_d \), \( A_p \) and \( A_V \) of this paper, are of the same order of magnitude as \( A_V \). Then, we ignore both of them in this paper.

There are also pieces of experimental evidence that the electron-phonon interaction arising from the modulation of \( \epsilon_d \) or \( t_{ij} \) by phonons is irrelevant in cuprates. Hwang, Timusk and Gu investigated life-time widths of quasiparticles instead of kinks; life-time widths depend on temperature and dopings. Their observation implies that kinks are large only in metallic cuprates where AF and SC fluctuations are well developed. The softening of phonons is also large in such metallic cuprates; no significant softening is observed in over-doped cuprates. It is difficult to explain these observations in terms of the electron-phonon interaction arising from the modulation of \( \epsilon_d \) or \( t_{ij} \) by phonons. On the other hand, these observations are pieces of evidence that the electron-phonon interaction that can couple directly with AF and SC channels is relevant and its enhancement by AF and SC fluctuations in metallic phase is crucial.

In insulating phases, only the contributions from Eq. (2.15) remains but those from Eqs. (2.16)-(2.18) vanish. Then, we cannot expect significant softening of phonons. This is also consistent with experiment.

Various physical properties are different or asymmetric between hole-doped and electron-doped cuprates. Within the theoretical framework of this paper, hole-doped and electron-doped cuprates must be, in essence, similar to each other. Phenomenologically, AF and SC fluctuations are relatively more developed in hole-doped cuprates than they are in electron-doped cuprates. If the asymmetry of the fluctuations can be explained, we can explain that of phonon properties. It is pointed out in another paper that the asymmetry of disorder can play a crucial role in the asymmetry between hole-doped and electron-doped cuprates.

In cuprate oxide superconductors, the exchange interaction arising from the virtual exchange of pair excitations of quasiparticles is less effective than the superexchange interaction; the pairing interaction arising from phonons can play no significant role. Then, the main pairing interaction \( I^*_1 \) must arise from the superexchange interaction, which is enhanced by spin fluctuations.

As is discussed in Introduction, the superexchange interaction arises from the virtual exchange of pair excitations of electrons across the lower and upper Hubbard bands. As is shown in Eqs. (2.30) and (2.32), the spin-fluctuation mediated pairing interaction is essentially the same as the superexchange interaction if high-energy spin fluctuations, whose energies are as large as the Hubbard onsite repulsion \( U \), are properly included. However, it is physically different from the superexchange interaction if only low-energy spin fluctuations are included.

The SSA is rigorous for Landau’s Fermi-liquid states in infinite dimensions so that the theory of Kondo lattices can be regarded as a 1/d expansion theory, with \( d \) being the spatial dimensionality. One may suspect that the 1/d expansion theory cannot be applied to quasi-two-dimensional cuprates. Any perturbative theory relies on the analytical continuity a perturbed state must be of the symmetry as an unperturbed state is. Normal states in over-doped or optimal-doped cuprates are certainly Landau’s normal Fermi liquids. Because there is no evidence that any symmetric change occurs between normal states in over-doped or optimal-doped cuprates and exotic normal states in under-doped cuprates, we can argue that the analytical continuity holds so that the 1/d expansion theory or the theory of Kondo lattices can be applied to exotic normal states in cuprates.

V. CONCLUSION

The electron-phonon interaction arising from the modulation of the superexchange interaction by phonons is relevant for strongly correlated electron liquids in the vicinity of the Mott-Hubbard transition. It is shown with the help of the theory of Kondo lattices that it can be enhanced by spin, superconducting, and charge bond-order fluctuations as well as charge fluctuations. The enhanced electron-phonon interaction is responsible for not only the softening of phonons but also kinks in the dispersion relation of quasiparticles in cuprate oxide high-temperature superconductors. However, it can never be the main Cooper-pair interaction. The main one must be the superexchange interaction.

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APPENDIX A: VARIOUS EXPRESSIONS FOR THE ELECTRON-PHONON INTERACTION

Equation (2.11) is also written in another form:
\[ \mathcal{P}_\Gamma(q) = \frac{1}{2N} \sum_{kpq} \sum_{\alpha\beta\gamma\delta} \eta_T(q') \left( s^{\alpha\beta}, s^{\gamma\delta} \right) a^\dagger_{(k+q preemptive+q')\alpha} a_{(k-q preemptive+q')\beta} a^\dagger_{(p-q preemptive+q')\gamma} a_{(p+q preemptive+q')\delta}. \] (A1)

This expression is useful to obtain Eqs. (A14) and (A30). When we replace variables in Eq. (A1) in such a way that \( k + \frac{1}{2} q' = k_1 + \frac{1}{2} q_1, k - \frac{1}{2} q' = p_1 + \frac{1}{2} q_1, \) and \( p + \frac{1}{2} q' = k_1 - \frac{1}{2} q_1, \) Eq. (A1) turns out to

\[ \mathcal{P}_\Gamma(q) = \frac{1}{2N} \sum_{kp_1q_1} \sum_{\alpha\beta\gamma\delta} \eta_T(k_1 - p_1) \left( s^{\alpha\beta}, s^{\gamma\delta} \right) a^\dagger_{(k_1+q_1+q_1)\alpha} a_{(p_1+q_1)\beta} a^\dagger_{(p_1-\frac{1}{2} q_1+\frac{1}{2} q_1)\gamma} a_{(k_1-\frac{1}{2} q_1)\delta}. \] (A2)

Matrix elements of \( \alpha = \delta = \gamma = \beta = \gamma \) are relevant for CBO channels, and they are the same as those given by

\[ \mathcal{P}'_\Gamma(q) = \frac{1}{2N} \sum_{kp_1q_1} \sum_{\alpha\beta\gamma\delta} \eta_T(k_1 - p_1) \left[ -3 \rho_c(k_1 + \frac{1}{2} q_1 + \frac{1}{2} q_1, k_1 - \frac{1}{2} q_1) \rho_c(p_1 - \frac{1}{2} q_1 + \frac{1}{2} q_1, p_1 + \frac{1}{2} q_1) \right] + \cdots, \] (A3)

with

\[ \rho_c(k_1, k_2) = a^\dagger_{k_1} a_{k_2}, \quad \rho_s(k_1, k_2) = a^\dagger_{k_1} a_{k_2} - a^\dagger_{k_2} a_{k_1}. \] (A4)

except for those given by what appear through the commutation of operators, which are not shown here. This expression is useful to obtain Eqs. (A47) and (A59). When we replace variables in Eq. (A2) in such a way that \( k_1 + \frac{1}{2} q_1 = k_2 + \frac{1}{2} q_2, p_1 + \frac{1}{2} q_1 = p_2 + \frac{1}{2} q_2, \) and \( k_1 - \frac{1}{2} q_1 = -p_2 + \frac{1}{2} q_2, \) Eq. (A2) turns out to

\[ \mathcal{P}_\Gamma(q) = \frac{1}{2N} \sum_{kp_2q_2} \sum_{\alpha\beta\gamma\delta} \eta_T(k_2 - p_2) \left( s^{\alpha\beta}, s^{\gamma\delta} \right) a^\dagger_{(k_2+q_2+\frac{1}{2} q_2)\alpha} a_{(p_2+q_2)\beta} a^\dagger_{(-k_2+\frac{1}{2} q_2+\frac{1}{2} q_2)\gamma} a_{(-p_2+\frac{1}{2} q_2)\delta}. \] (A5)

Matrix elements of \( \gamma = -\alpha \) and \( \delta = -\beta \) are relevant for singlet SC channels, and they are the same as those given by

\[ \mathcal{P}'_\Gamma(q) = \frac{1}{2N} \sum_{kp_2q_2} \sum_{\alpha\beta\gamma\delta} \eta_T(k_2 - p_2) \left[ -3 \rho^\dagger_{c}(k_2 + \frac{1}{2} q_2 + \frac{1}{2} q_2, -k_2 + \frac{1}{2} q_2 + \frac{1}{2} q_2) \rho_1(p_2 + \frac{1}{2} q_2, p_2 + \frac{1}{2} q_2) \right] + \cdots, \] (A6)

with

\[ \rho^\dagger_{c}(k_1, k_2) = a^\dagger_{k_1} a^\dagger_{k_2}, \quad \rho_3(k_1, k_2) = a^\dagger_{k_1} a^\dagger_{k_2} + a^\dagger_{k_1} a^\dagger_{k_2}. \] (A7)

except for those given by what appear through the commutation of operators, which are not shown here. This expression is useful to obtain Eqs. (A46) and (A51). The following relation is also useful:

\[ 2 \eta_s(k - p) = \eta_s(k) \eta_s(p) + \eta_d(k) \eta_d(p) + \eta_x(k) \eta_x(p) + \eta_y(k) \eta_y(p). \] (A8)

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