Electron-phonon interaction in cuprate-oxide superconductors

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We propose a novel electron-phonon interaction arising from the modulation of the superexchange interaction by phonons. It is enhanced by spin and superconducting fluctuations, which are developed mainly because of the superexchange interaction. It must be responsible for the softening of phonons and kinks in the dispersion relation of quasi-particles. However, the superexchange interaction must be mainly responsible for the formation of Cooper pairs.

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It is an important issue to elucidate the mechanism of high-$T_c$ superconductivity occurring on CuO$_2$ planes. Two observations, the softening of phonons and kinks in the quasi-particle dispersion, imply the relevance of the electron-phonon interaction. One may argue that it must be responsible for high-$T_c$ superconductivity. Its origin and role should be clarified.

Doped holes mainly go into O ions. This implies that the charge susceptibility of 3d electrons on Cu ions is much smaller than that of 2p electrons on O ions and charge fluctuation of 3d electrons can never be developed. Then, the conventional electron-phonon interaction, which directly couples with charge fluctuations, can play no crucial role. On the other hand, antiferromagnetic spin (AFS) and superconducting (SC) fluctuations are certainly developed. One may argue that their developments are because of the superexchange interaction. It is shown in early papers that the condensation of $d_{\gamma}$-wave Cooper pairs bound by the superexchange interaction can explain observed $T_c$. It is shown in a previous paper that pseudo-gaps appear because of large lifetime widths of quasi-particles due to SC fluctuations. Suggested by these arguments, we propose in this letter an electron-phonon interaction arising from the modulation of the superexchange interaction by phonons.

It is shown in another previous paper that Gutzwiller’s quasi-particle band lies between the lower and upper Hubbard bands in metallic phases in the vicinity of the Mott-Hubbard transition. The superexchange interaction arises from the virtual exchange of pair excitations of electrons in spin channels across the lower and upper Hubbard bands; as long as the Hubbard splitting is significant, it works between Gutzwiller’s quasi-particles or their renormalized ones. When nonzero bandwidths of the lower and upper Hubbard bands are ignored, the exchange constant between nearest-neighbor Cu ions is given by

$$J = -4V^4 \frac{1}{(\epsilon_d + U - \epsilon_p)^2} \left[ \frac{1}{\epsilon_d + U - \epsilon_p + 1} \right],$$

with $V$ the transfer integral between $3d$ and $2p$ orbits on adjacent Cu and O ions, and $\epsilon_d$ and $\epsilon_p$ their energy levels. The exchange constant depends on $V$, $\epsilon_p$ and $\epsilon_d$’s of adjacent Cu ions in such a way that

$$\Delta J = \frac{V^4}{(\epsilon_d + U - \epsilon_p)^3} \left[ \frac{6}{\epsilon_d + U - \epsilon_p + 4} \right] \times (\Delta \epsilon_{d|i} + \Delta \epsilon_{d|j} - 2\Delta \epsilon_{p|ij}) + 2\frac{J}{V}(\Delta V_{i|i} + \Delta V_{j|ij}),$$

with $\Delta \epsilon_{d|i}$ a variation of $\epsilon_d$ of the $i$th Cu ion, $\Delta \epsilon_{p|ij}$ a variation of $\epsilon_p$ of the $|ij|$th O ion that lies between the $i$th Cu ion and the $|ij|$th Cu ion, and $\Delta V_{ij}$ that of $V$ between the $i$th Cu ion and the $|ij|$th O ion. When we take the $x$- and $y$-axes along Cu-O-Cu bonds, they are given by

$$\Delta \epsilon_{d|i} = A_d \{ e_x \cdot (u_{i,x,+} - u_{i,x,-}) + e_y \cdot (u_{i,y,+} - u_{i,y,-}) \},$$

$$\Delta \epsilon_{p|ij} = A_p \{ e_x \cdot (u_{i} - u_{j}) \},$$

$$\Delta V_{i|i} + \Delta V_{j|ij} = A V \{ e_y \cdot (u_{i} - u_{j}) \},$$

with $A_d$, $A_p$ and $A V$ being constants, $u_i$ the displacement of the $i$th Cu ion, $u_{i,\epsilon}$ of an O ion on the adjacent side $s = +$ or $s = -$ side along the $\xi$-axis of the $i$th Cu ion, $e_x = (1, 0)$, $e_y = (0, 1)$, and $e_{ij} = (R_i - R_j)/|R_i - R_j|$, with $R_i$ the position of the $i$th Cu ion. Displacements of the $i$th Cu and the $|ij|$th O ions are given by

$$u_i = \sum_{\lambda q} \frac{\hbar v_{d,\lambda \lambda q}}{2N M_p \omega_{\lambda q}} e^{i q \cdot R_i} \epsilon_{\lambda q} \{ b_{\lambda q}^\dagger - b_{\lambda q} \},$$

$$u_{ij} = \sum_{\lambda q} \frac{\hbar v_{p,\lambda \lambda q}}{2N M_p \omega_{\lambda q}} e^{i q \cdot R_{ij}} \epsilon_{\lambda q} \{ b_{\lambda q}^\dagger + b_{\lambda q} \},$$

with $R_{ij} = (R_i + R_j)/2$, $M_d$ the mass of Cu ions, $M_p$ 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, $\epsilon_{\lambda q}$ unit polarization vectors, and $N$ the number of unit cells. The $q$ dependence of $v_{d,\lambda q}$ and $v_{p,\lambda q}$ can play a crucial role; $v_{d,\lambda q} = 0$ for the breeding modes that bring no changes in adjacent Cu-Cu distances while $v_{p,\lambda q} \approx 1$ for such modes.

The electronic part can be well described by the $t$-$J$ model on a square lattice: $\mathcal{H} = -\sum_{ij} t_{ij} d_{i\alpha}^\dagger d_{j\sigma}^\dagger - (J/2) \sum_{ij} (s_i \cdot s_j) + U \sum_i n_{i\uparrow} n_{i\downarrow}$, with the summation over $\langle ij \rangle$ restricted to nearest neighbors, $s_i = \ldots$
\( (1/2) \sum_{\alpha} \sum_{\beta} \left( \sigma_{\alpha x} \sigma_{\beta y} + \sigma_{\alpha y} \sigma_{\beta x} \right) d_{\alpha \alpha}^\dagger d_{\beta \beta} \), with \( \sigma_x, \sigma_y \) and \( \sigma_z \) the Pauli matrices, and \( n_d = d_{\alpha \alpha}^\dagger d_{\alpha \alpha} \). An infinitely large on-site repulsion, \( U_\infty |t_{ij}| \rightarrow +\infty \), is introduced to exclude any doubly occupied sites. According to Eq. 3, there are two types of electron-phonon interactions. When only longitudinal phonons are considered or when \( \varepsilon_{\alpha \beta} = (q_s, q_y, q_z)/q \) is assumed, they are given by

\[
H_p = iC_p \sum_{q_s} \frac{\hbar \Omega_{\alpha \beta} \eta_l(q_s)}{2N M \varepsilon_{\alpha \beta}} \sum_{\theta} \eta_l(\theta |q_s\rangle \eta_l(\theta^\dagger |q_s\rangle^\dagger), \tag{5a}
\]

\[
H_d = iC_d \sum_{q_s} \frac{\hbar \Omega_{\alpha \beta} \eta_l(q_s)}{2N M \varepsilon_{\alpha \beta}} \sum_{\theta} \eta_l(\theta |q_s\rangle \eta_l(\theta^\dagger |q_s\rangle), \tag{5b}
\]

with \( \eta_l(q_s) = (1/\sqrt{N}) \sum_{\kappa} \sigma_{\alpha \beta} \left( 1/2 \right) \sigma_{\alpha \beta} d_{\kappa \kappa}^\dagger d_{\kappa \kappa} \).

The form factors of \( p \) waves are defined by

\[
\frac{1}{4} I_{\Gamma}^{p}(\omega_l, q) = \frac{1}{1 - \frac{1}{4} I_{\Gamma}^{s}(\omega_l, q) \chi_{\Gamma}(\omega_l)}, \tag{9}
\]

Because of these equations, we call \( I_{\Gamma}^{s}(\omega_l, q) \) a bare exchange interaction, \( I_{\Gamma}^{s}(\omega_l, q) \) an enhanced one, and \( \phi_s \) an effective three-point vertex function in spin channels.

The enhanced one is expanded as \( I_{\Gamma}^{s}(\omega_l, q) = I_{\Gamma}^{p} + 2I_{\Gamma}^{s} \eta_l(q) + \cdots \). The nearest-neighbor \( I_{\Gamma}^{s} \) is mainly responsible for the development of not only SC but also charge bond-order (CBO) fluctuations \( \eta_l(q) \). Because contributions from \( |\omega_l| \ll k_B T_K \) are the most effective, we ignore its energy dependence. An effective SC susceptibility, which is multiplied by \( \phi_s^2 \), is calculated in the ladder approximation with respect to \( I_{\Gamma}^{s} \):

\[
\chi_{\Gamma}(\omega_l, q) = \frac{2W_{\omega_l}^{2s} \chi_{\Gamma}(\omega_l, q)}{1 + 3 \cdot \frac{1}{4} W_{\omega_l}^{2s} \chi_{\Gamma}(\omega_l, q)} \tag{10}
\]

for \( \Gamma = d \) wave, with

\[
\pi_{\Gamma}^{(s)}(\omega_l, q) = \frac{k_B T}{N} \sum_{n k} \eta_l^2(k) \frac{1}{\varepsilon_n - \xi(k + \frac{q}{2})} \times \frac{1}{-\varepsilon_n - \omega_l - \xi(\varepsilon - k + \frac{q}{2})}. \tag{11}
\]

Only d-wave SC fluctuation are considered in this Letter. An effective CBO susceptibility is similarly given by

\[
\chi_{\Gamma}^{(CBO)}(\omega_l, q) = \frac{2W_{\omega_l}^{2s} \chi_{\Gamma}^{(CBO)}(\omega_l, q)}{1 + 3 \cdot \frac{1}{4} W_{\omega_l}^{2s} \chi_{\Gamma}^{(CBO)}(\omega_l, q)} \tag{12}
\]

for \( \Gamma = s, p \) and \( d \) waves, with

\[
\pi_{\Gamma}^{(CBO)}(\omega_l, q) = \frac{k_B T}{N} \sum_{n k} \eta_l^2(k) \frac{1}{\varepsilon_n - \xi(k - \frac{q}{2})} \times \frac{1}{-\varepsilon_n + \omega_l - \xi(\varepsilon - k + \frac{q}{2})}. \tag{13}
\]

The form factors of \( p \) waves are defined by \( \eta_l^2(k) = \sqrt{2} \sin(k_x a) \) and \( \eta_l^2(k) = \sqrt{2} \sin(k_y a) \).
A renormalized Green function for phonons is given by \( D_\lambda(i\omega, \mathbf{q}) = 2\omega_\lambda / [\Delta^2 + 2\omega_\lambda] \), with \( \Delta_\lambda(i\omega, \mathbf{q}) = -(\hbar^2/2M_\lambda\omega_\lambda) S(i\omega, \mathbf{q}) \). Because phonons are renormalized by AFS, SC and CBO fluctuations as well as pair excitations of quasi-particles in charge channels or charge density fluctuations, we consider four processes shown in Fig. 1. When only the part of \( \Gamma = s \) in Eq. (3) is considered, it follows that \( S = S_s + S_{sc} + S_{cbo} + S_c \), with

\[
S_s(i\omega, \mathbf{q}) = \frac{3}{4\pi} Y_s^2(q) \frac{k_B T}{N} \sum_{l'q'} \eta_s^2(q') \chi_s(i\omega_l + i\omega_r, q' + \frac{1}{2}\mathbf{q}) \chi_s(i\omega_l - i\omega_r, -q' + \frac{1}{2}\mathbf{q}),
\]

\[
S_{sc}(i\omega, \mathbf{q}) = \frac{3}{4\pi} Y_s^2(q) \frac{k_B T}{N} \sum_{l'q'} \chi_{sc}^s(i\omega_l + i\omega_r, q' + \frac{1}{2}\mathbf{q}) \chi_{sc}^s(i\omega_l - i\omega_r, -q' + \frac{1}{2}\mathbf{q}),
\]

\[
S_{cbo}(i\omega, \mathbf{q}) = \frac{3}{4\pi} Y_s^2(q) \sum_{l'q'} \chi_{cbo}^s(i\omega_l + i\omega_r, q' + \frac{1}{2}\mathbf{q}) \chi_{cbo}^s(i\omega_l - i\omega_r, -q' + \frac{1}{2}\mathbf{q}),
\]

\[
S_c(i\omega, \mathbf{q}) = -\frac{3}{4\pi} \Phi_s^4 \frac{k_B T}{N} \sum_{n\sigma} Z^2(2\epsilon_n, i\omega; k, q) \frac{1}{i\epsilon_n - \xi(k)} \frac{1}{i\epsilon_n + i\omega_l - \xi(k+\mathbf{q})},
\]

with \( Y_s(q) = \tilde{\eta}_s(q) \left[ C_{v_p,\lambda} \eta_s(q) + C_{v_d,\lambda} \sqrt{M_p/M_d} \right] \). Here, \( Z(i\epsilon_n, i\omega; k, q) \) is a vertex function in the charge-density channel. It is also enhanced by AFS, SC and CBO fluctuations; \( Z = Z_s + Z_{sc} + Z_{cbo} + \cdots \), with

\[
Z_s(i\epsilon_n, i\omega; k, q) = \frac{k_B T}{N} \sum_{l'q'} \eta_s(q') K_s(i\omega_l + i\omega_r, q' + \frac{1}{2}\mathbf{q}) K_s(-i\omega_l + i\omega_r, -q' + \frac{1}{2}\mathbf{q}),
\]

\[
Z_{sc}(i\epsilon_n, i\omega; k, q) = \frac{1}{2} Y_s(q) \frac{k_B T}{N} \sum_{l'q'} \eta_{sc}(q') \eta_{sc}(k - \frac{1}{2}\mathbf{q} + \frac{3}{2}\mathbf{q}),
\]

\[
Z_{cbo}(i\epsilon_n, i\omega; k, q) = \frac{1}{2} Y_s(q) \frac{k_B T}{N} \sum_{l'q'} \eta_{sc}(q') \eta_{cbo}(k + \frac{1}{2}\mathbf{q} + \frac{3}{2}\mathbf{q}),
\]

with

\[
K_s(i\omega_l, q) = \frac{1}{1 - \frac{T}{2} (i\omega_l, q) \chi_s(i\omega_l)}, \quad K_{sc}(i\omega_l, q) = \frac{-2}{1 + \frac{T}{2} \pi_{sc}^d(i\omega_l, q)}, \quad K_{cbo}(i\omega_l, q) = \frac{-2}{1 + \frac{T}{2} \pi_{cbo}^d(i\omega_l, q)}.
\]

No softening occurs for \( q = 0 \) because \( \tilde{\eta}_s(q \to 0) \propto |q| \). When \( q \) goes from \( \Gamma \) point to the zone boundary, the softening must increase first. However, it is unlikely that the softening is the largest at the zone boundary. For example, consider the breathing mode at X point, \( q_X = (\pm \pi/a, 0) \). Because \( v_{d,\lambda} \) is zero, the electron-phonon interaction described by Eq. (5) vanishes. For \( q \neq q_X \), \( v_{d,\lambda} \) is nonzero. This implies that the softening may not be the largest at X point along \( \Gamma-X \) line. In actual, several experimental data show that the softening is the largest for \( q \) a little different from \( q_X \).

Because a low-energy scale is \( k_B T_K \), we put

\[
S(i\omega_l, q) \simeq s/k_B T_K, \quad \text{with } s = O(1) \text{ a dimensionless constant. It follows that}
\]

\[
\Delta\omega_\lambda(\omega_{qX}, q_X) \simeq -15sc^2_{ph} \text{ meV},
\]
When the experimental value $21$ is used, we obtain

$$\Delta \omega_\lambda(\omega_{\lambda q}, q_x) \simeq -10 \text{ meV},$$

(21)

can be explained. It should be examined whether $sc_p^2$ is actually as large as 1.

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

$$\frac{1}{\phi_i} \Delta \Sigma(i \varepsilon, k) = -k_B T \sum_{\lambda q} \bar{g}_\lambda^2 (i \varepsilon, i \omega l; k, q) D_\lambda (i \omega l, q) \times \frac{1}{i \varepsilon - i \omega l - \xi(k + q),}$$

(22)

with

$$g_\lambda (i \varepsilon, i \omega l; k, q) = C_p \frac{h}{2M_p c \omega_{\lambda q}} \frac{3}{4} \bar{W}_q^2 Z (i \varepsilon, i \omega l; k, q).$$

(23)

It is likely that the contribution of Fig. 1(d) dominate those of the other three, Figs. 1(a)–(c). In such a case,

$$g_\lambda (i \varepsilon, i \omega l; k, q) \simeq \sqrt{k_B T_K |\Delta \omega_\lambda(\omega_{\lambda q}, q_x)|}. \quad \text{(24)}$$

When the experimental value $21$ is used, we obtain

$$g_\lambda (i \varepsilon, i \omega l; k, q) \simeq 30 \text{ meV}. \quad \text{(25)}$$

This is large enough for optical phonons to cause kinks in the dispersion relation of quasi-particles. 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 cannot explain the other type of kinks observed only in SC phases.

The phonon-mediated pair interaction is given by $g_\lambda^2 (0, 0; k, q) D_\lambda (0, 0)$ or $-2g_\lambda^2 (0, 0; k, q) / \omega_{\lambda q}$. The softening of phonons is the largest for $q \simeq q_x$ along $\Gamma$–$X$ line. This implies that the pair interaction by phonons is attractive between nearest neighbors. The nearest-neighbor part of $-2g_\lambda^2 (0, 0; k, q) / \omega_{\lambda q}$ should be included in $\frac{3}{4} |I_1^*|$. According to the argument in this Letter, it follows that

$$-2g_\lambda^2 (0, 0; k, q_x) / \omega_{\lambda q} \simeq -20 \text{ meV}. \quad \text{(26)}$$

The phonon-mediated interaction cannot be ignored in cuprate-oxide superconductors. However, it is smaller than $\frac{3}{4} |I_1^*| \simeq 100 \text{ meV}$. The main Cooper-pair interaction must be the superexchange interaction.

There are two other types of electron-phonon interactions. Note that $\phi_i$ and $1/\phi_i$ are small parameters in the vicinity of the Mott-Hubbard transition. The conventional one arising from the modulation of 3d-electron levels, which can directly couples with charge fluctuations, gives renormalization effects higher order in $\phi_i$ and $1/\phi_i$. The interaction arising from the modulation of $t_{ij}$ gives renormalization effects higher order in $1/\phi_i$. Then, we ignore both of them. On the other hand, what are considered in this Letter are of the order of $(\phi_i)^0 (1/\phi_i)^0$.

In conclusion, we propose the electron-phonon interaction arising from the modulation of the superexchange interaction by phonons, which is only relevant for strongly correlated electron liquids in the vicinity of the Mott-Hubbard transition. Its novel property is that it can be enhanced by spin, superconducting, and charge bond-order fluctuations as well as charge density fluctuations. A phenomenological argument where parameters are determined from the observed softening of phonons implies that the enhanced electron-phonon interaction is also responsible for kinks in the dispersion relation of quasi-particles in cuprate-oxide high-Tc superconductors. However, it can never be the main Cooper-pair interaction. The main one must be the superexchange interaction.

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