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ORIGINAL PAPER

The Interplay of Phonon and Magnetic Mechanism of Pairing in Strongly Correlated Electron System of High-T_c Cuprates

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Abstract We consider magnetic mechanism of superconducting pairing in the effective low energy $t-t'-t''-J^*$ model with all parameters calculated ab initio. Interaction of strongly correlated electrons with different phonon modes is also incorporated. In a BCS type theory, the $d_{x^2-y^2}$ gap is given by a sum of magnetic and phonon contributions. The main contribution to the only fitting parameter G is determined by a competition of the breathing and buckling modes. Fitting the parameter G from the isotope effect, we obtain that magnetic and phonon contributions to the critical temperature T_c work together and are of the same order of magnitude.

Keywords High-T_c superconductivity · Strong correlated electron systems · Mechanisms of superconducting pairing

1 Introduction

A microscopic approach based on the conventional ab initio local density approximation (LDA) is not valid in the underdoped region of the cuprate phase diagram due to the strong electron correlations (SEC) effects [1, 2]. In general, the problem of strong electron correlations is not solved.

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The multielectron generalized tight-binding (GTB) method has been proposed [3] which describes electrons as the quasiparticle excitations between the local multielectron configurations with the interatomic hopping resulting in the dispersion and the band structure. The hybrid LDA+GTB method [4] takes the advantages of both ab initio single electron and multielectron approaches. The low energy effective Hamiltonian generated by the quasiparticle electronic structure is given by the $t-t'-t''-J^*$ model (here, star means that the three-site correlated hopping $\sim J$ is included) with all parameters calculated ab initio [4].

A self-consistent consideration of the electronic structure and spin correlation functions within the $t-t'-t''-J^*$ model with parameters of $La_{2-x}Sr_xCuO_4$ results in the doping evolution of the hole Fermi surface from small pockets around $(\pi/2,\pi/2)$ at $x<x_{cr}$ to large hole surface around (π,π) at $x>x_{cr}$ with quantum phase transition [5] at $x_{cr}\approx 0.15$. In this paper, we extend this approach to the superconducting phase taking into account both magnetic pairing within the $t-t'-t''-J^*$ model and electron-phonon interaction (EPI). In spite of the large number of different phonon modes, only a few of them have large EPI including the apical oxygen breathing mode (apical oxygen displacement perpendicular the CuO_2 plane which modifies the Madelung energy), the in-plane oxygen breathing/half-breathing mode, and the buckling mode with in-plane oxygen ions moving perpendicular to the CuO_2 plane [6, 7]. Recent ab initio study of the electronic structure and EPI in $La_{2-x}Sr_xCuO_4$ has also proved that these three modes contribution to the hole self-energy is more than 80% of the total self-energy [8].

The multiband pd-model at low energies is reduced to the effective Hubbard model with two Hubbard subbands. The lower and upper Hubbard bands (LHB and UHB) are the bands of the Hubbard fermions created by

the X-operators $X_f^{0\sigma}$ and $X_f^{-\sigma,2}$ at the site f, correspondingly, $X_f^{pq} = |p\rangle\langle q|$. Here, $|0\rangle$, $|\sigma = \pm 1/2\rangle$ and $|2\rangle$ are the multielectron eigenstates of the CuO_6 unit cell that includes CuO_4 in-plane atoms and 2 apical oxygens. The corresponding configurations are $d^{10}p^6$ with number of holes $n_h = 0$, $d^9p^6 + d^{10}p^5$ with $n_h = 1$, and $d^8p^6 + d^9p^5 + d^{10}p^4$ with $n_h = 2$. In the hole language, the electrons in the valence band correspond to the holes in the UHB. The amplitudes of interatomic hopping in the LHB and UHB are t_{fg}^{00} and t_{fg}^{11}, while the interband hopping is given by t_{fg}^{01}, $f \neq g$. When we eliminate the LHB and interband excitations through the charge transfer gap U_{eff} by the standard unitary transformation, the effective Hamiltonian for holes in the UHB is given by [9, 10] $H_{t-J^*} = H_{t-J} + H_{(3)}$ with

$$H_{t-J} = \sum_{f\sigma}\left((\varepsilon-\mu)X_f^{\sigma\sigma} + 2(\varepsilon-\mu)X_f^{22}\right) + \sum_{fg\sigma} t_{fg}^{11} X_f^{2,-\sigma} X_g^{-\sigma,2} + \sum_{fg} J_{fg}\left(\vec{S}_f\cdot\vec{S}_g - \frac{1}{4}n_f n_g\right),$$

$$H_{(3)} = \sum_{fmg\sigma} \frac{t_{fm}^{01} t_{mg}^{01}}{U_{\text{eff}}}\left(X_f^{2,\bar{\sigma}} X_m^{\sigma,\sigma} X_g^{\bar{\sigma},2} - X_f^{2,\sigma} X_m^{\sigma,\bar{\sigma}} X_g^{\bar{\sigma},2}\right).$$

Here, $J_{fg} = (t_{fg}^{01})^2/U_{\text{eff}}$ is the super exchange interaction. Distance dependent hopping parameters t_{fg}^{11} have been calculated up to 6th neighbors and it was revealed that contributions of the fourth and more distant neighbors are negligibly small [4]. This is the microscopic justification of the $t - t' - t'' - J^*$ model with 3 hopping parameter t_{fg}^{11} ($t = 0.932$, $t' = -0.120$, $t'' = 0.152$, $J = 0.298$, $J' = 0.003$, $J'' = 0.007$); all parameters are in eV. Due to stronger suppression of the t_{fg}^{01} with distance the second and third neighbor exchange, parameters J' and J'' are negligibly small. The last term $H_{(3)}$ corresponds to the three-site correlated hopping that has the same order as the exchange term J and has to be included in the theory of superconductivity [11].

In the strong electron correlation regime, the EPI is the interaction of phonon (with wave vector $\mathbf{q}$, frequency $\omega_{\mathbf{q}\nu}$, and mode ν) and Hubbard fermions [12] with wave vector $\mathbf{k}$. The effective total Hamiltonian is given by $H_{\text{eff}} = H_{t-J^*} + H_{\text{el-ph-el}}$, where Fröhlich interaction

$$H_{\text{el-ph-el}} = \sum_{\mathbf{kk'q}}\sum_{\sigma\sigma'} V_{\mathbf{kk'q}} X_{\mathbf{k+q}}^{2,\bar{\sigma}} X_{\mathbf{k'-q}}^{2,\bar{\sigma}'} X_{\mathbf{k'}}^{\bar{\sigma}',2} X_{\mathbf{k}}^{\bar{\sigma},2}$$

contains two Hubbard fermion creation $X_{\mathbf{k}}^{2\bar{\sigma}}$ and annihilation $X_{\mathbf{k}}^{\bar{\sigma}2}$ operators. The effective interaction neglecting retardation effects is given by

$$V_{\mathbf{kk'q}} = -\sum_{\upsilon} g_{\upsilon}(\mathbf{k},\mathbf{q}) g_{\upsilon}(\mathbf{k}',-\mathbf{q})/\omega_{\mathbf{q},\upsilon}.$$

For anisotropic $d_{x^2-y^2}$-gap, the wave vector dependence of the EPI matrix elements is crucial. Maximal EPI for the breathing/half-breathing mode at large $\mathbf{q} \sim \pi/a$ results in depairing effect of this mode, while the buckling mode with maximum of interaction at $\mathbf{q} = 0$ supports the $d_{x^2-y^2}$ pairing. This conclusion has been obtained by different approaches [6, 13, 14] and results from a simple physics: large $\mathbf{q}$ EPI changes the phase of the $d_{x^2-y^2}$-gap on the Fermi surface while small $\mathbf{q}$ EPI does not change the phase.

It should be emphasized that mean-field theory in the X-operator methods differs from standard mean field treatment of the Coulomb interaction like $Un_1n_2 \to Un_1\langle n_2\rangle$, where n_i is a number of particles in i state. For the superconducting state, the mean field theory has been developed in the X-operator representation that is reliable in the strong correlation regime [15]. Double occupation is prohibited in this approach by the local constraint formulated in the X-operator representation similar to the local constraint in the slave boson approach. Contrary to the slave boson mean field theory where the local constraint is violated, in our mean field theory the X-operator algebra provides the local constraint in all stages of calculations.

2 Isotope Effect

In the BCS-type approach to superconductivity, a spin singlet pairing of the Hubbard fermions is given by the anomalous average [15] $B_{\mathbf{q}} = \langle X_{-\mathbf{q}}^{\sigma,2} X_{\mathbf{q}}^{\bar{\sigma},2}\rangle$. For the $d_{x^2-y^2}$-pairing, the gap equation reads [13]

$$\Delta_{\mathbf{k}} = \frac{2\varphi_{\mathbf{k}}}{N}\sum_{\mathbf{q}} \lambda_{\text{tot}}(\mathbf{q}) \frac{2\Delta_{\mathbf{q}}\varphi_{\mathbf{q}}}{\xi_{\mathbf{q}} - \mu} \tanh\left(\frac{\xi_{\mathbf{q}} - \mu}{2\tau}\right) \tag{1}$$

where $\tau = k_BT$, k_B is Boltzmann constant, and T is temperature, $\varphi_{\mathbf{q}} = (\cos q_x a - \cos q_y a)/2$ is the angle-dependent part of the gap $\Delta_{\mathbf{q}} = \Delta_0\varphi_{\mathbf{q}}$. The θ-function as usual means that phonon pairing occurs in a narrow energy window of the width ω_D near the Fermi energy. The superconducting state dispersion of the BCS-type $\xi_{\mathbf{q}}$ takes into account the spin correlation function $c_{\mathbf{q}}$, and three-site interaction; the chemical potential μ is calculated self-consistently for the carrier concentration x in $La_{2-x}Sr_xCuO_4$. Without phonon contribution, the similar gap equation was obtained by the diagram technique [16] for Hubbard operators. Previously, the same equation was obtained in the RVB theory [17]. The phonon coupling parameter is given by $\lambda_{ph} = f(x)G$, where dimensionless function $f(x)$ is $f(x) = (1+x)(3+x)/8 - 3c_{01}/4$,

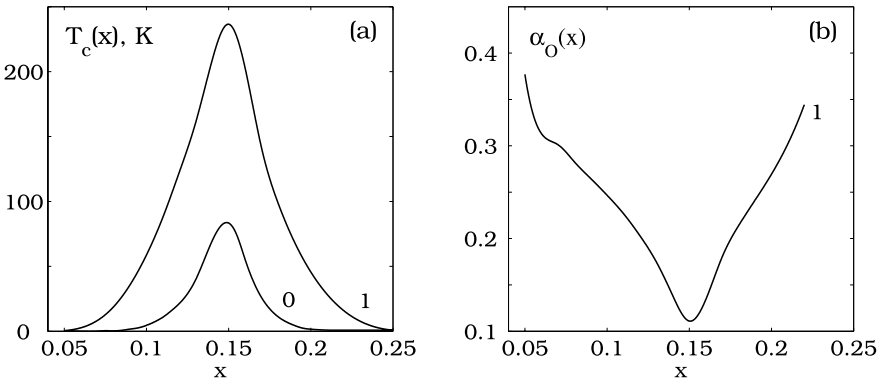

Fig. 1 The critical temperature (**a**) and the doping dependence of the oxygen isotope exponent (**b**) for the effective EPI parameter G/J indicated near the curves

and the parameter G is determined by the bare EPI matrix elements $G = (g^2_{\text{buck}}/\omega_{\text{buck}} - g^2_{\text{breath}}/\omega_{\text{breath}})$ [13].

The concentration dependence of both magnetic and phonon couplings stems from the unusual statistics of the Hubbard fermions. Contrary to the free electron band with two electrons per atom, the Hubbard subbands have the odd number of states which depend on concentration via total number of holes $n_h = 1 + x$ and the nearest neighbor spin correlation function c_{01}. Due to the antiferromagnetic type of correlation, c_{01} is negative and its contribution to λ_{ph} is positive. The appearance of the spin correlation function in the phonon coupling means some interference of the magnetic and phonon mechanisms of pairing. This function $c_{01} = 2\langle S^z_0 S^z_1\rangle = \langle S^+_0 S^-_1\rangle$ characterizes the spin liquid properties of the underdoped cuprate and is concentration dependent [5].

All parameters in the gap equation (1) but G have been obtained within ab initio LDA+GTB approach. The precision of modern calculations of the EPI matrix elements for strongly correlated electrons seems to be not enough. Thus, in this paper, we consider the parameter G as the only fitting parameter. To find the value of G, we calculate T_c using (1) and then the isotope effect exponent determining as $\alpha_O = -\frac{\mathrm{d}\ln(T_c)}{\mathrm{d}\ln(M_O)}$ (Fig. 1).

We have found that the positive (negative) sign of G results in positive (negative) sign of the exponent α_O. The value $G/J = 1$ provides $\alpha_O = 0.11$ close to the $La_{2-x}Sr_xCuO_4$ experimental data at the optimal doping [18, 19]. The increase of the isotope exponent away from the optimal doping is obtained. $T_c(x)$ dependence reproduces the general structure of the superconducting dome well with the optimal doping at $x = 0.15$ and disappearance of superconductivity in the underdoped region below $x = 0.05$. The absolute value of T_c is too large and this is the general drawback of the mean field theory. We have obtained that with positive parameter G magnetic and phonon contributions to pairing work together and are of the same order of magnitude. Then we would like to discuss the effect of the strong EPI with apical oxygen breathing mode. This interaction is poorly screened. The direct experimental proof of its importance is demonstrated by the colossal lattice expansion along c-axis in $La_2CuO_{4+\delta}$ under femtosecond intense light pulses [20]. Nevertheless, in our theory, this large EPI does not contribute to the superconducting d-pairing due to the orthogonality of the in-plane electron momentum and c-axis phonon wave number for the apical oxygen breathing mode [13]. The site selective isotope substitution confirms the absence of the isotope effect when the isotope is in the apical oxygen position [21, 22]. Previously, the absence of the apical oxygen breathing mode contribution to the $d_{x^2-y^2}$ pairing has been obtained in the paper [6].

We have restricted ourselves to the tetragonal lattice with pure $d_{x^2-y^2}$ pairing symmetry. Due to orthorhombic distortion, the mixed $(s + d_{x^2-y^2})$ symmetry is possible. Several experiments indicate substantial amount of s-wave gap in YBCO [23, 24] and Bi2212 [25, 26]. It is very likely that the strong experimentally observed Cu and O isotope effects are indicative of very strong EPI. Taking into account that the spin-polaron bandwidth $W \sim J$, we find for our EPI parameter $G = W$ that results in the dimensionless EPI coupling constant $\lambda \approx 1$. The additional s-wave pairing will probably increase the isotope effect exponent in the underdoped orthorhombic region.

Summarizing our discussion, we want to emphasize that both magnetic and phonon mechanisms of $d_{x^2-y^2}$-pairing should be considered in realistic theory of superconductivity in cuprates. Many authors have previously discussed separately the magnetic mechanisms of pairing generated by strong electron correlations or phonon pairing which explains the isotope effect. Here, we have shown that both mechanisms may work together increasing each other. Our theory is almost parameter-free. All parameters of the electronic structure and the magnetic mechanisms of pairing have been calculated within the ab initio LDA+GTB approach. The only parameter entering our theory is the combination of bare electron-phonon matrix elements G. Its sign $G > 0$ is required to have the positive oxygen isotope exponent α, its value can be fitted to get the proper concentration dependence of $\alpha(x)$. The ab initio calculation of the electron-phonon matrix elements in the regime of strong

electron correlations still remains the important unsolved problem.

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