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Effect of Interlayer Single-Particle Hoppings on the Superconducting Transition Temperature

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It is well known that the superconducting transition temperature of high-T_c cuprates depends on the number of CuO_2 planes in the unit cell. The multilayer structure implies the possibility of interlayer hopping. Under the assumption that the interlayer hopping can be specified by the parameter $t_\perp(\mathbf{k}) = t_\perp(\cos(k_x) - \cos(k_y))^2$, the quasiparticle excitation spectrum for the bilayer cuprate in the superconducting state has been determined in the framework of the $t - t' - t'' - t_\perp - J^*$ model using the generalized mean-field approximation. It turns out that the interlayer hoppings does not create any additional mechanism of the Cooper paring and does not lead to an increase in T_c. The splitting of the upper Hubbard quasiparticle band attributed to the interlayer hoppings is manifested as two peaks in the doping dependence of the superconducting transition temperature at temperatures below the maximum T_c value for a single-layer cuprate. It has been found that antiferromagnetic interlayer correlations suppress the interlayer splitting. This probably leads to the common doping dependence of T_c for both single-layer and bilayer cuprates.

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1. The nature of superconductivity in high-T_c cuprates is still one of the most challenging problems in condensed matter physics. Currently, pairing due to the antiferromagnetic exchange in the CuO_2 plane seems to be the most probable candidate for the role of the superconductivity mechanism. However, in the framework of this mechanism, it is still impossible to explain certain important effects. In particular, it is not clear why there is a quite large difference between the superconducting transition temperatures (T_c) for the compounds with the same number of layers (for $La_{2-x}Sr_xCuO_4$, $T_c = 40$ K and $HgBa_2CuO_4$, $T_c = 90$ K) and why T_c increases in all cuprate families with the number of layers n up to $n = 3$ [1]. The difference in T_c for the single-layer cuprates is attributed to the absence or presence of structural defects and to the degree of curvature of the CuO_2 plane [2]. The dependence of T_c on the number of CuO_2 layers can be related both to a change in the structural imperfection owing to the addition of one layer or directly to the processes characteristic only of multilayer systems. In this work, we consider interlayer hole hoppings that is the most obvious and important process of this type. To clarify how the interlayer hoppings affect T_c without an admixture of other effects, we study the superconducting phase of the YBCO-type bilayer cuprate. The stoichiometric composition of the bilayer cuprate corresponds to one hole per CuO_2 plane. If we do not take into account the absence of one apical oxygen atom, each layer reproduces a unit cell of $La_{2-x}Sr_xCuO_4$ whose electron structure was studied in detail in [3, 4]. This determines our approach to the study of the bilayer system under consideration. We assume that the addition of the second copper–oxygen layer does not change the electron structure of CuO_2 layers, but provides the possibility of the interlayer hopping of quasiparticles leading to the splitting of bands of one layer into bonding and antibonding bands ("bilayer splitting") [5–11].

2. We start with the t–t'–t''–$t_\perp$–J^* model (i.e., from the t–J model [12], taking into account the neighboring atoms up to the third coordination sphere, the three-site intraplane hoppings, and interplane hoppings), which is an effective low-energy model for cuprates in the limit of strong electron correlations. In the case of the bilayer cuprate, the Hamiltonian of the t–t'–t''–$t_\perp$–J^* model written in terms of the Hubbard operators $X_f^{\sigma S}$ has the form

$$H_{t-t'-t''-t_\perp-J^*}$$

$$= \sum_{f\alpha\sigma}(\varepsilon_1 - \mu)X_{f\alpha}^{\sigma\sigma} + \sum_{f\alpha}(\varepsilon_2 - 2\mu)X_{f\alpha}^{SS}$$
$$+ \sum_{fg\alpha\sigma} t_{fg}X_{f\alpha}^{S\sigma}X_{g\alpha}^{\sigma S} + \sum_{fg\alpha\sigma} J_{fg}(X_{f\alpha}^{\sigma\bar{\sigma}}X_{g\alpha}^{\bar{\sigma}\sigma} - X_{f\alpha}^{\sigma\sigma}X_{g\alpha}^{\bar{\sigma}\bar{\sigma}})$$
$$- \sum_{mln\alpha\sigma} \frac{\tilde{t}_{ml}\tilde{t}_{ln}}{E_{ct}}(X_{m\alpha}^{S\sigma}X_{l\alpha}^{\sigma\bar{\sigma}}X_{n\alpha}^{\bar{\sigma}S} - X_{m\alpha}^{S\sigma}X_{l\alpha}^{\bar{\sigma}\bar{\sigma}}X_{n\alpha}^{\sigma S}) + H_{\text{bil}}. \quad (1)$$

Here and further on, subscript α denotes the upper (u) and lower (d) CuO_2 planes, $J_{fg} = 2\tilde{t}_{fg}^2/E_{ct}$ is the parameter characterizing the effective exchange interaction due to virtual hopping to the lower Hubbard band and back, t_{fg} are the intraband hopping integrals between the unit cells, $\tilde{t}_{fg}$ are the interband hopping integrals between the unit cells, E_{ct} is the charge-transfer bandgap, and ϵ_1 and ϵ_2 are the energies of one- and two-hole states of the cell, respectively. Interlayer hopping is taken into account by adding the corresponding term to the Hamiltonian

$$H_{\text{bil}} = \sum_{f_u f_d \sigma} t_\perp(f_u, f_d)(X_{f_u}^{S\sigma}X_{f_d}^{\sigma S} + \text{H.c.}), \quad (2)$$

where the $t_\perp(f_u, f_d)$ factor is the Fourier transform of $t_\perp(\mathbf{k}) = t_\perp(\cos(k_x) - \cos(k_y))^2$ determining the dependence of the interlayer hopping integral on the distance to the cell in the neighboring plane to which the hopping takes place. The typical form of $t_\perp(\mathbf{k})$ as a function of the two-dimensional wave vector was found based on the band calculations [13] taking into account the effective overlapping of copper d_x orbitals involving the actual overlapping of the s orbitals and was confirmed by the ARPES experiments [6, 7]. For each CuO_2 layer, we used the parameters of the t–t'–t''–J^* model calculated in [4] in the framework of the LDA + GTB method (the ab initio LDA calculations + the generalized tight-binding method). For such a model, the spectrum of charge carriers (holes) and the Fermi surface in the normal phase with the bilayer splitting were studied in [5]. In this work, using the band structure reported in [5], we study the superconducting phase in the framework of the generalized mean-field theory.

3. To calculate the energy characteristics, such as dispersion and the superconducting gap, we use the equations of motion for the intraplane two-time retarded Green's function $G_{k\sigma}^u = \langle\langle X_k^{\sigma S} | X_k^{S\sigma}\rangle\rangle$. The equations of motion deduced using the method of irreducible Mori operators [4, 14–18] contain the higher-order Green's functions, which are projected onto the basis of normal $G_{k\sigma} = \langle\langle X_k^{\sigma S} | X_k^{S\sigma}\rangle\rangle$ and anomalous $F_{k\sigma} = \langle\langle X_{-k}^{S\bar{\sigma}} | X_k^{S\sigma}\rangle\rangle$ Green's functions. As a result, we find the anomalous averages $B_q = \langle X_q^{\sigma S}X_{-q}^{\bar{\sigma}S}\rangle$, the anomalous interlayer averages $B_{\perp q} = \langle X_{(u)q}^{\sigma S}X_{(d)-q}^{\bar{\sigma}S}\rangle$, and bandgap, which includes all possible interactions potentially leading to the pairing of two particles

$$\Delta_k = -\frac{1}{N}\frac{1}{p_\sigma + x}\sum_q \Big[\Big(2t_q - p_\sigma(J_{k+q} + J_{k-q}) + 2p_\sigma\frac{\tilde{t}_q^2}{E_{ct}} - 4(p_\sigma + x)\frac{\tilde{t}_k\tilde{t}_q}{E_{ct}}\Big)B_q + 2\tilde{t}_{\perp q}B_{\perp q}\Big], \quad (3)$$

where p_σ is the occupation number of a single-particle state, x is the number of doping holes per unit cell, and the expression

$$\tilde{t}_{\perp q} = (p_\sigma + x)t_\perp(\cos(q_x) - \cos(q_y))^2 \times\Big(1 + \frac{3}{2}\frac{C_\perp}{(p_\sigma + x)^2}\Big) \quad (4)$$

determines the bilayer splitting for the quasiparticle band in a single CuO_2 layer, in which $C_\perp = \langle X_{fu}^{\sigma\bar{\sigma}}X_{fd}^{\bar{\sigma}\sigma}\rangle$ is the interlayer spin correlation function. The first part in (3) corresponding to the interlayer Cooper pairing in the CuO_2 plane was deduced in [15, 16, 19]. The second part results from introducing the hopping between CuO_2 layers. Both these terms still allow the possibility of the pairing with any type of symmetry. Relationship (3) is valid for both CuO_2 planes, since the superconducting gaps for the upper and lower layers are completely identical, having the same absolute value and phase (the method for determining a general form of the gap is described in detail in [20]). In the superconducting state, the dispersion laws for the bands can be written as

$$E_k^{1,2} = \pm\sqrt{(\xi_k + \tilde{t}_{\perp k})^2 + \Delta_k^2},$$
$$E_k^{3,4} = \pm\sqrt{(\xi_k - \tilde{t}_{\perp k})^2 + \Delta_k^2}, \quad (5)$$

where ξ_k is the dispersion law for the normal phase including the kinematic and spin correlation functions. Assuming the $d_{x^2-y^2}$ symmetry of the gap, $\Delta_k = (\Delta_0/2)(\cos(k_x) - \cos(k_y))$, we can transform the equation for T_c to the form (if we take into account only the nearest-neighbor exchange J_{01})

$$1 = \frac{1}{N}p_\sigma J_{01}\sum_q \frac{(\cos(k_x) - \cos(k_y))^2}{2} \times\Big(\frac{1}{\xi_q + \tilde{t}_{\perp q}}\tanh\frac{\xi_q + \tilde{t}_{\perp q}}{2kT} + \frac{1}{\xi_q - \tilde{t}_{\perp q}}\tanh\frac{\xi_q - \tilde{t}_{\perp q}}{2kT}\Big). \quad (6)$$

4. The solution of Eq. (6) describing the dependence of T_c on x has rather unexpected form for high-T_c cuprates. For all cuprates, it is well known that the superconducting region in the phase diagram is characterized by a single peak in T_c corresponding to the

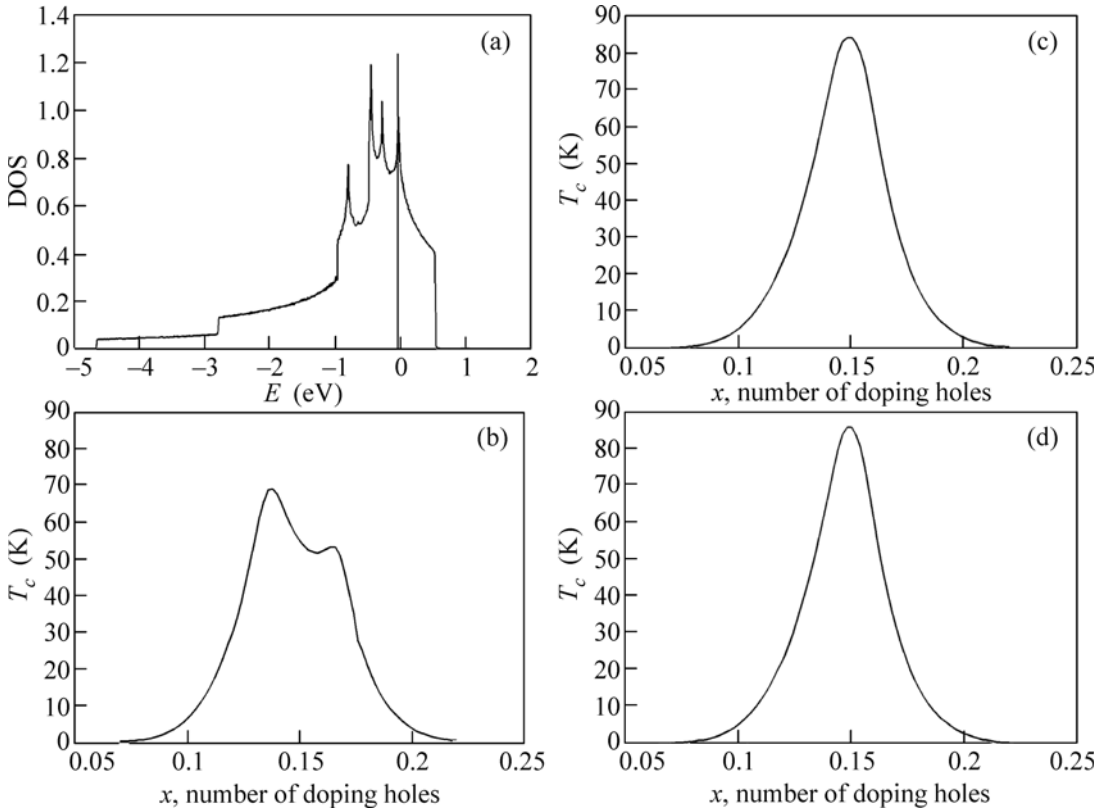

Fig. 1. (a) Density of states at $x = 0.125$ and $t_\perp = 0.1$ eV for a bilayer cuprate (the vertical lines indicates the chemical potential); and T_c versus x at $t_\perp =$ (b) 0.1 and (c) 0.02 eV, as well as (d) for a single-layer cuprate.

optimal doping level. In the case of bilayer cuprates with $t_\perp = 0.1$ eV, one can clearly see two peaks in T_c (Fig. 1b). The origin of these peaks is quite clear. Due to the bilayer splitting, instead of a single band in a CuO_2 plane, we have two bands, bonding and antibonding, giving rise to two van Hove singularities in the density of states (Fig. 1a) [5, 21]. With the change in doping, the peaks in the density of states are displaced and their intensity changes, but the two-peak structure itself remains unchanged. The coincidence of the chemical potential with each of the van Hove singularities results in its own peak in T_c. A sufficiently large intracell interlayer hopping integral $t_\perp = 0.1$ eV results in a large band splitting and, hence, in a large difference in the doping levels corresponding to these peaks. The first and second peaks are observed at $x =$ 0.125 and 0.178, respectively. With a decrease in the bilayer splitting, the peaks become closer, but remain distinguishable down to $t_\perp = 0.05$ eV. Further on, we see only a single broad peak, which becomes narrower with the decrease in $t_\perp$ (Fig. 1c); at $t_\perp = 0.01$ eV, the plot becomes nearly identical to that for the single-layer cuprates (Fig. 1d). For bilayer cuprates, the maximum value of T_c is lower than that for single-layer cuprates. The T_c value for single-layer compounds is the limiting value for the maximum T_c value in the bilayer ones increasing with the decrease in the coupling between CuO_2 layers. The main cause preventing an increase in T_c with the number of layers is a factor of 1/2 in the sum of anomalous averages for the bonding and antibonding bands in Eq. (6), whereas in comparison to the single-layer compound, no additional pairing mechanism appears.

The height of the T_c peaks also changes, which seems to be rather strange at first glance. However, there actually are even two factors affecting the absolute value of T_c. First, the bilayer splitting manifests itself not only in the separation of the band energies but also in the difference in the set of wavevectors forming the Fermi contour for a given band. In other words, the band splitting in energy is accompanied by a shift in the wave vectors. Thus, the terms (in the sum over **q**) in equation (6) for T_c giving the maximum contribution to the formation of one peak differ from those forming another peak, first of all, in the set of wave vectors **q**. Since the sum includes a factor with the difference of cosines, the different sets of wave vectors make different contributions. Second, the number of contributions from the different regions of the **k** space to the sum over **q** depends on the position of the chemical potential. For example, in the quantum transition point at $x = 0.125$, the maximum contribution to the sum comes from the nodal direction, which

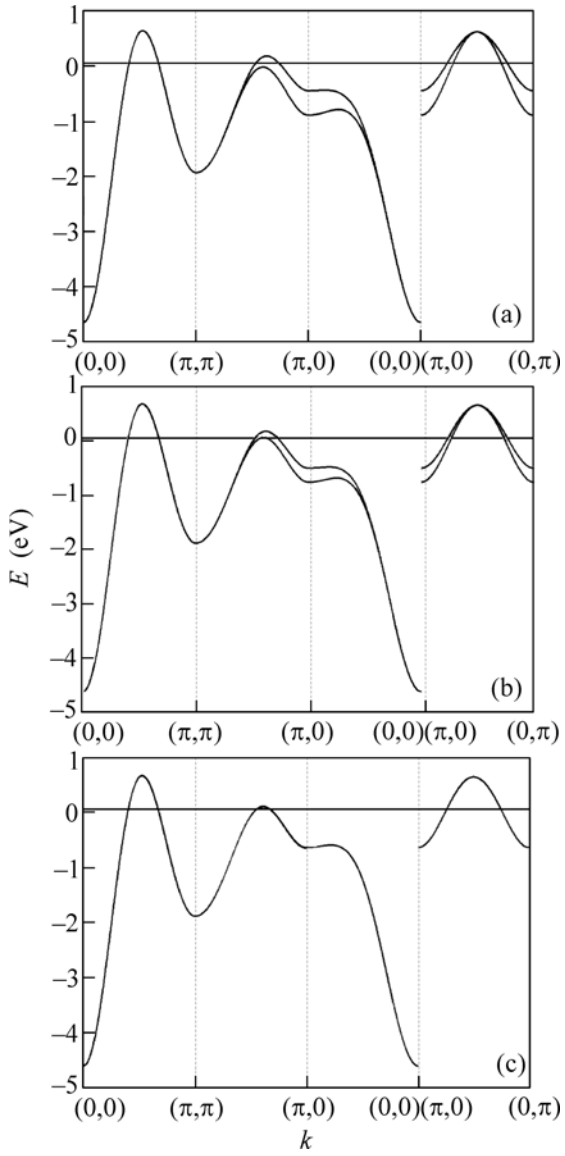

Fig. 2. Band structure at different values of interlayer antiferromagnetic correlations: $C_\perp$ = (a) −0.01, (b) −0.1, and (c) −0.22.

intersects the chemical potential, as well as directly from the saddle point (the point of tangency of the antibonding band with the chemical potential) located in the (π, π)–(π, 0) direction. At the point of the second quantum phase transition (x = 0.178), the chemical potential again crosses the band at the nodal direction, touches the bonding band, but in this case, it additionally crosses the antibonding band. Therefore, the sum over **q** should include more significant contributions leading to the lowering of the transition temperature.

5. In addition to the interlayer hopping, multilayer compounds exhibit also magnetic correlations along the c axis. We neglect the intercell magnetic correlations due to the large distance between the neighboring bilayers along the c axis (0.8 nm) in comparison to the distance between one bilayer (0.3 nm) and keep only the intracell interlayer spin correlation function. The value of this correlation function was calculated by the exact diagonalization for the bilayer cluster. We considered the unit cell of a bilayer cuprate consisting of two CuO_5 pyramids and took explicitly into account all interactions within them. In the obtained basis of two-particle states corresponding to one hole per layer, the ground state is a singlet, which can be written in the form $(1/\sqrt{2})(a^+_{fu\downarrow}a^+_{fd\uparrow} + a^+_{fd\downarrow}a^+_{fu\uparrow})$. This state corresponds to the antiferromagnetic spin ordering in the neighboring layers. Such antiferromagnetic interlayer ordering was confirmed by the neutron diffraction experiments [22]. For the underdoped case, at $T = 0$, our calculations demonstrate that the characteristic interlayer spin correlation function $\langle X^{\sigma\bar{\sigma}}_{(u)}X^{\bar{\sigma}\sigma}_{(d)}\rangle$ is equal to −0.1 (recall that the correlation function for the nearest neighbors inside the CuO_2 layer is $C_{01} \approx -0.2$ [4, 23, 24]). According to (4), the spin correlations contribute to the energy of the coupling between CuO_2 layers; at first glance, it seems that they should result in an increase in the energy. However, due to the negative sign of the correlation function, this contribution to energy leads to lowering of the coupling energy; that is, the antiferromagnetic correlations suppress, in fact, the bilayer splitting. Indeed, the assumption of the existence of the antiferromagnetic spin ordering in the neighboring CuO_2 layers in the cell means that single-particle states with spin up and down are occupied in the first and second layers, respectively. In its turn, this imposes a limitation to the form of possible quasiparticles and hence to the possible interlayer hopping; for example, a quasiparticle with spin up cannot come to the neighboring plane since the latter has the occupied single-particle state with the same spin and, therefore, only intraplane quasiparticle transitions with the opposite spins are possible.

An effect of the antiferromagnetic correlations leading to a pronounced decrease in the bilayer splitting is illustrated in Fig. 2. Figure 2a shows the band structure for the system with the interlayer coupling mediated only by the interlayer quasiparticle hopping. In the other limiting case, $C_\perp = -0.22$ (Fig. 2c), when the absolute value of the spin correlation function is close to the maximum possible one for an undoped composition, namely to 0.25, the band splitting can disappear at all. The effect of magnetic correlations on the magnitude of the bilayer splitting manifests itself, of course, in the concentration dependence of T_c. The growth of magnetic correlations up to $C_\perp = -0.22$ leads to the complete disappearance of the two-peak structure of $T_c(x)$. Thus, the mechanism underlying the preservation of the single-peak shape of the $T_c(x)$ curve is related just to the antiferromagnetic exchange between the CuO_2 layers.

Doping leads to an increase in the charge carrier density and, hence, in the kinetic energy of the system,

resulting in the smearing of magnetic correlations. This is confirmed by the calculations of the dependence of the spin correlation functions on doping x for the single-layer cuprates [4]. It is evident that the interlayer spin correlation function will also be decreasing with an increase in the density of charge carriers appearing due to the doping. In addition, the contribution of this spin correlation function to the bilayer splitting will decrease due to the denominator $p_\sigma + x$. This decrease will lead to an increase in both the interlayer coupling and bilayer splitting. This is clearly seen in the ARPES images of the Fermi surface. The observation of the bilayer splitting turned out to be possible just for overdoped samples [25].

Thus, the conventional parabolic shape of the phase diagram characteristic of the superconducting state of the bilayer cuprates can be not only a consequence of the limitations on the typical hopping integrals, but can also be due to the strong antiferromagnetic correlations suppressing the interlayer hopping.

6. The similarity in the shape of the concentration dependence of T_c for the bilayer cuprates with that of the $T_c(x)$ curve for single-layer cuprates can be interpreted as a consequence of a pronounced suppression of the bilayer splitting, related to the quasiparticle hopping between the CuO_2 layers, by the intracell antiferromagnetic interlayer correlations. The absence of the growth in the maximum T_c value due to the interlayer hopping suggests that such hopping between CuO_2 layers cannot play a key role in the mechanism of high-T_c superconductivity. The experimentalists come to the same conclusion, based on the pressure dependence of T_c in the directions of three crystallographic axes. It turns out that T_c depends on pressure only slightly in the direction perpendicular to the CuO_2 plane and, hence, only slightly depends on the interplanar distance [26–28]. The analysis of the high-pressure data for $La_{2-x}Sr_xCuO_4$ reported in [2] leads to the conclusion that the weak dependence of T_c on the number of CuO_2 layers in the unit cell related to the inhomogeneities and defects, since it is well known that the compounds with high T_c values have the most "regular" structure in contrast to the systems with relatively low T_c values characterized by different kinds of distortions.

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