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Superconductivity in the doped "pseudo-ladder" compound $CaCu_2O_3$

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Abstract. An effective anisotropic t-J model for the "pseudo-ladder" compound $CaCu_2O_3$ is proposed based on recent experimental studies and band structure calculations. Superconducting pairing mediated by the exchange interaction in the model is investigated as a function of doping away from the antiferromagnetic insulating state. It is shown that strong anisotropy in the electronic spectrum suppresses superconducting temperature in comparison with conventional copper-oxide superconductors with square lattices.

PACS. 74.20.-z Theories and models of superconducting state – 74.20.Mn Nonconventional mechanisms (spin fluctuations, polarons and bipolarons, resonating valence bond model, anyon mechanism, marginal Fermi liquid, Luttinger liquid, etc.) – 74.72.-h Cuprate superconductors (high-T_c and insulating parent compounds)

1 Introduction

The study of ladder compounds reveals interesting physics caused by a complex interplay between spin and charge degrees of freedoms in these particular class of strongly correlated electronic systems (for a review see Ref. [1]). The most intriguing phenomenon observed in the two-leg compound $Sr_{14-x}Ca_xCu_{24}O_{41}$ is superconductivity at high pressure [2] which possibly correlates with closing of the spin gap [3] (however, see also Ref. [4], where the closing of the spin gap has been doubted). On the other hand, under high pressure a crossover from one to two dimensions is observed [5] which shows that the superconductivity in this system occurs in a highly anisotropic two dimensional CuO_2 plane.

In recent experimental and theoretical studies of the electronic structure of the "pseudo-ladder" cuprate compound $CaCu_2O_3$ an unusual non-planar hole distribution was observed at variance with conventional ladder compounds [6]. It results from the strong interlayer coupling which is responsible for the missing spin gap generic for other two-leg ladder cuprates [7]. Contrary to the undoped two-leg ladder compounds, the undoped $CaCu_2O_3$ is an antiferromagnet (although with a relatively low Néel temperature $T_N = 25$ K [7]) as in other quasi-two-dimensional parent cuprates. Therefore this compound can be considered as an anisotropic bilayer compound and a candidate for high temperature superconductivity at hole doping away from the antiferromagnetic insulating state investigated so far.

In the present paper we propose an effective anisotropic t-J model and calculate the superconducting transition temperature as a function of doping. It is shown that anisotropy of the electronic spectrum in the copper-oxide plane suppresses the superconductivity mediated by the exchange interaction in comparison with conventional cuprates having square lattice.

2 Effective t-J model

The crystal structure of the $CaCu_2O_3$ compound can be viewed as corner-shared CuO_2 zigzag chains running along the b-axis which are tilted by nearly 29° from a straight Cu-O-Cu bond with the neighboring zigzag chains forming this way positively and negatively buckled ladders with "kinked" rungs in a-direction (see Fig. 1). This layers are packed along c-direction in a three-dimensional crystal. Each stack of pseudoladders forms a bilayer. Taking into account the results of recent experimental and theoretical studies of the electronic structure of this "pseudo-ladder" cuprate compound [6], we propose the following anisotropic t-J model:

$$H_{t-J} = -\sum_{ij\sigma\alpha\beta} t_{ij}^{\alpha\beta} \tilde{a}_{i\alpha\sigma}^{+} \tilde{a}_{j\beta\sigma} + \frac{1}{2}\sum_{ij\sigma\alpha\beta} J_{ij}^{\alpha\beta}\left(S_{i\alpha}S_{j\beta} - \frac{1}{4}n_{i\alpha}n_{j\beta}\right), \quad (1)$$

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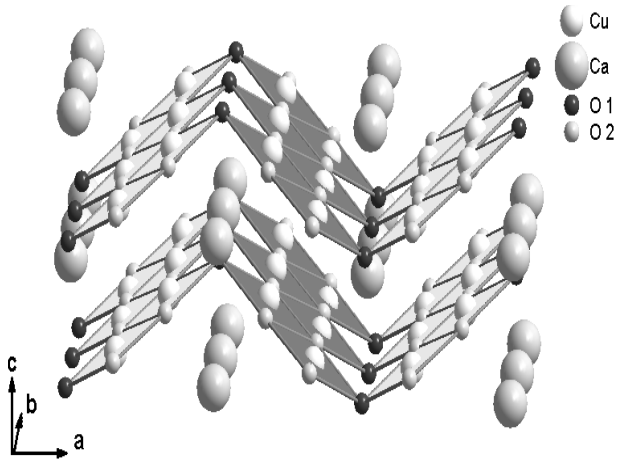

Fig. 1. The crystal structure of the undoped $CaCu_2O_3$ compound [6].

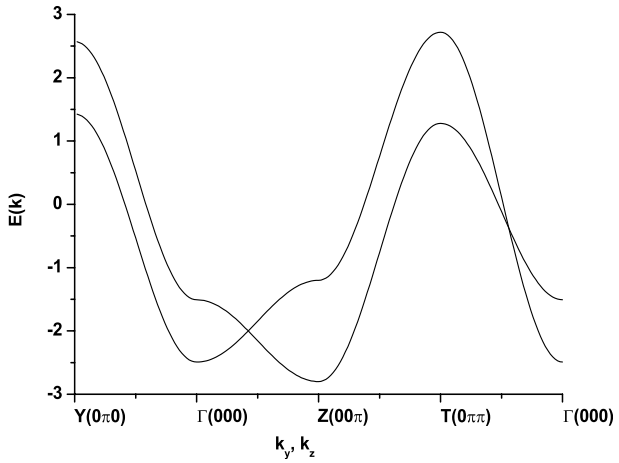

Fig. 2. The tight binding spectrum of the model, equations (2), (4) in units of $t = t_b = 430$ meV.

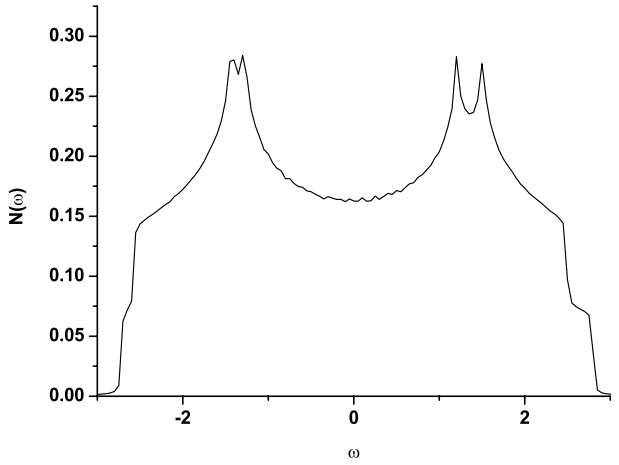

Fig. 3. The density of state for the spectrum shown in Figure 2.

where $\tilde{a}^+_{i\alpha\sigma} = a^+_{i\alpha\sigma}(1 - n_{i\alpha,-\sigma})$ are projected electron operators, $n_{i\alpha} = \sum_\sigma \tilde{a}^+_{i\alpha\sigma}\tilde{a}_{i\alpha\sigma}$ and $S^\gamma_{i\alpha} = (1/2)\sum_{s,s'} \tilde{a}^+_{i\alpha s}\sigma^\gamma_{s,s'}\tilde{a}_{i\alpha s'}$ – are the number and the spin operators for the lattice site $i\alpha = \mathbf{R}_i + \alpha a$, where the coordinates in the (b,c)-plane are defined as $\mathbf{R}_i = i_b b + i_c c$, while the parameter $\alpha(\beta) = 0, 1$ numbers two nearest neighbor planes along the "kinked" rung in the a-direction and $2a, b, c$ are the corresponding lattice parameters. The hopping integrals $t^{\alpha\beta}_{ij}$ and the exchange energy $J^{\alpha\beta}_{ij}$ can be written in the form

$$t^{\alpha\beta}_{ij} = \delta_{\alpha\beta}t_b\delta_{ji\pm b} + (1-\delta_{\alpha\beta})(t_a\delta_{ij} - t_c\delta_{ji\pm c} + t'\delta_{ji\pm b}), \quad (2)$$

$$J^{\alpha\beta}_{ij} = \delta_{\alpha\beta}(J_b\delta_{ji\pm b} + J_c\delta_{ji\pm c}) + (1-\delta_{\alpha\beta})J_a\delta_{ij}. \quad (3)$$

Here the nearest neighbor hopping and exchange parameters according to [6] can be estimated as (in meV):

$$t_b = 430,\ t_c = 140,\ t_a = 50,\ t' = 9,$$
$$J_b = 170,\ J_c = 20,\ J_a = 50. \quad (4)$$

The hopping parameter and the exchange interaction along the chains are close to those of the related ladder compound $SrCu_2O_3$ [8], while the interchain couplings are quite different. The electronic dispersions along the several symmetry directions are shown in Figure 2. The tight binding approximation, equation (2), describes the LDA spectrum reasonably well, except the small splittings along the $\Gamma \to Y$ and $\Gamma \to Z$ directions due to weak interladder interactions in (a,b) plane which we ignore for the sake of simplicity. The corresponding density of electronic state for the tight binding model is shown in Figure 3. To take into account rigorously the projected character of electron operators, we employ the Hubbard operator (HO) technique. The HO are defined as $X^{n,m}_{i\alpha} = |i\alpha, n\rangle\langle i\alpha, m|$ for three possible states at a lattice site $i\alpha$: $|i\alpha, n\rangle = |i\alpha, 0\rangle$, $|i\alpha, \sigma\rangle$ for an empty site and for a singly occupied site by an electron with spin $\sigma/2$ ($\sigma = \pm 1$, $\bar{\sigma} = -\sigma$). They obey the completeness relation

$$X^{00}_{i\alpha} + \sum_\sigma X^{\sigma\sigma}_{i\alpha} = 1, \quad (5)$$

which rigorously preserves the constraint of no double occupation at each lattice site by any quantum state $|i\alpha, n\rangle$. In terms of the HO the model (1) reads:

$$H_{t-J} = -\mu\sum_{i\sigma\alpha} X^{\sigma\sigma}_{i\alpha} - \sum_{ij\sigma\alpha\beta} t^{\alpha\beta}_{ij} X^{\sigma 0}_{i\alpha} X^{0\sigma}_{j\beta} + \frac{1}{4}\sum_{ij\sigma\alpha\beta} J^{\alpha\beta}_{ij}\left(X^{\sigma\bar{\sigma}}_{i\alpha}X^{\bar{\sigma}\sigma}_{j\beta} - X^{\sigma\sigma}_{i\alpha}X^{\bar{\sigma}\bar{\sigma}}_{j\beta}\right). \quad (6)$$

Here we have introduced the chemical potential μ which depends on the average number of electrons on one site:

$$n = \sum_\sigma \langle X^{\sigma\sigma}_{i\alpha}\rangle, \quad (7)$$

which does not depends on $\alpha = 0, 1$ since the two planes within a bilayer are equivalent. The model (6) describes

two anisotropic copper-oxygen planes which can be called as a "pseudo-ladder" compound due to quite a large coupling of the ladders along the c-axis [6]. Therefore, to estimate the superconducting transition temperature T_c in the model we can apply the theory of superexchange pairing developed in [9,10] for a copper-oxygen plane.

3 Green functions

To discuss the superconducting pairing within the model (6) we consider the matrix Green function (GF)

$$\hat{G}_{i\alpha,j\beta,\sigma}(t-t') = \left\langle\left\langle \Psi_{i\alpha\sigma}(t)|\Psi^{\dagger}_{j\beta\sigma}(t')\right\rangle\right\rangle, \qquad (8)$$

in terms of the Nambu operators:

$$\Psi_{i\alpha\sigma} = \begin{pmatrix} X^{0\sigma}_{i\alpha} \\ X^{\bar{\sigma}0}_{i\alpha} \end{pmatrix}, \qquad \Psi^{\dagger}_{j\beta\sigma} = \left(X^{\sigma 0}_{j\beta}\ X^{0\bar{\sigma}}_{j\beta}\right),$$

where Zubarev's notation for the anticommutator Green function (8) has been used [11]. To simplify the notation we omit further the subscripts α, β by taking $i\alpha \equiv i$, $j\beta \equiv j$.

By differentiating the GF (8) with respect to the time t we get for its ω-Fourier component the following equation

$$\omega\hat{G}_{ij\sigma}(\omega) = \delta_{ij}\hat{Q}_{\alpha\sigma} + \left\langle\left\langle \hat{Z}_{i\sigma} \mid \Psi^{\dagger}_{j\sigma}\right\rangle\right\rangle_{\omega}, \qquad (9)$$

where $\hat{Z}_{i\sigma} = [\Psi_{i\sigma}, H]$ and $\hat{Q}_{\alpha,\sigma} = \langle\{\Psi_{i\alpha\sigma}, \Psi^{\dagger}_{i\alpha\sigma}\}\rangle = \langle X^{00}_{i\alpha} + X^{\sigma\sigma}_{i\alpha}\rangle = Q\hat{\tau}_0$. We consider a paramagnetic state and therefore the correlation function in equation (9) $Q_{\alpha,\sigma} = \langle 1 - X^{\bar{\sigma}\bar{\sigma}}_{i\alpha}\rangle = 1 - n/2$ depends only on the average number of electrons n.

To close the system of equations for the single-electron GF (9) we apply the projection technique for the equation of motion for GF. We project the many–particle GF in (9) on the single-electron GF by introducing the irreducible (irr) part of $\hat{Z}_{i\sigma}$ operator which is orthogonal to the single-electron operator:

$$\left\langle\left\langle \hat{Z}_{i\sigma} \mid \Psi^{\dagger}_{j\sigma}\right\rangle\right\rangle = \sum_{l}\hat{E}_{il\sigma}\left\langle\left\langle \Psi_{l\sigma} \mid \Psi^{\dagger}_{j\sigma}\right\rangle\right\rangle + \left\langle\left\langle \hat{Z}^{(irr)}_{i\sigma} \mid \Psi^{\dagger}_{j\sigma}\right\rangle\right\rangle,$$

$$\left\langle\left\{\hat{Z}^{(irr)}_{i\sigma}, \Psi^{\dagger}_{j\sigma}\right\}\right\rangle = \left\langle \hat{Z}^{(irr)}_{i\sigma}\Psi^{\dagger}_{j\sigma} + \Psi^{\dagger}_{j\sigma}\hat{Z}^{(irr)}_{i\sigma}\right\rangle = 0. \qquad (10)$$

From this equation the definition of the energy matrix follows as

$$\hat{E}_{ij\sigma} = \left\langle\left\{[\Psi_{i\sigma}, H], \Psi^{\dagger}_{j\sigma}\right\}\right\rangle\ Q^{-1}. \qquad (11)$$

The frequency matrix (11) defines the zero-order GF in the generalized MFA:

$$\hat{G}^{0}_{ij\sigma}(\omega) = Q\left\{\omega\hat{\tau}_0\delta_{ij} - \hat{E}_{ij\sigma}\right\}^{-1}, \qquad (12)$$

where $\hat{\tau}_0$ is the Pauli matrix.

In the present study we neglect self-energy corrections which stem from the essentially many-particle GF $\langle\langle \hat{Z}^{(irr)}_{i\sigma} \mid \Psi^{\dagger}_{j\sigma}\rangle\rangle$ in equation (10) defined by the irreducible part of the operator $Z^{(irr)}_{i\sigma}$. As was shown in [9] these corrections, though giving quite a substantial contribution to the electronic spectrum and superconducting pairing, do not change qualitatively the results for the superconducting transition temperature T_c. Therefore, for a comparative study of superconductivity in compounds with nearly tetragonal, "symmetric", 2D copper-oxide planes and the highly anisotropic "pseudo-ladder" compound under consideration, we can apply the MFA given by the zero-order GF (12).

To calculate the energy matrix (11) we should consider the equation of motion for the HO:

$$\left(i\frac{d}{dt} + \mu\right)X^{0\sigma}_{i} = -\sum_{l} t_{il}B_{i\sigma\sigma'}X^{0\sigma'}_{l} + \frac{1}{2}\sum_{l} J_{il}(B_{l\sigma\sigma'} - \delta_{\sigma\sigma'})X^{0\sigma'}_{i}, \qquad (13)$$

where we introduced the operator

$$B_{i\sigma\sigma'} = (X^{00}_{i} + X^{\sigma\sigma}_{i})\delta_{\sigma'\sigma} + X^{\bar{\sigma}\sigma}_{i}\delta_{\sigma'\bar{\sigma}} = \left(1 - \frac{1}{2}n_i + \sigma S^{z}_{i}\right)\delta_{\sigma'\sigma} + S^{\bar{\sigma}}_{i}\delta_{\sigma'\bar{\sigma}}. \qquad (14)$$

The Bose-like operator (14) describes electron scattering on spin and charge fluctuations caused by the nonfermionic commutation relations for the HO (the first term in (13) – the kinematic interaction) and by the exchange spin-spin interaction (the second term in (13)).

By using equation of motion (13) and performing the corresponding commutations for the Hubbard operators in the energy matrix (11) we can write the normal, $E^{11}_{i\alpha,j\beta,\sigma} = -E^{22}_{j\beta,i\alpha,\bar{\sigma}}$, and anomalous, $E^{12}_{i\alpha,j\beta,\sigma} = (E^{21}_{j\beta,i\alpha,\sigma})^{+}$, matrix components in the form:

$$E^{11}_{i\alpha,j\beta,\sigma} = -t^{\alpha\beta}_{ij}\frac{1}{Q}\chi^{\alpha\beta}_{ij} - \frac{1}{2Q}J^{\alpha\beta}_{ij}\left\langle X^{\bar{\sigma}0}_{j\beta}X^{0\bar{\sigma}}_{i\alpha}\right\rangle + \delta_{ij}\delta_{\alpha\beta}(-\mu + \delta\mu), \qquad (15)$$

$$\delta\mu = \frac{1}{Q}\sum_{l\gamma}\left(t^{\alpha\gamma}_{il}\left\langle X^{\bar{\sigma}0}_{i\alpha}X^{0\bar{\sigma}}_{l\gamma}\right\rangle + \frac{1}{2}J^{\alpha\gamma}_{il}(\chi^{\alpha\gamma}_{il} - 1)\right),$$

$$E^{12}_{i\alpha,j\beta,\sigma} = J^{\alpha\beta}_{ij}\frac{1}{Q}\left\langle X^{0\sigma}_{i\alpha}X^{0\bar{\sigma}}_{j\beta}\right\rangle, - \delta_{ij}\delta_{\alpha\beta}\frac{2}{Q}\sum_{l\gamma} t^{\alpha\gamma}_{il}\left\langle X^{0\sigma}_{i\alpha}X^{0\bar{\sigma}}_{l\gamma}\right\rangle, \qquad (16)$$

where we introduced the spin-charge correlation function

$$\chi^{\alpha\beta}_{ij} = \left\langle\left(1 - \frac{n_{i\alpha}}{2}\right)\left(1 - \frac{n_{j\beta}}{2}\right)\right\rangle + \langle\mathbf{S}_{i\alpha}\mathbf{S}_{j\beta}\rangle \simeq Q^2 + \langle\mathbf{S}_{i\alpha}\mathbf{S}_{j\beta}\rangle = Q^2 + \chi^{s}_{i\alpha,j\beta}. \qquad (17)$$

In the last approximate expression we neglect the charge-charge fluctuations $\langle\delta n_{i\alpha}\delta n_{j\beta}\rangle$, $\delta n_{i\alpha} = n_{i\alpha} - \langle n_{i\alpha}\rangle$. We stress, however, that the short-range spin-spin antiferromagnetic correlation, $\chi^{s}_{i\alpha,j\beta} = \langle\mathbf{S}_{i\alpha}\mathbf{S}_{j\beta}\rangle$, gives a substantial contribution to the narrowing of the quasiparticle

bandwidth in the low doping region and cannot be disregarded (see [9]).

By introducing the $\mathbf{q}$-representation in (b,c)-plane for the GF (12) and the energy matrix (11) as follows

$$\hat{G}^0_{i\alpha,j\beta,\sigma}(\omega) = \frac{1}{N}\sum_{\mathbf{q}} \mathrm{e}^{i\mathbf{q}(\mathbf{R_i}-\mathbf{R_j})}\, \hat{G}^0_{\alpha\beta,\sigma}(\mathbf{q},\omega), \quad (18)$$

where N is the number of lattice sites in one (b,c)-plane, we can write the GF (12) in the form

$$\hat{G}^0_{\alpha\beta,\sigma}(\mathbf{q},\omega) = Q\left\{\omega\hat{\tau}_0\delta_{\alpha\beta} - \hat{E}_{\alpha\beta,\sigma}(\mathbf{q})\right\}^{-1} = \begin{pmatrix} G_{\alpha\beta}(\mathbf{q},\omega) & F_{\alpha\beta,\sigma}(\mathbf{q},\omega) \\ F^{\dagger}_{\beta\alpha,\sigma}(\mathbf{q},\omega) & -G_{\beta\alpha}(\mathbf{q},-\omega)\end{pmatrix}, \quad (19)$$

where the energy matrix is given by the equation:

$$\hat{E}_{\alpha\beta,\sigma}(\mathbf{q}) = \begin{pmatrix} \varepsilon_{\alpha\beta}(\mathbf{q}) & \Delta_{\alpha\beta,\sigma}(\mathbf{q}) \\ \Delta^{*}_{\beta\alpha,\sigma}(\mathbf{q}) & -\varepsilon_{\beta\alpha}(\mathbf{q})\end{pmatrix}. \quad (20)$$

The normal state energy matrix $\varepsilon_{\alpha\beta}(\mathbf{q})$ which does not depend on spin σ and the gap matrix which is an odd function of the spin σ: $\Delta_{\alpha\beta,\sigma}(\mathbf{q}) = -\Delta_{\alpha\beta,\bar{\sigma}}(\mathbf{q})$, can be written in the form:

$$\begin{aligned}\varepsilon_{\alpha\beta}(\mathbf{q}) &= \delta_{\alpha\beta}\,\varepsilon(\mathbf{q}) - (1-\delta_{\alpha\beta})\,\tilde{t}_{\perp}(\mathbf{q}) \\ &= -\delta_{\alpha\beta}\,2\tilde{t}_b\cos q_y + (1-\delta_{\alpha\beta})(\tilde{t}_a - 2\tilde{t}_c\cos q_z \\ &\quad + 2\tilde{t}'\cos q_y) - \mu - \delta\mu. \end{aligned} \quad (21)$$

$$\Delta_{\alpha\beta,\sigma}(\mathbf{q}) = \delta_{\alpha\beta}\,\Delta_{\sigma}(\mathbf{q}) + (1-\delta_{\alpha\beta})\,\Delta_{\sigma,\perp}\,, \quad (22)$$

where for calculation of the quasiparticle energy for one plane $\varepsilon(\mathbf{q})$ and the interplane coupling $\tilde{t}_{\perp}(\mathbf{q})$ we have used equation (15) and introduced the renormalized hopping parameters $\tilde{t}_{\alpha}$. For the gap functions we get from equation (16) the following equations for the in-plane gap $(\alpha=\beta)$ and the rung gap $(\alpha\neq\beta)$:

$$\begin{aligned}\Delta_{\sigma}(\mathbf{q}) &= \frac{1}{NQ}\sum_{\mathbf{k}} J(\mathbf{q}-\mathbf{k})\left\langle X^{0\sigma}_{\mathbf{k}\alpha}X^{0\bar{\sigma}}_{-\mathbf{k}\alpha}\right\rangle, \\ &\quad - \frac{2}{NQ}\sum_{\mathbf{k}\gamma} t^{\alpha\gamma}(\mathbf{k})\,\left\langle X^{0\sigma}_{\mathbf{k}\alpha}X^{0\bar{\sigma}}_{-\mathbf{k}\gamma}\right\rangle, \end{aligned} \quad (23)$$

$$\Delta_{\sigma,\perp} = J_a\frac{1}{NQ}\sum_{\mathbf{k}}\left\langle X^{0\sigma}_{\mathbf{k}\alpha}X^{0\bar{\sigma}}_{-\mathbf{k}\bar{\alpha}}\right\rangle. \quad (24)$$

To calculate the normal, $G_{\alpha\beta}(\mathbf{q},\omega)$, and the anomalous, $F_{\alpha\beta,\sigma}(\mathbf{q},\omega)$ components of the GF in equation (19) we consider the (2×2) matrix equations:

$$\begin{aligned}&\{\omega\delta_{\alpha\beta} - \varepsilon_{\alpha\beta}(\mathbf{q})\}G_{\beta\alpha}(\mathbf{q},\omega) - \Delta_{\alpha\beta,\sigma}(\mathbf{q})F^{\dagger}_{\beta\alpha,\sigma}(\mathbf{q},\omega) = Q, \\ &\Delta^{*}_{\beta\alpha,\sigma}(\mathbf{q})G_{\beta\alpha}(\mathbf{q},\omega) - \{\omega\delta_{\alpha\beta} + \varepsilon_{\alpha\beta}(\mathbf{q})\}F^{\dagger}_{\beta\alpha,\sigma}(\mathbf{q},\omega) = 0.\end{aligned}$$

After some algebra we get the following solution for the GF:

$$G_{\alpha\beta}(\mathbf{q},\omega) = Q\frac{A_{\alpha\beta}(\mathbf{q},\omega)}{[\omega^2 - E^2_1(\mathbf{q})][\omega^2 - E^2_2(\mathbf{q})]}, \quad (25)$$

$$F^{\dagger}_{\alpha\beta,\sigma}(\mathbf{q},\omega) = Q\frac{B_{\alpha\beta}(\mathbf{q},\omega)}{[\omega^2 - E^2_1(\mathbf{q})][\omega^2 - E^2_2(\mathbf{q})]}, \quad (26)$$

where the quasiparticle energy for the two bands in the superconducting state are

$$\begin{aligned}&E^2_{1(2)}(\mathbf{q}) = \varepsilon^2_{1(2)}(\mathbf{q}) + \Delta^2_{1(2)\sigma}(\mathbf{q}), \\ &\varepsilon_{1(2)}(\mathbf{q}) = \varepsilon(\mathbf{q}) \pm \tilde{t}_{\perp}(\mathbf{q}), \quad \Delta_{1(2)\sigma}(\mathbf{q}) = \Delta_{\sigma}(\mathbf{q}) \mp \Delta_{\sigma,\perp}.\end{aligned} \quad (27)$$

The coefficient in the numerator of equations (25, 26) for the diagonal GF reads

$$\begin{aligned}A_{\alpha\alpha}(\mathbf{q},\omega) &= (\omega-\varepsilon(\mathbf{q}))\left[(\omega+\varepsilon(\mathbf{q}))^2 - \tilde{t}^2_{\perp}(\mathbf{q})\right] \\ &\quad - \left[(\omega+\varepsilon(\mathbf{q}))(\Delta^2_{\sigma}(\mathbf{q}) + \Delta^2_{\sigma,\perp}) + 2\tilde{t}_{\perp}(\mathbf{q})\Delta_{\sigma,\perp}\Delta_{\sigma}(\mathbf{q})\right],\end{aligned}$$

and for the nondiagonal GF equals to

$$\begin{aligned}A_{\alpha\bar{\alpha}}(\mathbf{q},\omega) &= -\tilde{t}_{\perp}(\mathbf{q})\left[(\omega+\varepsilon(\mathbf{q}))^2 - \tilde{t}^2_{\perp}(\mathbf{q})\right] \\ &\quad + \left[(\omega+\varepsilon(\mathbf{q}))2\Delta_{\sigma,\perp}\Delta_{\sigma}(\mathbf{q}) + \tilde{t}_{\perp}(\mathbf{q})(\Delta^2_{\sigma}(\mathbf{q}) + \Delta^2_{\sigma,\perp}))\right].\end{aligned}$$

The coefficient in the numerator of equation (26) for the anomalous diagonal GF reads

$$\begin{aligned}B_{\alpha\alpha}(\mathbf{q},\omega) &= -2\Delta_{\sigma,\perp}\,\tilde{t}_{\perp}(\mathbf{q})\,\varepsilon(\mathbf{q}) \\ &\quad + \left[\omega^2 - (\varepsilon(\mathbf{q})^2 + \tilde{t}^2_{\perp}(\mathbf{q}) + \Delta_{\sigma}(\mathbf{q})^2 - \Delta^2_{\sigma,\perp})\right]\Delta_{\sigma}(\mathbf{q}),\end{aligned}$$

and for the anomalous nondiagonal GF equals to

$$\begin{aligned}B_{\alpha\bar{\alpha}}(\mathbf{q},\omega) &= -2\Delta_{\sigma}(\mathbf{q})\,\tilde{t}_{\perp}(\mathbf{q})\,\varepsilon(\mathbf{q}) \\ &\quad + \left[\omega^2 - (\varepsilon(\mathbf{q})^2 + \tilde{t}^2_{\perp}(\mathbf{q}) + \Delta_{\sigma}(\mathbf{q})^2 - \Delta^2_{\sigma,\perp})\right]\Delta_{\sigma,\perp}.\end{aligned}$$

As we see from the equations for the GF and the quasiparticle spectra, equation (27), the coupling between the planes due to the effective interaction $\tilde{t}_{\perp}(\mathbf{q})$ in equation (21) results in the splitting of the two bands in the bilayer: $\varepsilon_{1(2)}(\mathbf{q}) = \varepsilon(\mathbf{q}) \pm \tilde{t}_{\perp}(\mathbf{q})$, while the exchange coupling between the planes, J_a, results in the gap splitting: $\Delta_{1(2)\sigma}(\mathbf{q}) = \Delta_{\sigma}(\mathbf{q}) \mp \Delta_{\sigma,\perp}$. Therefore, to study superconductivity in the model we should consider a system of equations for the two gaps, $\Delta_{1(2)\sigma}(\mathbf{q})$.

4 Gap equation

To obtain a self-consistent system of equations for the superconducting gaps, equations (23, 24), we have to calculate the anomalous correlation function:

$$\langle X^{\sigma 0}_{\beta\mathbf{k}}X^{\bar{\sigma}0}_{-\mathbf{k}\alpha}\rangle = \int_{-\infty}^{+\infty}\frac{\mathrm{d}\omega}{\mathrm{e}^{\,\omega/T}+1}\left[-\frac{1}{\pi}\mathrm{Im}F^{\dagger}_{\alpha\beta,\sigma}(\mathbf{k},\omega+i\delta)\right].$$

By using GF (26) and taking into account the symmetry relation for the anomalous correlation functions:

$$\left\langle X^{\sigma 0}_{\beta\mathbf{k}}X^{\bar{\sigma}0}_{-\mathbf{k}\alpha}\right\rangle = -\left\langle X^{\bar{\sigma}0}_{-\mathbf{k}\alpha}X^{\sigma 0}_{\beta\mathbf{k}}\right\rangle = -\left\langle X^{0\sigma}_{\beta\mathbf{k}}X^{0\bar{\sigma}}_{-\mathbf{k}\alpha}\right\rangle,$$

we obtain the following equation for the in-plane gap (23)

$$\Delta_{\sigma}(\mathbf{q}) = \frac{1}{N}\sum_{n,\mathbf{k}} J(\mathbf{q}-\mathbf{k})\frac{\Delta_{n,\sigma}(\mathbf{k})}{4E_n(\mathbf{k})}\,\tanh\frac{E_n(\mathbf{k})}{2T}, \quad (28)$$

where the sum over $n = 1, 2$ runs over two bands with the quasiparticle energy (27), and an analogous equation for the rung gap, equation (24). In equation (28) we disregarded the contribution from the kinematic interaction, the second term in equation (23), since it gives a **q**-independent contribution to the in-plane gap. This results in a significant double occupancy of one lattice site which is energetically unfavorable for a strongly correlated system such as considered here.

From equations (24), (28) we obtain the following equation for the gaps in two bands, $n = 1, 2$:

$$\Delta_{n,\sigma}(\mathbf{q}) = \frac{1}{N}\sum_{m,\mathbf{k}} J_{n,m}(\mathbf{q}-\mathbf{k})\frac{\Delta_{m,\sigma}(\mathbf{k})}{4E_m(\mathbf{k})}\tanh\frac{E_m(\mathbf{k})}{2T}, \tag{29}$$

where the exchange interaction

$$J_{nn}(\mathbf{q}) = J(\mathbf{q}) + J_a, \quad J_{n\neq m}(\mathbf{q}) = J(\mathbf{q}) - J_a,$$
$$J(\mathbf{q}) = 2J_b\cos q_y b + 2J_c\cos q_z c. \tag{30}$$

In deriving equation (29) we neglected small contributions of the order of $(\Delta_\sigma(\mathbf{q})\Delta_{\sigma,\perp}/\varepsilon(\mathbf{q})\tilde{t}_\perp(\mathbf{q}))$ which appear in the equation for the rung gap, $\Delta_{\sigma,\perp}$.

5 Results and discussions

To calculate T_c we should consider a linear system of equations (29) for the gaps by neglecting the gap contribution in the quasipartical energy: $E_n(\mathbf{q}) = \varepsilon_n(\mathbf{q})$. The highest eigenvalue of this linear equation determines the superconducting temperature T_c, while the eigenfunction should give the symmetry of the order parameter of the superconducting state. However, a straightforward solution of the problem is difficult to obtain. Instead we employ a variational ansatz for the gap function suggested by the **q**-dependence of the pairing interaction (30). This is a conventional approach in the theory of superconductivity. Thus, we consider the following two band gap model $(n = 1, 2)$:

$$\Delta_{n,\sigma}(\mathbf{k}) = \Delta_y\cos k_y + \Delta_z\cos k_z + \Delta_x(-1)^n, \tag{31}$$

where we used the dimensionless wave vectors: $(-\pi \leq k_y, k_z \leq \pi)$. By using this model in the linearized gap equation (29) we obtain the following system of equations for the parameters Δ_ξ $(\xi = y, z, x)$:

$$\Delta_\xi = \sum_\nu F_{\xi\nu}(T)\,\Delta_\nu. \tag{32}$$

The function $F_{\xi\nu}(T)$ is given by the equation

$$F_{\xi\nu}(T) = \frac{1}{N}\sum_{m,\mathbf{q}} f_{\xi\nu}(m,\mathbf{q})\frac{1}{2\varepsilon_m(\mathbf{q})}\tanh\frac{\varepsilon_m(\mathbf{q}))}{2T}, \tag{33}$$

where the matrix $f_{\xi\nu}$ reads

$$f_{\xi\nu}(n,\mathbf{q}) = \begin{pmatrix} J_b\cos^2 q_y & J_b\cos q_y\cos q_z & J_b\cos q_y(-1)^n \\ J_c\cos q_y\cos q_z & J_c\cos^2 q_z & J_c\cos q_z(-1)^n \\ \frac{1}{2}J_a(-1)^n\cos q_y & \frac{1}{2}J_a(-1)^n\cos q_z & \frac{1}{2}J_a \end{pmatrix}.$$

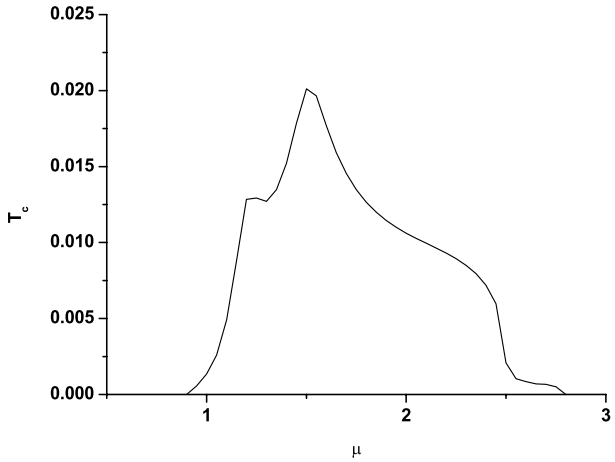

Fig. 4. $T_c(\mu)$ for the model of hole doped $CaCu_2O_3$, equations (1–4). T_c and μ are given in units of $\tilde{t} \simeq 2500$ K.

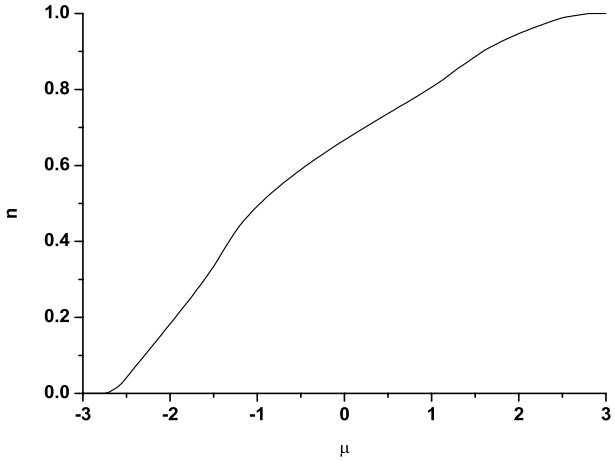

Fig. 5. Band filling vs. chemical potential, $n(\mu)$.

The nonzero solution of the linear system of equations (32) exists when the determinant of the matrix $||F_{\xi\nu}(T_c) - \delta_{\xi,\nu}||$ equals to zero. The results of a numerical solution of this equation for T_c as a function of the chemical potential μ are shown in Figure 4 for the following parameters of the model: $\tilde{t_b} = \tilde{t}$, $\tilde{t_c} = 0.323\tilde{t}$, $\tilde{t_a} = 0.114\tilde{t}$, $\tilde{t'} = 0.02\tilde{t}$, $J_b = 0.8\tilde{t}$, $J_c = 0.11\tilde{t}$, $J_a = 0.22\tilde{t}$. T_c and μ are measured in units of $\tilde{t} = t_b/2 \simeq 2500$ K. This renormalization by a factor of two of the LDA hopping parameters takes into account the band narrowing due to strong correlation as follows from equation (15). It depends on the doping (in the simple Hubbard-I approximation as $1 - n/2$) which has been ignored for the small doping range considered here (close to half-filling, $n = 1$).

The maximum for $T_c \simeq 0.02\tilde{t} \simeq 50$ K occurs at $\mu \simeq 1.5$ that corresponds to the doping $\delta = 1-n \simeq 0.12$ as follows from the $n(\mu)$ dependence shown in Figure 5. We consider this estimate of T_c as an optimistic upper bound of the superconducting temperature which should be suppressed by ferromagnetic interladder interaction (in (a, b)-plane) as well as fluctuation effects beyond the mean field approximation used here. The ratio of the gap components

are: $\Delta_a/\Delta_b = -0.1$ and $\Delta_c/\Delta_b = -0.1$ which shows a weak coupling in the rung and along the c-axis. At small doping the gap exhibits no nodes in both bands as a consequence of strong anisotropy of the dispersion and of the exchange interaction. In this context an observation of the Hebel–Slichter peak in the NMR experiments [4]) in the related highly anisotropic ladder compound $Sr_{14-x}Ca_xCu_{24}O_{41}$ is in accord with our finding. A more comprehensive theoretical analysis of superconductivity within our approach for ladder compounds will be given elsewhere.

To summarize, in the present paper we considered a theory for superconducting pairing due to the exchange interaction in the doped "pseudo-ladder" compound $CaCu_2O_3$. The calculations show that in spite of the large coupling along the chain direction ($J_b \simeq 170$ meV) the anisotropy of electron spectra suppresses T_c which explains experimental findings that the highest superconducting T_c values are observed in cuprates with an ideal square lattice as in the mercury compounds (see, e.g., [12]). The maximum of T_c is obtained at the highest density of state close to the Van Hove singularity which is achieved at relatively small hole doping. This might be realized if one could partially substitute the divalent Ca^{2+} ions for monovalent alkaline ions, say e.g. Na^+, in our title compound.

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