Dependence of the Critical Temperature of High-Temperature Cuprate Superconductors on Hoppings and Spin Correlations between CuO$_2$ Planes

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Abstract—The influence of interlayer hoppings on the superconducting transition temperature (T_c) in bilayer cuprates has been studied. The parameter of hopping between layers is expressed as $t_\perp(\mathbf{k}) = t_\perp(\cos(k_x) - \cos(k_y))^2$ and treated as a small perturbation for the states of two CuO$_2$ planes described by the t–t'–t''–J^* model. In the generalized mean field approximation for $d_{x^2-y^2}$ symmetry of the superconducting gap, neither the interlayer hopping or exchange interaction, nor the pair hopping between CuO$_2$ layers provides an additional mechanism of Cooper pair formation or an increase in T_c. In the concentration dependence of T_c, the bilayer splitting of the upper Hubbard band of quasi-holes is manifested as two peaks with temperatures slightly lower than the maximum T_c for a single-layer cuprate. Interlayer antiferromagnetic spin correlations suppress bilayer splitting.

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1. INTRODUCTION

It is known that all high-temperature cuprate superconductors consist of alternating conducting and dielectric layers, the former containing various numbers (n) of CuO$_2$ planes. The importance of coupling between CuO$_2$ layers was established shortly after the discovery of high-temperature superconductivity, since it was found that the superconducting transition (critical) temperature T_c increased in each cuprate family (homologous series of Bi, Tl, and Hg-based superconductors) when the number of CuO$_2$ planes was changed from $n = 1$ to 3. Based on these findings, it could be expected that, by increasing the number of CuO$_2$ planes to $n \sim 10$ (which is allowed in crystal chemistry), it would be possible to reach $T_c \approx 300$ K. The creation of artificial multilayer structures of the Bi-22($n - 1$) system with T_c = 250 K for Bi$_2$Sr$_2$Ca$_7$Cu$_8$O$_{20+x}$ (Bi-2278) [1] seemed to confirm this hypothesis. However, these structures turned out to be unstable. Later, stable Bi-2278 structures were created using molecular beam epitaxy (MBE), but their T_c values did not exceed 60 K [2]. Moreover, it was also demonstrated [2] that a Bi-2212 film of unit-cell thickness (with n =2 CuO$_2$ planes) has T_c = 70 K.

The subsequent progress in MBE technology revealed the role of individual LaSrCuO layers, as parts of a multilayer La$_{1.55}$Sr$_{0.45}$CuO$_4$/La$_2$CuO$_4$ metal−dielectric heterostructure, in the formation of the superconducting state of the whole sample [3]. It was found that suppression of the superconductivity in a single La$_{2-x}$Sr$_x$CuO$_4$ layer (assumed to be doped to a nearly optimum level) significantly influences T_c of the whole structure. These results indicate that each individual CuO$_2$ layer plays an important role in the achievement of superconductivity in a volume sample. The nature of the T_c dependence on the number of CuO$_2$ planes in the unit cell is still not completely clear.

In this study, we will not consider the role of tunneling between superconducting layers through dielectric interlayers in the unit cell (according to the "high-temperature cuprate superconductor as heterostructure" model [4]). We restrict ourselves to the influence of the presence of two CuO$_2$ planes in a single superconducting metallic layer.

Generally speaking, the addition of a second CuO$_2$ plane permits growth of T_c by two types of mechanisms. The first type, which can be called dynamic, is related to interplanar interactions and hopping. The second type is based on specific features of the structure and the distribution of impurities and, hence, can be called impurity mechanisms. The present study is devoted to the dynamic mechanisms of single-electron hopping, interplanar exchange interaction, and interplanar hopping of quasi-particle pairs.

Experimental NMR data revealed the inequivalence of two external and $n - 2$ internal CuO_2 planes in the structures with $n \geq 3$ [5]. For this reason, we will restrict ourselves to two-layer structures of the $YBa_2Cu_3O_7$ (YBCO) and Bi-2212 types with equivalent CuO_2 planes. Chakravarty et al. [6] proposed an effective theoretical mechanism of the increase in T_c in these structures based on the postulated tunneling of Cooper pairs between CuO_2 planes with a tunneling probability amplitude of $T_J \sim 10\Delta_0$, where Δ_0 is the superconducting gap in one plane. However, Schneider and Singer [7] demonstrated the inapplicability of this approach to real high-temperature cuprate superconductors by estimating from experimental data the ratio (η) of the free energy due to interplanar coupling to the total energy of a superconductor for various families of cuprates. In particular, this ratio was $\eta \sim 10^{-3}$ for YBCO and $\eta \sim 10^{-4}$ for Hg cuprates. The smallness of η is evidence in favor of the model of a Josephson structure with weak coupling that does not influence the superconducting properties of separate CuO_2 planes.

Recently, we studied theoretically the role of hopping between CuO_2 planes in the normal phase and obtained bilayer splitting of the Fermi surface that was known earlier from experimental angle-resolved photoelectron spectroscopy (ARPES) data [9, 10]. In the present study, the bilayer system is considered using the $t-J$ model in a regime of strong electron correlations. A superconducting phase for $d_{x^2-y^2}$ symmetry of the gap with a magnetic mechanism of pairing is described using a generalized mean field theory of the Bardeen–Cooper–Schrieffer (BCS) type. It will be shown that the interplanar hopping does not increase the critical temperature. Thus, we conclude that the dependence of T_c on the number of CuO_2 planes should be searched in the class of impurity mechanisms.

The structure of this article is as follows. Section 2 describes the $t-t'-t''-t_\perp-J^*-J_\perp$ model with interlayer hopping ($t_\perp$), interplanar exchange ($J_\perp$), and interplanar pair hopping.

Section 3 gives the main relations of the generalized mean field theory for a superconducting phase with allowance for the short-range antiferromagnetic order, and Section 4 presents the results of numerical simulating the influence of interlayer hopping ($t_\perp$) on the T_c value. Section 5 considers the behavior of the isotopic effect parameter in systems with interlayer splitting. In Section 6, the results are discussed and compared to experimental data. Preliminary results of this investigations were reported in part in [11].

2. BILAYER CUPRATES: $t-t'-t''-t_\perp-J^*-J_\perp$ MODEL

It is commonly accepted that the electron structure and all important characteristics of high-temperature cuprate superconductors in both normal and superconducting phases are determined by the behavior of particles inside the CuO_2 layer, while the role of all other atoms in the cell is entirely reduced to supplying current carriers to the copper–oxygen layer. The main argument in favor of the possibility of ignoring the atomic environment of the CuO_2 layer is based on the fact that the valence shell energies in atoms of these metals are significantly lower than the characteristic band energies in the CuO_2 plane. In the copper–oxygen plane, the dynamics of electrons is realized on the $3d$ orbitals of copper and $2p$ orbitals of oxygen, so that a multiband $p-d$ model offers a natural basis for describing the electron structure in this plane. In the presence of strong electron correlations, it is necessary to modify the usual one-electron approach to the description of these systems [12, 13]. Because of strong Coulomb repulsion on one atom, states with numbers of particles differing by unity have significantly different energies. A realistic multiband Hubbard model constructed on the basis of one- and two-particle states determined in the $p-d$ model gives a more adequate description in this case. In the region of low-energy excitations in the limit of strong electron correlations, this model reduces to the $t-t'-t''-J^*$ model [14–19]. As for the superconducting phase, we are primarily interested in states near the Fermi level, while states deep in the band are less important. Therefore, it is expedient to use the $t-t'-t''-J^*$ model for the superconducting state as well [16, 17].

The stoichiometric composition of a bilayer superconducting cuprate in the absence of doping (e.g., for $YBa_2Cu_3O_7$) corresponds to one hole in each CuO_2 plane. Except for the case of one missing apical oxygen, each CuO_5 pyramid repeats the unit cell of an $La_2Sr_{2-x}CuO_4$ crystal. For this reason, we assume that the electron structure of the bilayer system differs from that of a single layer [19] only by the splitting of bands in each layer into bonding and antibonding ones (bilayer splitting) [9, 20–25] as a result of interlayer interactions. Allowance for interlayer hopping and exchange interaction modifies the $t-t'-t''-J^*$ model into the $t-t'-t''-t_\perp-J^*-J_\perp$ model.

For a superconducting electron fluid, the fraction of the free energy density along the c axis relative to the total free energy density in cuprates is very small ($\eta \sim 0.001$) [7, 26–31]. This indicates that multilayer cuprates are quasi-two-dimensional systems and, hence, allows us to ignore processes related to single-particle hopping and pair tunneling between unit cells along the c axis. For this reason, we will only consider hopping along the c axis between two CuO_2 planes inside one bilayer within a single unit cell. A similar approach was used earlier to investigate multilayer structures [32–38]. Hopping is formally treated as transitions from a band of the upper CuO_2 plane to a band of the lower plane and vice versa. In the Hamiltonian, this process is represented as a term with the characteristic dependence on the two-dimensional

(2D) wave vector: $t_\perp(\mathbf{k}) = t_\perp(\cos k_x - \cos k_y)^2$. This form of the hopping integral as a function of the 2D wave vector follows from the results of band calculations [39] and is consistent with ARPES experiments [9, 20]. The square of the difference of cosines appearing in the expression for $t_\perp(\mathbf{k})$ is related to an effective overlap of the $d_{x^2-y^2}$ orbitals of copper, which is provided by real overlap of the s orbitals and by the $s-p$ and $p-d$ hybridization. Direct overlap of the $d_{x^2-y^2}$ orbitals and p_x, p_y orbitals of the adjacent layers is extremely small because the major electron density fraction of these orbitals is distributed in the CuO_2 plane. As a result, the absolute value of the interlayer hopping integral is smaller by an order of magnitude than that for the intraplane hopping, which makes it possible to consider the former hopping as a small perturbation between the two CuO_2 planes. The presence of quasi-particle hopping between planes in the $t-J$ model automatically leads to the appearance of interlayer exchange interactions, but these—as will be shown below—do not play any significant role in the mechanism of superconductivity. In describing the superconducting phase, it is also important to take into account the hopping of quasi-particle pairs between layers, i.e., the hopping of a Cooper pair as the whole. Note that the hopping of Cooper pairs between layers is analogous to the Josephson effect for a weak contact between two superconductors.

The Hamiltonian of the $t-t'-t''-t_\perp-J^*-J_\perp$ model is written in terms of Hubbard operators, which provide a natural and convenient algebra for describing systems with strong electron correlations. The Hubbard operator $X_f^{\sigma S}$ corresponds to quasi-particle excitations from a two-hole Zhang–Rice state $|S\rangle$ to a one-hole state $|\sigma\rangle$ on the fth site, which form the upper Hubbard hole band. Thus, in the case of a bilayer cuprate, the total Hamiltonian of the $t-t'-t''-t_\perp-J^*-J_\perp$ model can be written as follows:

$$H_{t-t'-t''-t_\perp-J^*-J_\perp} = \sum_{f\alpha\sigma}(\varepsilon_1 - \mu)X_{f\alpha}^{\sigma\sigma}$$

$$+ \sum_{f\alpha}(\varepsilon_2 - 2\mu)X_{f\alpha}^{SS} + \sum_{fg\alpha\sigma}t_{fg}X_{f\alpha}^{S\sigma}X_{g\alpha}^{\sigma S}$$

$$+ \sum_{fg\alpha\sigma}J_{fg}(X_{f\alpha}^{\sigma\bar\sigma}X_{g\alpha}^{\bar\sigma\sigma} - X_{f\alpha}^{\sigma\sigma}X_{g\alpha}^{\bar\sigma\bar\sigma}) \tag{1}$$

$$- \sum_{mln\alpha\sigma}\frac{\tilde{t}_{ml}\tilde{t}_{ln}}{E_{ct}}(X_{m\alpha}^{S\sigma}X_{l\alpha}^{\sigma\bar\sigma}X_{n\alpha}^{\bar\sigma S} - X_{m\alpha}^{S\sigma}X_{l\alpha}^{\bar\sigma\bar\sigma}X_{n\alpha}^{\sigma S})$$

$$+ H_{t_\perp} + H_{\text{exch}} + H_{\text{pair}},$$

$$H_{t_\perp} = \sum_{m_u n_d \sigma} t_\perp(m_u, n_d)(X_{m_u}^{S\sigma}X_{n_d}^{\sigma S} + X_{n_d}^{S\sigma}X_{m_u}^{\sigma S}), \tag{2}$$

$$H_{\text{exch}} = \sum_{m_u n_d \sigma} J_\perp(m_u, n_d) \tag{3}$$

$$\times (X_{m_u}^{\sigma\bar\sigma}X_{n_d}^{\bar\sigma\sigma} - X_{m_u}^{\sigma\sigma}X_{n_d}^{\bar\sigma\bar\sigma}),$$

$$H_{\text{pair}} = \sum_{\substack{u_1 u_2 \\ d_1 d_2 \\ \sigma}} T_\perp(u_1, u_2, d_1, d_2) \tag{4}$$

$$\times (X_{u_1}^{S\bar\sigma}X_{u_2}^{S\sigma}X_{d_1}^{\sigma S}X_{d_2}^{\bar\sigma S} + \text{H.c.}).$$

Here, subscript "α" refers to up (u) and down (d) CuO_2 planes; $J_{fg} = 2\tilde{t}_{fg}^2/E_{ct}$ is the parameter of the effective exchange interaction associated with hoppings to the lower Hubbard band and back; t_{fg} are the intraband hoppings between unit cells; $\tilde{t}_{fg}$ are the interband hoppings between unit cells; E_{ct} is the dielectric gap with charge transfer; and ε_1 and ε_2 are the energies of local states for the cell with one and two holes, respectively. The values of model parameters for a single CuO_2 layer were calculated earlier [19] ab initio using the local density approximation (LDA) with the generalized tight binding (GTB) model. Hamiltonians $H_{t_\perp}$, H_{exch}, and H_{pair} describe interlayer hopping, interlayer exchange interaction, and interlayer pair hopping, respectively. In the latter Hamiltonian, u_1, u_2 and d_1, d_2 refer to pairs of sites in the up and down CuO_2 planes, respectively. The coefficient $t_\perp(m_u, n_d)$ in expression (2) is the Fourier transform $t_\perp(\mathbf{k})$ of the integral of interlayer hopping between sites in the up (m_u) and down (n_d) planes. The characteristic values of the intracell hopping integral $t_\perp$ that can be extracted from LDA calculations [39] ($t_\perp = 0.25/4 = 0.06$ eV) or from ARPES data [40] ($t_\perp = 0.5 \times 0.057 \approx 0.029$ eV) are two orders of magnitude lower than the maximum integral t_{pd} of in-plane hopping between d_x orbitals of copper and p orbitals of oxygen. It is also necessary to bear in mind that, on the passage from description of the usual fermions to Hubbard's fermions, the effective value of the interlayer hopping integral decreases as a result of multiplication by the Clebsch–Gordan and genealogical coefficients. Figure 1 presents the coordinate dependence of this integral plotted as $t_\perp(\mathbf{R}) = t_\perp(m_u, n_d)$.

The dependence of the interlayer exchange parameter $J_\perp(m_u, n_d)$ on the distance between sites in the up (m_u) and down (n_d) CuO_2 planes is determined by the form of this function in the $\mathbf{k}$ space:

$$J_\perp(\mathbf{k}) = \frac{t_\perp^2(\mathbf{k})}{E_{ct}} = \frac{t_\perp^2(\cos k_x - \cos k_y)^4}{E_{ct}}. \tag{5}$$
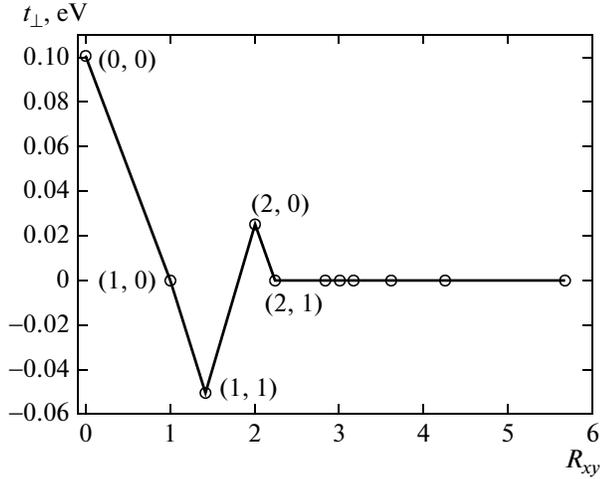
Fig. 1. Coordinate dependence of interlayer hopping integral (R_{xy} is the distance in plane between $(0, 0)$ site in one layer to (x, y) site in the adjacent layer, $t_\perp$ is assumed to be 0.1 eV).

The interlayer pair hopping in the reciprocal space is described by the following Hamiltonian:

$$H_{\text{pair}} = \sum_{\mathbf{k}} T_\perp(\mathbf{k})(X_{\mathbf{k}}^{S\sigma} X_{-\mathbf{k}}^{S\bar{\sigma}} X_{-\mathbf{k}}^{\bar{\sigma}S} X_{\mathbf{k}}^{\sigma S} + \text{H.c.}), \qquad (6)$$

where the hoping integrals $T_\perp(\mathbf{k})$ are determined by the $t_\perp^2(\mathbf{k})/t_{01}$ values [6] as

$$T_\perp(\mathbf{k}) = \frac{t_\perp^2(\mathbf{k})}{t_{01}}(\cos k_x - \cos k_y)^4. \qquad (7)$$

The parameters of the $t–t'–t''–t_\perp–J^*–J_\perp$ model Hamiltonian (borrowed from [19] are as follows (in electronvolts):

$$\varepsilon_2 - \varepsilon_1 = -0.091, \quad \varepsilon_2 = 2\varepsilon_1 + E_{\text{ct}}, \quad E_{\text{ct}} = 2,$$

$$t \equiv t_{01} = 0.93, \quad t' \equiv t_{11} = -0.12, \quad t'' \equiv t_{02} = 0.15,$$

$$J \equiv J_{01} = 0.295, \quad J' \equiv J_{11} = 0.003,$$

$$J'' \equiv J_{02} = 0.007,$$

$$\tilde{t} \equiv \tilde{t}_{01} = 0.77, \quad \tilde{t}' \equiv \tilde{t}_{11} = -0.08, \quad \tilde{t}'' \equiv \tilde{t}_{02} = 0.12.$$

Note that, in fact, we need to speak about a certain region of possible parameters for the reduction of various realistic models (e.g., the multiband $p–d$ model) to the $t–t'–t''–J^*$ model. Variation of the model parameters in this region would mostly be related to choosing the number of energy levels to be taken into account in the initial (nonreduced) Hamiltonian. The problem of determining these intervals of parameters has been considered in much detail [41, 42].

3. DESCRIPTION OF THE SUPERCONDUCTING PHASE

The energy characteristics, such as the dispersion and superconducting gap, have been calculated using the method of motion equations for the two-time retarded four-component Green's function

$$G_{\mathbf{k}\sigma} = \langle\langle X_{\mathbf{k}}^{\sigma S} | X_{\mathbf{k}}^{S\sigma} \rangle\rangle,$$

which consists of normal and anomalous in-plane components,

$$G_{\mathbf{k}\sigma}^{u} = \langle\langle X_{(u)\mathbf{k}}^{\sigma S} | X_{(u)\mathbf{k}}^{S\sigma} \rangle\rangle, \quad F_{\mathbf{k}\sigma}^{u} = \langle\langle X_{(u)-\mathbf{k}}^{S\bar{\sigma}} | X_{(u)\mathbf{k}}^{S\sigma} \rangle\rangle$$

and interlayer components,

$$G_{\mathbf{k}\sigma}^{du} = \langle\langle X_{(d)\mathbf{k}}^{\sigma S} | X_{(u)\mathbf{k}}^{S\sigma} \rangle\rangle, \quad F_{\mathbf{k}\sigma}^{du} = \langle\langle X_{(d)-\mathbf{k}}^{S\bar{\sigma}} | X_{(u)\mathbf{k}}^{S\sigma} \rangle\rangle.$$

The equation of motion contains high-order Green's functions, which can be projected using the method of irreducible Mori operators [42, 43] onto the basis set of normal Green's functions,

$$G_{\mathbf{k}\sigma} = \langle\langle X_{\mathbf{k}}^{\sigma S} | X_{\mathbf{k}}^{S\sigma} \rangle\rangle$$

and anomalous Green's functions,

$$F_{\mathbf{k}\sigma} = \langle\langle X_{-\mathbf{k}}^{S\bar{\sigma}} | X_{\mathbf{k}}^{S\sigma} \rangle\rangle.$$

As a result, we obtain the anomalous means

$$B_{\mathbf{q}} = \langle X_{\mathbf{q}}^{\sigma S} X_{-\mathbf{q}}^{\bar{\sigma} S} \rangle,$$

anomalous interlayer means

$$B_{\perp\mathbf{q}} = \langle X_{(u)\mathbf{q}}^{\sigma S} X_{(d)-\mathbf{q}}^{\bar{\sigma} S} \rangle$$

and two energy gaps, which include all possible interactions leading to the potential pairing of particles:

$$\Delta_{\mathbf{k}} = -\frac{1}{N}\frac{1}{p_\sigma + x}\sum_{\mathbf{q}}\Bigg[\left(2t_{\mathbf{q}} - p_\sigma(J_{\mathbf{k}+\mathbf{q}} + J_{\mathbf{k}-\mathbf{q}})\right.$$
$$\left. + 2p_\sigma\frac{\tilde{t}_{\mathbf{q}}^2}{E_{\text{ct}}} - 4(p_\sigma + x)\frac{\tilde{t}_{\mathbf{k}}\tilde{t}_{\mathbf{q}}}{E_{\text{ct}}}\right)B_{\mathbf{q}} - 2\tilde{t}_{\perp\mathbf{q}}B_{\perp\mathbf{q}}\Bigg], \qquad (8)$$

$$\Delta_{\perp\mathbf{k}} = \frac{1}{N}\frac{1}{p_\sigma + x}\sum_{\mathbf{q}}(p_\sigma(J_{\perp\mathbf{k}+\mathbf{q}} + J_{\perp\mathbf{k}-\mathbf{q}}) + ((p_\sigma + x)T_\perp)B_{\perp\mathbf{q}}), \qquad (9)$$

where $p_\sigma = \langle X^{\sigma\sigma} \rangle$ and x is the concentration of doping holes. The first term on the right-hand side of Eq. (8) reflects the kinematic mechanism of pairing[44], the second term is related to the exchange, the third and fourth are due to three-center interactions in one CuO_2 plane, and the last term allows for the hoppings between CuO_2 layers. The appearance of superconducting gap (9) is due to the possible pairing of quasiparticles from different planes by means of interlayer exchange interaction. The symmetry of the gap will be considered below. In the general case, the superconducting gap in each CuO_2 plane has the form of $\Delta^{u(d)} = \Delta_0^{u(d)} e^{i\theta^{u(d)}}$, where phase θ is the sum of the mean phase θ_0 and phase fluctuation $\delta\theta$.

For multilayer compounds, the form of the superconducting gap taking into account the mean phase was determined in [45]. That self-consistent calculation using a system of equations for each CuO_2 plane of the multilayer compound with allowance for the interaction between neighboring layers gave the following expression [45]:

$$\Delta_{j,k} = 2i\Delta_k \sin\left(\frac{\pi j}{p+1}\right),$$

where j runs through the numbers of CuO_2 layers and p is the total number of these layers. For example, in our case $p = 2$ and, hence, $\Delta_1 = \Delta_2$. Below we will rely on this result and assume mean phases in the neighboring layers to be the same and equal to zero. Phase fluctuations in the order parameters begin at temperatures about 15 K above T_c, and the phase rigidity grows with decreasing temperature [46] to reach a maximum upon the Berezinskii–Kosterlitz–Thouless (BKT) transition, where the system becomes two-dimensional. On passing toward higher temperatures, phase fluctuations at the BKT point break the 2D superconductivity. The phase difference between the adjacent planes along the c axis in single-layer cuprates vanishes due to the pair tunneling between planes, which leads to the establishment of phase coherence and thus forms the 3D superconductivity. For this reason, the 3D superconductivity is retained above T_{BKT} up to T_c. Since the region of 3D superconductivity (dome-shaped for both single- and multilayer cuprates) is qualitatively the same as the concentration dependence of T_c obtained in our calculations and only exhibits quantitative differences, we use the mean field approximation without taking into account fluctuations in the order parameter. The real parts of superconducting gaps for the up and down layer are assumed to the same, while the phase is assumed to be fixed and equal to zero.

The system of the equations of motion for both normal and anomalous in-plane and interlayer Green functions is as follows:

$$\begin{pmatrix} E-\xi & -t_\perp & -\Delta & -\Delta_\perp \\ -t_\perp & E-\xi & -\Delta_\perp & -\Delta \\ -\Delta^* & -\Delta_\perp^* & E+\xi & t_\perp \\ -\Delta_\perp^* & -\Delta^* & t_\perp & E+\xi \end{pmatrix} \begin{pmatrix} G_{k\sigma}^u \\ G_{k\sigma}^{du} \\ F_{k\sigma}^u \\ F_{k\sigma}^{du} \end{pmatrix}$$

$$= \begin{pmatrix} p_\sigma + x \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad (10)$$

where

$$\xi = \varepsilon_2 - \varepsilon_1 - \mu + (p_\sigma + x)t_k + p_{\bar{\sigma}}J_0$$
$$+ p_{\bar{\sigma}}(p_\sigma + x)\tilde{t}_k^2/E_{ct} + \Sigma(k) \quad (11)$$

is the law of dispersion in the normal phase;

$$\Sigma(k) = \frac{1}{p_\sigma + x}\frac{1}{N}$$

$$\times \sum_q \left[Y_1(k,q)K_q + \frac{3}{2}Y_2(k,q)C_q + t_\perp(q)K_q^\perp \right] \quad (12)$$

is the self-energy operator expressed via the in-plane kinematic correlators $K_q = \langle X_q^{S\sigma} X_q^{\sigma S} \rangle$, in-plane spin correlators $C_q = \langle X_q^{\bar{\sigma}\sigma} X_q^{\sigma\bar{\sigma}} \rangle$, and interlayer kinematic correlators $K_q^\perp = \langle X_{(u)q}^{S\sigma} X_{(d)q}^{\sigma S} \rangle$ with the coefficients

$$Y_1(k,q) = t_q - p_\sigma J_{k-q} - x\frac{\tilde{t}_q^2}{E_{ct}} - (p_\sigma + x)\frac{2\tilde{t}_q\tilde{t}_k}{E_{ct}}, \quad (13)$$

$$Y_2(k,q) = t_{k-q} - p_\sigma J_q + p_\sigma\frac{\tilde{t}_{k-q}^2}{E_{ct}}$$
$$- (p_\sigma + x)\frac{2\tilde{t}_k\tilde{t}_{k-q}}{E_{ct}}, \quad (14)$$

and

$$\tilde{t}_{\perp q} = (p_\sigma + x)t_\perp(\cos q_x - \cos q_y)^2$$
$$\times \left(1 + \frac{3C_\perp}{2(p_\sigma + x)^2}\right) \quad (15)$$

is the bilayer splitting of the quasi-particle band of one CuO_2 layer with the interlayer spin correlator $C_\perp = \langle X_{(u)}^{\bar{\sigma}\sigma} X_{(d)}^{\sigma\bar{\sigma}} \rangle$.

In expressions (8)–(15), $p_\sigma + x = \langle X^{\sigma\sigma} \rangle + \langle X^{SS} \rangle$ is the occupation factor of the band under consideration. The occupation numbers of local states can be determined by jointly solving the chemical potential equation,

$$1 + x = \sum_\sigma p_\sigma + 2\langle X^{SS} \rangle,$$

where x is the degree of hole doping per CuO_2 layer, with the basis set completeness condition

$$\sum_\sigma X^{\sigma\sigma} + X^{SS} = 1.$$

The total number of states for a one-particle sector of the Hilbert space is

$$\sum_\sigma p_\sigma = 1 - x.$$

Since we are considering a paramagnetic phase, the probability of filling of one-particle states with spins

up ($p_\sigma = \langle X_f^{\sigma\sigma} \rangle$) and those with spins down ($p_{\bar\sigma} = \langle X_f^{\bar\sigma\bar\sigma} \rangle$) is the same: $p_\sigma = p_{\bar\sigma} = (1-x)/2$. The doping level is assumed to be the same in both CuO_2 layers and, hence, the occupation numbers are equal as well.

The interlayer kinematic correlators are calculated self-consistently together with the in-plane kinematic correlators and the chemical potential. The interlayer spin correlator was calculated using exact diagonalization of a bilayer cuprate cluster as described in the next section.

Solving system of equations (10) gives the dispersion of quasi-particle bands in the superconducting state,

$$E_{\mathbf{k}}^{1,2} = \pm\sqrt{(\xi_{\mathbf{k}} + \tilde{t}_{\perp\mathbf{k}})^2 + \Delta_{\mathbf{k}}^{(+)2}},$$
$$E_{\mathbf{k}}^{3,4} = \pm\sqrt{(\xi_{\mathbf{k}} - \tilde{t}_{\perp\mathbf{k}})^2 + \Delta_{\mathbf{k}}^{(-)2}}, \tag{16}$$

where $\Delta_{\mathbf{k}}^{(+)} = \Delta_{\mathbf{k}} + \Delta_{\perp\mathbf{k}}$ and $\Delta_{\mathbf{k}}^{(-)} = \Delta_{\mathbf{k}} - \Delta_{\perp\mathbf{k}}$, and determines the Green's functions

$$G_{\mathbf{k}\sigma}^{u} = \frac{p_\sigma + x}{(E - E_{\mathbf{k}}^1)(E - E_{\mathbf{k}}^2)(E - E_{\mathbf{k}}^3)(E - E_{\mathbf{k}}^4)}$$
$$\times [((E + \xi_{\mathbf{k}})^2 - \tilde{t}_{\perp\mathbf{k}}^2)(E - \xi_{\mathbf{k}})$$
$$- (\Delta_{\mathbf{k}}^2 + \Delta_{\perp\mathbf{k}}^2)(E + \xi_{\mathbf{k}}) + (\Delta\Delta_{\perp}^* + \Delta_{\perp}\Delta^*)\tilde{t}_{\perp\mathbf{k}}], \tag{17}$$

$$G_{\mathbf{k}\sigma}^{du} = \frac{p_\sigma + x}{(E - E_{\mathbf{k}}^1)(E - E_{\mathbf{k}}^2)(E - E_{\mathbf{k}}^3)(E - E_{\mathbf{k}}^4)}$$
$$\times [((E + \xi_{\mathbf{k}})^2 - \tilde{t}_{\perp\mathbf{k}}^2 - \Delta_{\mathbf{k}}^2 - \Delta_{\perp\mathbf{k}}^2)\tilde{t}_{\perp\mathbf{k}}$$
$$+ (E + \xi_{\mathbf{k}})(\Delta\Delta_{\perp}^* + \Delta_{\perp}\Delta^*)], \tag{18}$$

$$F_{\mathbf{k}\sigma}^{u} = \frac{p_\sigma + x}{(E - E_{\mathbf{k}}^1)(E - E_{\mathbf{k}}^2)(E - E_{\mathbf{k}}^3)(E - E_{\mathbf{k}}^4)}$$
$$\times [(E^2 - \xi_{\mathbf{k}}^2 - \tilde{t}_{\perp\mathbf{k}}^2 - \Delta_{\mathbf{k}}^2)\Delta_{\mathbf{k}}^*$$
$$+ (\Delta\Delta_{\perp}^* + 2\xi_{\mathbf{k}}\tilde{t}_{\perp\mathbf{k}})\Delta_{\perp}^*)], \tag{19}$$

$$F_{\mathbf{k}\sigma}^{du} = \frac{p_\sigma + x}{(E - E_{\mathbf{k}}^1)(E - E_{\mathbf{k}}^2)(E - E_{\mathbf{k}}^3)(E - E_{\mathbf{k}}^4)}$$
$$\times [(E^2 - \xi_{\mathbf{k}}^2 - \tilde{t}_{\perp\mathbf{k}}^2 - \Delta_{\perp\mathbf{k}}^2)\Delta_{\perp\mathbf{k}}^*$$
$$+ (\Delta^*\Delta_{\perp} + 2\xi_{\mathbf{k}}\tilde{t}_{\perp\mathbf{k}})\Delta^*)]. \tag{20}$$

According to the spectral theorem, the interlayer anomalous means are related to the interlayer Green function $F_{\mathbf{k}\sigma}^{du}$ as

$$B_{\perp\mathbf{k}} = \langle X_{(u)\mathbf{k}}^{\sigma S} X_{(d)-\mathbf{k}}^{\bar\sigma S} \rangle$$
$$= -\frac{1}{\pi}\int_{-\infty}^{\varepsilon_F} f(E)\,\mathrm{Im}(\langle\langle X_{(d)-\mathbf{k}}^{S\bar\sigma}|X_{(u)\mathbf{k}}^{S\sigma}\rangle\rangle_{E+i\delta})\,dE. \tag{21}$$

As a result, the general expression for the superconducting gap takes the following form:

$$\Delta_{\mathbf{k}} = -\frac{1}{N}\frac{1}{p_\sigma + x}$$
$$\times \sum_{\mathbf{q}}\left(t_{\mathbf{q}} - p_\sigma(J_{\mathbf{k}+\mathbf{q}} + J_{\mathbf{k}-\mathbf{q}}) + 2p_\sigma\frac{\tilde{t}_{\mathbf{q}}^2}{E_{ct}}\right.$$
$$\left.- 4(p_\sigma + x)\frac{\tilde{t}_{\mathbf{k}}\tilde{t}_{\mathbf{q}}}{E_{ct}}\right)\left[\frac{\Delta_{\mathbf{q}}^{(+)}}{4E_{\mathbf{q}}^1}\tanh\frac{E_{\mathbf{q}}^1}{2\tau} + \frac{\Delta_{\mathbf{q}}^{(-)}}{4E_{\mathbf{q}}^3}\tanh\frac{E_{\mathbf{q}}^3}{2\tau}\right]$$
$$-\frac{1}{N}\frac{1}{p_\sigma + x}\sum_{\mathbf{q}}\left[\tilde{t}_{\perp\mathbf{q}}\left(\frac{\Delta_{\mathbf{q}}^{(+)}}{4E_{\mathbf{q}}^q}\tanh\frac{E_{\mathbf{q}}^1}{2\tau}\right.\right.$$
$$\left.\left.-\frac{\Delta_{\mathbf{q}}^{(-)}}{4E_{\mathbf{q}}^3}\tanh\frac{E_{\mathbf{q}}^3}{2\tau}\right)\right], \tag{22}$$

$$\Delta_{\perp\mathbf{k}} = \frac{1}{N}\frac{1}{p_\sigma + x}$$
$$\times \sum_{\mathbf{q}}(p_\sigma(J_{\perp\mathbf{k}+\mathbf{q}} + J_{\perp\mathbf{k}-\mathbf{q}}) + (p_\sigma + x)T_\perp) \tag{23}$$
$$\times \left[\frac{\Delta_{\mathbf{q}}^{(+)}}{4E_{\mathbf{q}}^1}\tanh\frac{E_{\mathbf{q}}^1}{2\tau} - \frac{\Delta_{\mathbf{q}}^{(-)}}{4E_{\mathbf{q}}^3}\tanh\frac{E_{\mathbf{q}}^3}{2\tau}\right],$$

where $\tau = k_B T$ and k_B is the Boltzmann constant.

For single-layer cuprates, it was shown [44, 47] that pairing within the $t-t'-t''-J^*$ model is possible due to the kinematic mechanism, exchange mechanism, and three-center hopping mechanism. It is known that the kinematic mechanism does not obey the condition of $d_{x^2-y^2}$ symmetry of the superconducting gap observed in the ARPES experiments [48] and scanning tunneling spectroscopy [49, 50]. Nevertheless, it should be noted that there is some evidence for deviations of the gap function from $\cos k_x - \cos k_y$ [51]. Expression (22) shows that the pairing of separate quasi-particles via interlayer hopping is impossible for the $d_{x^2-y^2}$ symmetry of the superconducting gap, since the product of $\tilde{t}_{\perp q}$ and Δ_q in this sum gives a third power of the difference of cosines and this term disappears upon summation. In the case of a bilayer cuprate, in contrast to the self-consistent equation for the superconducting gap in a single-layer cuprate, the Δ_k gap related to the in-plane pairing is supplemented by the $\Delta_{\perp k}$ gap, which reflects the interlayer pairing via exchange interaction. We can naturally assume that Δ_k, as well as the main superconducting gap $\Delta_{\perp k}$, possesses the $d_{x^2-y^2}$ symmetry. In the case of pairing in the CuO_2 plane, consideration is usually restricted to the exchange between nearest neighbors. For the interlayer exchange, the nearest neighbors are CuO_2 layers in the unit cell with

$(R_x, R_y) = (0, 0)$, for which the magnitude of exchange interaction is $J_{\perp 00} = 0.011$ eV. In this case, terms $J_{\perp 00}$ in the expansion of $J_{\perp \mathbf{k} \pm \mathbf{q}}$ will not contribute to the equation for T_c, since they cancel the dependence on $\mathbf{k}$ and $\mathbf{q}$ and, because of the $d_{x^2-y^2}$ symmetry of the gap, the summation over $\mathbf{q}$ eventually yields zero. Proceeding from the structure of its contribution to the expansion of $J_{\mathbf{k} \pm \mathbf{q}}$, exchange $J_{\perp 01}$ between the next-neighboring cells in the adjacent planes could potentially participate in pairing for the $d_{x^2-y^2}$ symmetry of the gap. However, the dependence of $J_\perp(\mathbf{k})$ on the wave vector resulted in the fact that $J_{\perp 01}$ was zero. Therefore, it can be seen that, in the adopted nearest-neighbor approximation, the mechanism of pairing via interlayer exchange interaction can be rejected.

In contrast to the hopping of separate quasi-particles, the anomalous Green's function in the case of pair tunneling,

$$F_{\mathbf{k}\sigma}^{du} = \langle\langle X_{(d)-\mathbf{k}}^{S\bar\sigma} | X_{(u)\mathbf{k}}^{S\sigma} \rangle\rangle$$

exhibits direct entanglement with the normal Green's function

$$G_{\mathbf{k}\sigma} = \langle\langle X_{\mathbf{k}}^{\sigma S} | X_{\mathbf{k}}^{S\sigma} \rangle\rangle,$$

which leads to an additional contribution to the superconducting gap $\Delta_\perp$. However, taking into account the $d_{x^2-y^2}$ symmetry of the gap, the contribution from the tunneling of quasi-particle pairs to the self-consistent equation for the $d_{x^2-y^2}$ symmetry of the gap disappears for the same reason as that of separate one-particle hopping. Indeed, the product of an even power (second for single-particle hopping and fourth for pair hopping) of the difference of cosines in the hopping integral and the $\cos k_x - \cos k_y$ factor due to the gap symmetry leads to vanishing of the sum with respect to $\mathbf{q}$.

Eventually, with allowance for the $d_{x^2-y^2}$ symmetry of the gap,

$$\Delta_\mathbf{k} = \frac{\Delta_0}{2}(\cos k_x - \cos k_y) = \Delta_0 \varphi_\mathbf{k}$$

in the approximation of J_{01} exchange between nearest neighbors in the CuO_2 layer, the equation for T_c can be transformed as follows:

$$1 = \frac{1}{N} p_\sigma J_{01}$$

$$\times \sum_q \frac{\varphi_q^2}{2}\left(\frac{1}{E_q^+}\tanh\frac{E_q^+}{2\tau} + \frac{1}{E_q^-}\tanh\frac{E_q^-}{2\tau} \right), \quad (24)$$

where $E_q^+ = \xi_\mathbf{q} + \tilde{t}_{\perp\mathbf{q}}$ and $E_q^- = \xi_\mathbf{q} - \tilde{t}_{\perp\mathbf{q}}$. As can be clearly seen, the only result of the inclusion of interlayer interactions into the initial model is the appearance of a sum of two terms (corresponding to the pres-
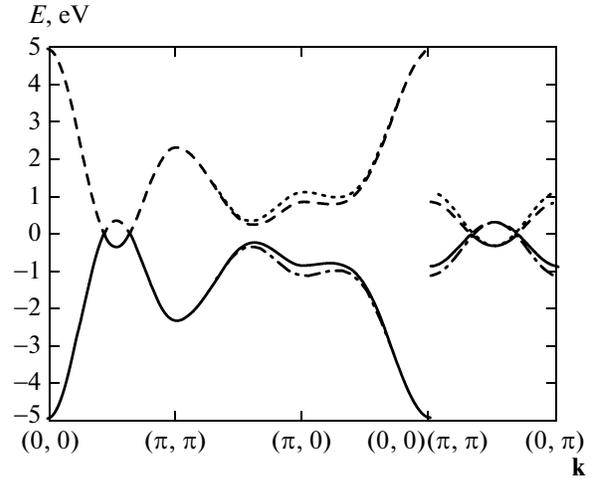
Fig. 2. Dispersion of quasi-particle bands for a bilayer cuprate with $x = 0.16$ in the superconducting phase.

ence of bonding and antibonding bands) in the expression for the anomalous means.

Using Eq. (17) at a fixed temperature, it is also possible to determine Δ_0. In the case under consideration, this value is 0.0195 eV at $T = 0$ for the parameters of Hamiltonian (1). For the given gap, the band structure in accordance with dispersion law (16) comprises four bands (Fig. 2).

4. INFLUENCE OF HOPPING INTEGRAL $t_\perp$ AND INTERLAYER SPIN CORRELATIONS ON T_c

4.1. Interlayer Hopping

Figures 3a and 3b show the concentration dependences of T_c for different values of single-particle interlayer hopping integral $t_\perp$. For realistic values of $t_\perp = -0.02$ eV and $C_\perp = -0.1$, the dependence of T_c on x (Fig. 3a) is almost the same as that for single-layer cuprates, the only difference being a small decrease in T_c at all concentrations of doping carriers. The main factor that prevents the increase in T_c with an increasing number of layers is redistribution of the density of states (DOS) of a single band (for single-layer cuprates) between two bands in the case of bilayer cuprates, which is manifested by the appearance of coefficient 1/2 in Eq. (24), while there are no additional mechanisms of pairing in bilayer system as compared to the single-layer case. Thus, in the framework of the generalized mean field approximation, it is impossible to speak of an increase in T_c due to the interlayer one-particle hopping. An increase in the hopping integral $t_\perp$ is accompanied by an increase in bilayer splitting between the bonding and antibonding bands and, hence, in the distance between two peaks in the DOS (Fig. 3c) [32]. Each peak corresponds to a certain van Hove singularity. With a change in the level of doping, the DOS peaks exhibit shifts and their
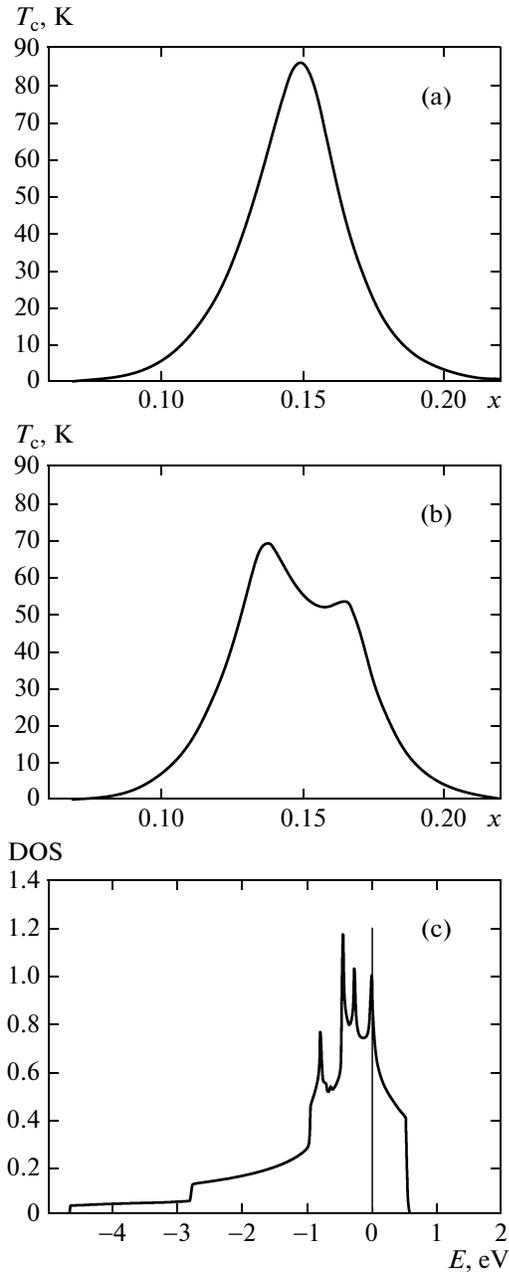
Fig. 3. Plots of (a, b) $T_c(x)$ versus x for $t_\perp = 0.02$ and 0.1 eV, respectively, and (c) density of states for $x = 0.137$ and $t_\perp = 0.1$ eV. All calculations were performed for an interplanar spin correlator $C_\perp = -0.1$.

intensities vary, but the two-peak structure is retained. Coincidence of the chemical potential with each of the van Hove singularities corresponds to a maximum in T_c. A rather large intracell interplanar hopping integral ($t_\perp = 0.1$ eV) leads to significant splitting of bands and the resulting difference of maxima with respect to the doping level (Fig. 3b). Indeed, the first maximum corresponds to $x = 0.137$, while the second corresponds to $x = 0.166$. No such two-peak structure in the concentration dependence of T_c has been observed in

experiments. Therefore, it may be concluded that the interlayer coupling never reaches this high a level in real bilayer cuprates.

The absolute values of maxima in T_c also vary, which might seem rather strange at first glance. However, there are two factors that can affect the absolute value of T_c. First, the bilayer splitting not only influences the energy difference between the bonding and antibonding bands (Fig. 4a), but also determines differences in the sets of wave vectors that form the Fermi contour for a certain band. This is well illustrated by the difference between regions of the Brillouin zone, in which a quantum phase transition takes place upon closing of the hole pockets (Fig. 4b). In other words, the energy splitting of the band takes place with a shift in respect to the wave vectors. Therefore, the terms in the sum over $\mathbf{q}$ in Eq. (24) for T_c, which give the maximum contribution to the formation of a single maximum, differ (primarily with respect to the set of $\mathbf{q}$) from the terms responsible for the second maximum. It should be noted that the maximum contribution to this sum is due to the points occurring close to the chemical potential, which is determined by the ratio of the hyperbolic tangent and deviation from the chemical potential, which enters $E^+(E^-)$ in Eq. (24). Since the sum contains a factor with the difference of cosines, various sets of wave vectors make different contributions.

Second, the number of contributions to the sum over $\mathbf{q}$ from different regions of the $\mathbf{k}$-space varies depending on the chemical potential. For example, at a point of the quantum phase transition for $x = 0.137$, the maximum contributions to the sum comes from the wave vectors along the nodal direction (crossed by the chemical potential) and directly from the saddle point (i.e., the point where the antibonding band touches the chemical potential) that occurs in the $(\pi, \pi)-(\pi, 0)$ direction. At the point of the second quantum phase transition ($x = 0.166$), the chemical potential once again crosses the band in the nodal direction and touches the bonding band, but now it also crosses the antibonding band, thus making more significant contributions to the sum over $\mathbf{q}$, so that the critical temperature should decrease.

4.2. Interlayer Spin Correlations

In the phase diagram of cuprates, the region of low doping corresponds to the antiferromagnetic phase. The zero doping level corresponds to the situation with a single hole with spin 1/2 per copper–oxygen plane in separate unit cells and long-range antiferromagnetic order in the entire crystal. As additional hole-type carriers are added, the long-range magnetic order is broken and replaced by a short-range order. The spin correlation functions that characterize the magnetic order very strongly influence the electron structure and spectrum of quasi-particle excitations [52–55]. In particular, allowance for the hole scatter-
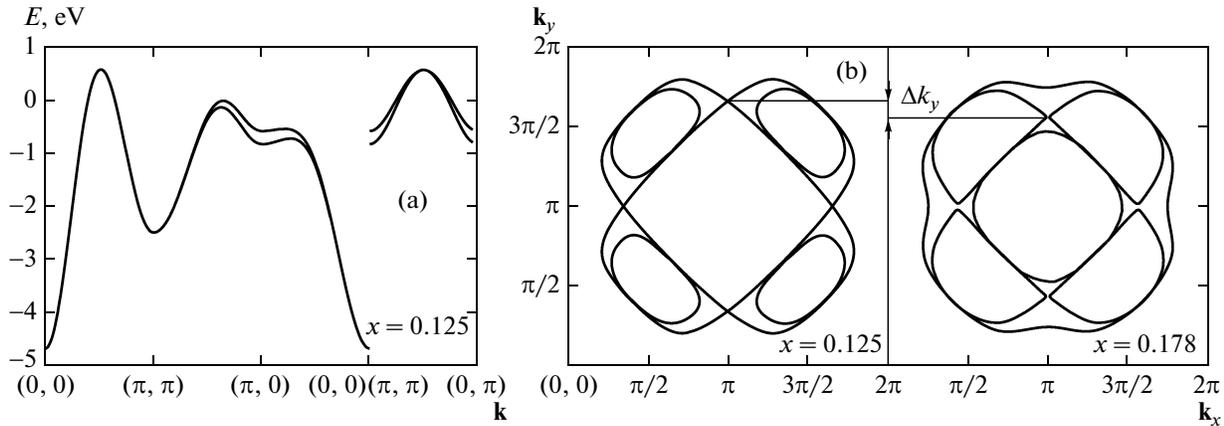
Fig. 4. (a) Bilayer splitting in the band structure of quasi-particle excitations in the normal state ($x = 0.125$); (b) Fermi surface at the points of quantum phase transitions ($x = 0.137$ and 0.166); Δk_y is the difference of wave vectors k_y for the two quantum phase transitions, which shows the shift of bands along wave vectors in the case of bilayer splitting.

ing on spin fluctuations leads to suppression of the spectral weight of the part of the pocket related to the shadow zone and the formation of an arc that is observed in ARPES [56]. Recent ARPES measurements with improved energy resolution actually revealed a pocket with sharply different spectral weights at various points of the Brillouin zone [57].

Bilayer cuprates exhibit magnetic correlations in the c axis. Ignoring the intercell spin correlations because of large distances (0.8 nm) between neighboring bilayers along the c axis as compared to interlayer intracell distance (0.3 nm), we retain only the intracell interlayer spin correlator. The magnitude of this correlator was determined by exact diagonalization of a bilayer cluster. For this purpose, a cell of bilayer cuprate consisting of two CuO_5 pyramids was considered and all interactions were exactly described. Then, the state with a minimum energy of the type $\frac{1}{\sqrt{2}}(a^+_{fu\downarrow}a^+_{fd\uparrow} - a^+_{fd\downarrow}a^+_{fu\uparrow})$ was separated in the basis of two-particle states. Since this state turned out to be singlet, the ground state in the undoped composition (with one hole per layer) must correspond to the antiferromagnetic state of two layers. The antiferromagnetic order of spins was experimentally confirmed by neutron diffraction [58]. Our calculations for the undoped composition at $T = 0$ showed that the characteristic interlayer spin correlator was $\langle X^{\sigma\bar\sigma}_{(u)} X^{\bar\sigma\sigma}_{(d)} \rangle = -0.1$. For comparison, it should be recalled that the spin correlation function for the nearest neighbors within the CuO_2 layer is $C_{01} \approx -0.2$ [19, 59, 60]. Spin correlations are part of the energy of binding between CuO_2 layers (16) and, at first glance, it might seem that their presence would increase this energy. However, because of the negative sign of the correlator, this contribution will decrease the binding energy so that, in

fact, the antiferromagentic correlations suppress bilayer splitting. Indeed, if the antiferromagentic ordering of spins were present in the neighboring CuO_2 layers of the cell, this would imply that a one-particle state with spin up is occupied in one layer and a state with spin down is occupied in the other layer. This, in turn, poses a limitation on the form of quasi-particles and, hence, on the possibility of hopping between layers: a quasi-particle with spin up cannot pass to the neighboring plane because the one-particle state with this spin is occupied, so that only in-plane transitions of quasi-particles with opposite spins are possible.

Figure 5 shows how strongly the antiferromagnetic correlations can decrease bilayer splitting. The band structure of a system in which a weak coupling between layers is provided only by the hopping of quasi-particles is shown in Fig. 5a. In the other limiting case of $C_\perp = -0.22$ (Fig. 5b), where the spin correlator for the undoped composition is close to maximum possible (0.25), the splitting of bands may completely vanish.

The effect of magnetic correlations on the magnitude of bilayer splitting is naturally manifested in the concentration dependence of T_c. An increase in the level of magnetic correlations to $C_\perp = -0.22$ leads to disappearance of the two-peak structure in $T_c(x)$. Thus, the antiferromagnetic exchange between CuO_2 layers provides the other mechanism (together with the small value of the interlayer hopping integral) that retains the shape of the $T_c(x)$ dependence with a single maximum. It should be emphasized that the suppression of bilayer splitting by spin correlations was obtained in the static mean field approximation. Allowance for the dynamic processes related, e.g., to the interaction with spin fluctuations can lead to a positive contribution to the interlayer coupling. For example, it was pointed out [61] that the interlayer
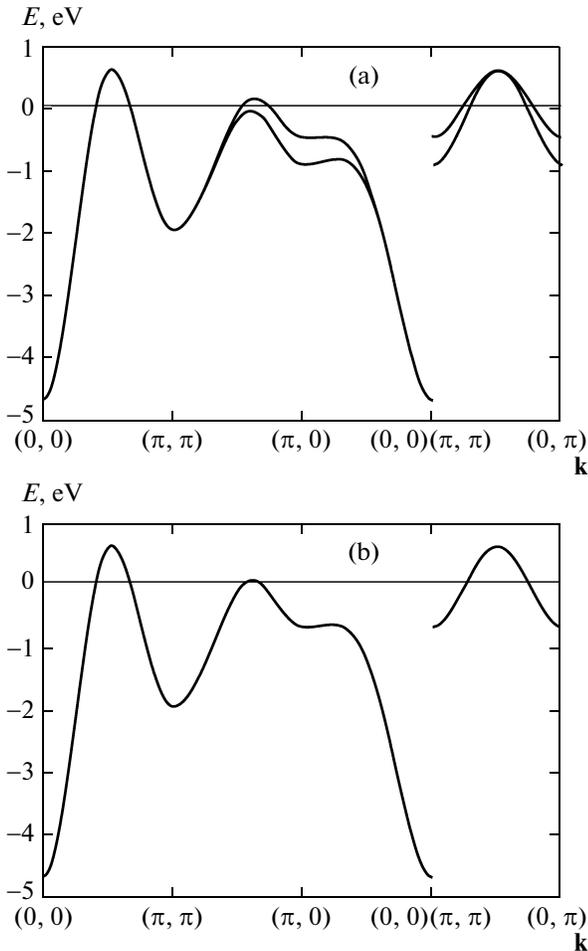
Fig. 5. Band structure for $t_\perp = 0.1$ eV and interlayer anti-ferromagnetic correlations $C_\perp = -0.01$ (a) and -0.22 (b).

spin−fluctuation interaction influenced the electron structure the most strongly and caused the appearance of kinks long the nodal direction. Thorough derivation of the exchange and spin−fluctuation mechanisms of superconductivity for a CuO_2 layer within the $p-d$ Hubbard model in the approximation of noncrossing diagrams [62] shows that (i) the spin−fluctuation mechanism of pairing becomes active in the case of allowance for the dynamic processes related to high-energy interband transitions and (ii) the mechanism of pairing due to scattering on spin fluctuations increases T_c.

5. INFLUENCE OF BILAYER SPLITTING ON THE ISOTOPE EFFECT EXPONENT WITH RESPECT TO THE TEMPERATURE

In addition to the concentration dependence of the critical temperature, another important characteristic of superconductivity is the isotope effect with respect to the temperature. In the results obtained above, it was assumed that a transition to the superconducting state was caused by the magnetic mechanism of Cooper pairing. In order to describe the isotope effect observed in cuprates, it is necessary to take into account the phonon mechanism as well. In a BCS-type theory, this leads to renormalization of the coupling constant in the equation for T_c, which will be the sum of the exchange and phonon contributions:

$$\lambda_{\mathbf{q}}^{tot} = p_\sigma J_{01} + \lambda_{ph}\theta(\omega_D - |E_{\mathbf{q}}^{+,-} - \mu|).$$

Here, as usual, the θ function restricts the phonon contribution to energies on the order of ω_D near the Fermi surface, while the parameter λ_{ph}, proportional to the matrix elements of electron−phonon interaction, is assumed to be free. It should be noted that the structure of this parameter in the used model is analogous to that in single-layer cuprates [63] because the final equation for the gap does not contain the inter-layer component $\Delta_{\perp\mathbf{k}}$. The difference appears in the expression for the isotope effect exponent. The determination of this parameter as $\alpha_o = -d\ln(T_c)/d\ln(M_o)$ leads to the following formula:

$$
\begin{aligned}
\alpha_o = {}& \lambda_{ph}\omega_D \sum_{\mathbf{q}} \delta(\omega_D - |E_{\mathbf{q}}^{+,-} - \mu|) \\
& \times \varphi_{\mathbf{q}}^2 \left[\frac{1}{E_{\mathbf{q}}^-}\tanh\left(\frac{E_{\mathbf{q}}^-}{2\tau_c}\right) + \frac{1}{E_{\mathbf{q}}^+}\tanh\left(\frac{E_{\mathbf{q}}^+}{2\tau_c}\right) \right] \\
& \times \left\{ \sum_{\mathbf{q}} (p_\sigma J_{01} + \lambda_{ph}\theta(\omega_D - |E_{\mathbf{q}}^{+,-} - \mu|)) \right. \\
& \left. \times \frac{\varphi_{\mathbf{q}}^2}{\tau_c}\left[\cosh^{-2}\left(\frac{E_{\mathbf{q}}^-}{2\tau_c}\right) + \cosh^{-2}\left(\frac{E_{\mathbf{q}}^+}{2\tau_c}\right) \right] \right\}^{-1}.
\end{aligned}
\tag{25}
$$

Evidently, the sums in square brackets correspond to the two van Hove singularities in the DOS. Since this parameter is inversely proportional to the DOS, each of these singularities is manifested by a minimum on the concentration dependence of $\alpha_o(x)$ at a sufficiently large value of the interband splitting (Fig. 6, solid curve). Experiments show a single minimum for both single-layer and bilayer cuprates [64]. In the model of interacting CuO_2 layers, this situation is achieved for $t_\perp \leq 0.035$ eV, which corresponds well to the hoping integral in real systems ($t_\perp^{exp} = 0.0285$ eV [40]; note that this value $t_\perp$ is not renormalized to the spin corre-lator; i.e., $t_\perp^{exp}$ coincides with the value used in our cal-culations at $C_\perp = 0$, see Eq. (15) for $\tilde{t}_\perp$). For these $t_\perp$ values, the minimum in α_o (in contrast to that for sin-gle-layer systems with $t_\perp = 0$) becomes wider and is located higher (Fig. 6). Thus, it can be seen that, in the mean field approximation, the interlayer splitting does not significantly affect the absolute values of T_c and α_o, although it can be among the possible reasons [65] for the broadening of the $T_c(x)$ and $\alpha_o(x)$ dependences.

In contrast to the results reported in [64], more recent investigation [66] revealed a strong dependence of α_o on the number of CuO_2 layers in a homologous series of bismuth cuprates. At the point of optimum doping, α_o decreases from 0.25 for $n = 1$ to 0.02 for $n = 3$. Note that, according to Eq. (25), this behavior cannot not only be the trivial consequence of a decrease in the phonon contribution to Cooper pairing, but can also be related to an increase in the magnetic contribution on the transition from single-layer to bilayer systems.

6. DISCUSSION OF RESULTS

The region of superconductivity in the phase diagrams of a large class of cuprates is inverse parabola with a maximum at the optimum doping level. Representatives of one family differ in the absolute values of T_c for a particular doping level, while the shape of the $T_c(x)$ curve remains qualitatively the same. Based on the results of calculations performed in the mean field approximation, we can conclude that the interlayer hopping does not increase the maximum T_c value as compared to that for single-layer compounds and, at a sufficiently large hopping integral, can change the $T_c(x)$ shape to a curve with two peaks. A two-peak concentration dependence was obtained earlier in [34], where the concentration dependence of the critical temperature of high-temperature bilayer cuprate superconductors was studied in the $t–J$ model, assuming that $t_\perp$ was nonzero only for the interlayer hopping inside the unit cell, i.e., that the hopping integral was independent of the 2D wave vector. The two-peak concentration dependence of T_c disappears for $t_\perp/t_{01} \approx 0.03$, replaced by a usual parabolic single-peak curve.

The absence of an increase in the maximum of T_c in the case of interlayer hopping suggests that the hopping of quasi-particles between CuO_2 layers cannot play a significant role in the formation of a high-temperature superconducting state. This agrees with the results of experiments on uniaxial pressure [67–70], which showed that a decrease in the spacing of CuO_2 layers under uniaxial pressure along the c axis influences T_c only via an increase in the concentration of carriers in the CuO_2 layers. In other words, an increase in the interlayer coupling weakly influences $T_{c(max)}$; i.e., dT_c/dP_c is decreased by an order of magnitude lower than the rate of change in $T_{c(max)}$ for compression in the plane: $dT_c/dP_a \approx -1.9$ K GPa^{-1} and $dT_c/dP_b \approx +2.2$ K GPa^{-1}. This is additional evidence for the decisive role of the CuO_2 layer in the formation of superconductivity. Pressure along the a and b axes leads to a decrease in the lattice parameters, which enhances coupling between the orbitals of copper and oxygen atoms and, hence, increases the hopping integral and exchange interactions. The exchange interactions between nearest neighbors in the plane, according to Eq. (23), directly influence T_c. It should be noted that the values of derivatives with respect to
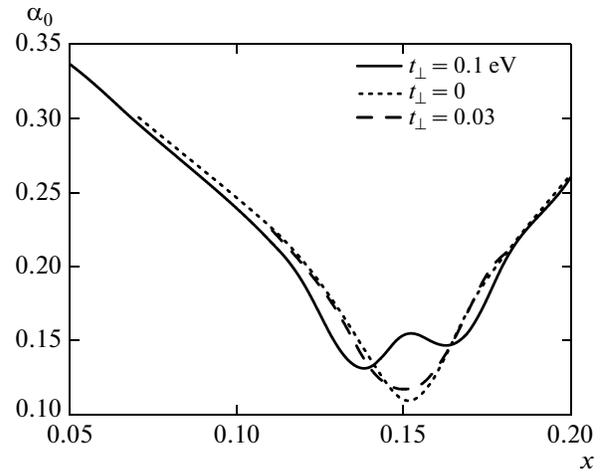
Fig. 6. Plot of the isotopic effect parameter α_o versus doping hole concentration for bilayer cuprates with various values of the interlayer hopping integral $t_\perp$.

pressure reflect the so-called "internal" properties of cuprates, i.e., changes in the atomic and electron structures without affecting the doping level in the CuO_2 plane. Schilling [71] used the terms of "healthy" and "pathological" cuprates, the latter being represented by the LaSrCuO and YBaCuO systems, in which the doping changes not only the hole concentration, but the structure as well. In contrast, the structures of healthy cuprates based on Tl and Hg are stable and doping only influences the concentration of holes. Experiments with pressure are performed in the latter families of cuprates—i.e., on compounds with the most planar and least curved CuO_2 planes. This choice is related to the absence of effects related to pressure-induced structural phase transitions. In addition, these compounds are characterized by the maximum T_c values among all cuprates. These facts suggest that defects such as the curves CuO_2 planes are not favorable for superconductivity. From the standpoint of microscopic theory, this can be explained by decreasing overlap (and, hence, interaction constants) for orbitals in this plane in the case of its deformation. However, this by no means implies that all other possible inhomogeneities are also unfavorable. It is quite possible that inhomogeneities and disorder in fact cause an increase in T_c upon the addition of CuO_2 layers to the unit cell with rearrangement of the atomic and electron structure of the reservoir of charge carriers and the introduction of new atoms. Indeed, an additional atom (e.g., Ca or Y) appears between copper–oxygen planes in bilayer cuprates in comparison to single-layer ones. A disorder that arises when divalent Ca^{2+} cation is replaced by trivalent Y^{3+} stabilizes the general cell structure due to the presence of an additional positive charge. Moreover, this substitution affects the electron structure of CuO_2 layers much more weakly as compared to the influence of disorder which takes

place with atomic substitutions near the apical oxygen [72]. In single-layer cuprates, the local substitutions of atoms located near the apical oxygen may displace this oxygen and deform the CuO_6 octahedron, since the opposite apical oxygen in this octahedron is fixed. Naturally, this deformation would modify the wavefunction and energy of the entire octahedron and, hence, affect the superconductivity. It was shown [72] for the family of bismuth cuprates that the partial replacement of Bi^{3+} by various lanthanide atoms (Ln—La, Pr, Sm, Eu. Gd) of the same valence significantly influenced T_c and greater the ion radius of substituted atoms corresponds the higher critical temperature. Reasons for the observed increase in T_c under these conditions are not completely clear, but it is evident that the presence of impurities and inhomogeneities in the atomic surrounding of CuO_2 layers influences the superconducting state either directly or indirectly (via apical oxygen). In multilayer cuprates, the influence of such inhomogeneities has an apparently softer character. In bilayer cuprates, there are two CuO_5 pyramids spaced by a relative large distance (0.3 nm) instead of one CuO_6 octahedron in single-layer compounds. The space between layers serves a kind of buffer that smoothens possible distortions in one of the two pyramids—probably, including the aforementioned curvature of CuO_2 planes—thus ensuring a more stable superconducting state and higher T_c values.

7. CONCLUSIONS

The existence of an experimentally observed dependence of the critical temperature of high-temperature cuprate superconductors depending on the number of CuO_2 layers per unit cell unambiguously indicates the presence of a relationship between the mechanism of superconductivity and effects related to the addition of CuO_2 layers. One of these effects is the appearance of possible intracell hopping between the copper—oxygen layers and other interlayer interactions. The present theoretical investigation showed in the framework of the generalized mean field approximation that allowance for the interlayer hopping treated as small perturbation leads to a decrease in the maximum T_c in bilayer cuprates. Therefore, it can be ascertained that the main effect of inclusion of the interlayer hopping—the band splitting and the resulting redistribution of the DOS—is not a factor that accounts for the increase in T_c in multilayer cuprate structures. Another consequence of the coupling between CuO_2 layers—the two-peak structure of the concentration dependence of T_c—is not achieved in bilayer cuprates because of small values of the interlayer hopping integral ($t_\perp \approx 0.027$ eV). Possible factors accounting for this smallness of $t_\perp$ are the weak overlap between the orbitals of adjacent CuO_2 planes and the presence of intracell interlayer antiferromagnetic correlations. Thus, the most probable reason for the

increase in T_c with the number of CuO_2 layers is the influence of various inhomogeneities. In comparison to single-layer cuprates, the bilayer ones exhibit changes in the curvature of CuO_2 planes, composition and structure of their atomic environment, way of doping, distribution of doping charge carriers, arrangement of defects and impurities, etc. We can naturally suggest that an increase in T_c in the case of bilayer compounds can be due to several of these factors.

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