Impact of Optical Modes on the Pairing Potential in Bilayer Cuprates

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Superconducting transition temperature is calculated for differently doped bilayer cuprates. Superexchange is assumed to be the dominating mechanism of high-temperature superconductivity, but the contribution from the phonon potential is not negligible, which qualitatively explains the observed weak isotopic effect. The calculated value $2\Delta_{\text{max}}/k_B T_C \simeq 4.5$ is close to the experiment in the case of optimum doping.

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I. INTRODUCTION

The High Temperature Superconductivity (HTSC) was discovered 11 years ago. None of the proposed HTSC mechanisms has been commonly accepted yet (see [1]). Unlike the case in normal low-temperature superconductors, the energy gap in HTSC materials is different at different points of the Brillouin zone. This dependence is important, for the understanding of the HTSC mechanism.

In [2,3] we found solutions of the Bardeen-Cooper-Schrieffer (BCS) equations taking copper spin superexchange into consideration. This interaction was found to lead to a reasonable critical temperature $T_C$ and $d$-symmetry of the energy gap in superconducting cuprates. The conclusion about the $d$-symmetry of the order parameter was confirmed by recent studies of photoemission spectra [4]. In the present work we additionally consider the electron - phonon interaction with optical buckling $A_{1g}$, $B_{1g}$ and breathing $A_g$, $E_g$ modes to explain the weak isotope effect in these compounds.

II. POTENTIAL OF CURRENT CARRIERS PAIRING THROUGH OPTICAL BUCKLING AND BREATHING MODES

In the compound YBa$_2$Cu$_3$O$_{7-x}$ holes interact most strongly with an electric field perpendicular to the CuO$_2$ plane. This field is mainly induced by triply charged yttrium ions [5]. The operator of binding energy with oscillations perpendicular to the CuO$_2$ plane has the form

$$H_{h-ph} = \epsilon \sum_{n\sigma} \left\{ E_x u_x \left( an + \frac{ax}{2} \right) p_{n\sigma}^{\sigma} + E_y u_y \left( an + \frac{ay}{2} \right) p_{n\sigma}^{\sigma} \right\},$$

where $p_{n\sigma}^{\sigma}$ and $p_{n\sigma}^{\sigma}$ are the Hubbard operators of oxygen holes, $u_x(n)$ and $u_y(n)$ are the displacements vectors of O(2) and O(3) positions in a unit cell with the number $a$, $x$ and $y$ are unit vectors of the axes $a$ and $b$ respectively, $a$ is the lattice constant, and $E_x = 1.2 \cdot 10^8$ V·cm$^{-1}$, $E_y = 1.5 \cdot 10^8$ V·cm$^{-1}$ are the components of electric field along the c axis, calculated in [6]. For simplicity, we put $E = E_x = E_y = 1.35 \cdot 10^8$ V·cm$^{-1}$. Then, calculating the commutator $[\psi_{\mathbf{k}+p\sigma}, H_{h-ph}]$ and using the expression
\[ \left[ \Psi^{\perp,pd}_k, H_{h-ph} \right] = \sum_{\alpha,q} V^{\alpha}(q) \Psi^{\perp,pd}_{k-q}(b_q + b^+_q), \]

where \( \Psi^{\perp,pd}_k \) is the quasiparticle operator of singlet-correlated oxygen holes, \( b^+_q \) and \( b_q \) are the phonon creation and annihilation operators, one finds

\[ V^{\alpha}(q) = \frac{e^2}{2} \sqrt{\frac{\hbar}{2m\omega_\alpha}} \left[ \cos \left( \frac{q_x a}{2} \right) \pm \cos \left( \frac{q_y a}{2} \right) \right], \tag{2} \]

where \( \omega_\alpha = \omega_{A_{1g}} = 440 \text{ cm}^{-1} \) and \( \omega_{B_{1g}} = 340 \text{ cm}^{-1} \) [7]. The plus and minus signs correspond to the modes \( A_{1g} \) and \( B_{1g} \) respectively, \( e \) is the electron charge, and \( m \) is the mass of the unit cell. Since the difference between \( \omega_{A_{1g}} \) and \( \omega_{B_{1g}} \) is not so important, they are put equal to \( \omega_G = 400 \text{ cm}^{-1} \).

Using the Frohlich procedure, the potential of current carriers interacting through the phonon field of buckling modes \( A_{1g} \) and \( B_{1g} \) is written as

\[ G(k' - k) = 2G_0^2 \frac{1 + \frac{1}{2} \left[ \cos (k'_x - k_x) + \cos (k'_y - k_y) \right]}{\left( \varepsilon_{k'} - \varepsilon_k \right)^2 - (\hbar \omega_G)^2} \hbar \omega_G, \tag{3} \]

where \( G_0 = 35 \text{ meV} \).

Assuming that the constant of interaction with the modes \( A_g \) and \( E_g \) (and their frequencies) are identical, the contribution to the pairing potential is written as

\[ B(k' - k) = 2B_0^2 \frac{1 + \frac{1}{2} \left[ \cos (k'_x - k_x) + \cos (k'_y - k_y) \right]}{\left( \varepsilon_{k'} - \varepsilon_k \right)^2 - (\hbar \omega_B)^2} \hbar \omega_B. \tag{4} \]

According to the estimate of [8], the constant \( B_0 \) is about 60 meV. The frequencies \( \omega_{A_g} \) and \( \omega_{E_g} \), taken from [9], are about 480 cm\(^{-1}\).

### III. EQUATION FOR THE GAP

The BCS equation for the energy gap, taking into account the interaction via the phonon field and the superexchange between copper spins, has the form

\[ \Delta_k = \sum_k \left\{ P^2 \left[ G(k' - k) + B(k' - k) \right] \theta(\hbar \omega_D - |\varepsilon_{k'} - \varepsilon_k|) - J^{dd}(k' - k) \right\} \langle \Psi^{\perp,pd}_k \Psi^{\perp,pd}_{-k} \rangle, \tag{5} \]

where \( J^{dd}(q) \) is the Fourier transform of the superexchange parameter \( J = 57 \text{ meV} \),

\[ J^{dd}(q) = 2J \left( \cos q_x a + \cos q_y a \right), \]

\( \omega_D = 500 \text{ cm}^{-1} \) is the Debye frequency, and \( P = \frac{1}{2} (1 + x) \). The correlation function is given by

\[ \langle \Psi^{\perp,pd}_k \Psi^{\perp,pd}_{-k} \rangle = \frac{\Delta_k}{2E_k} \tanh \left( \frac{E_k}{2k_B T} \right), \]

where \( E_k = \sqrt{(\varepsilon_k - \mu)^2 + \Delta_k^2} \). The chemical potential \( \mu \) and the hole concentration \( x \) for two copper sites in the bilayer (assuming that the antibonding band is empty) are related as

\[ x = P \sum_k \left[ \exp \left( \frac{\varepsilon_k - \mu}{k_B T} \right) + 1 \right]^{-1}. \]

At \( x = 0.33 \) the chemical potential is placed on 10 meV below the saddle singularity peak in the density of states. The dispersion \( \varepsilon_k \) is chosen as

\[ \varepsilon_k = P \left[ 2t_1 \left( \cos k_x a + \cos k_y a \right) + 2t_2 \cos k_x a \cos k_y a + 2t_3 \left( \cos 2k_x a + \cos 2k_y a \right) \right], \tag{6} \]

where \( t_1, t_2, \) and \( t_3 \) are the effective hopping integrals. All the calculations are carried out at \( t_1 = 70 \text{ meV}, t_2 = 0, \) and \( t_3 = 5 \text{ meV} \).
FIG. 1. Temperature dependence of the superconducting transition temperature in YBa$_2$Cu$_3$O$_{7-y}$ with doping: solid line (calculations) and the experimental points are sketched by open circles.

Figure 1 shows the dependence of the superconducting transition temperature of YBa$_2$Cu$_3$O$_{7-y}$ with doping. It is evident that the calculations qualitatively conform with the experimental data (normalized by the expression $T_C/T_{C,\text{max}} = 1 - 82.6(x - 0.32)^2$ [10]). However, their noncoincidence remains unexplained. Numerical solution of the energy gap equation yields a $d$-type symmetry of the order parameter $\Delta_k = \Delta_0 (\cos k_x a - \cos k_y a)$ and a nonstandard value of $2\Delta_{\text{max}}/k_B T_C \approx 4.5$ with the superconducting transition temperature $T_{C,\text{max}} \sim 100$ K. Note that solutions of (5) with $J = 0$ lead to the $s$-type symmetry of the gap, $\Delta_k = \Delta_0 (\cos k_x a + \cos k_y a)$. The conclusion of [11] that the $d$-symmetry of the gap arises from pairing only through optical buckling modes seems to be groundless.

IV. CONCLUSION

Self-consistent solutions of the BCS gap equation are found in the class of short-range pairing potentials for various chemical potentials. When the Fermi level $\varepsilon_F$ is near the bottom(top) of the band, the solutions correspond to the $s$-type pairing, while for $\varepsilon_F$ in the center of the band the solution are related to the $d$-type. The short-range potentials considered are (i) superexchange interaction, (ii) interaction of current carriers via optical oscillations, and (iii) breathing and buckling modes of oxygen atoms in CuO$_2$ planes. The superconducting transition temperature is calculated for various oxygen indices $x$.

The dominant HTSC mechanism is a superexchange. However, the contribution of the phonon pairing is not negligible, that qualitatively explains the observed weak isotope effect. The calculated value $2\Delta_{\text{max}}/k_B T_C \approx 4.5$ is close to the experiment.

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