Journal of Low Temperature Physics (2019) 196:242–252
https://doi.org/10.1007/s10909-018-02120-3

Influence of the Coulomb Repulsions on the Formation of the Superconducting Gap of the Spin-Polaron Quasiparticles in Cuprates

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Received: 1 July 2018 / Accepted: 9 December 2018 / Published online: 17 December 2018

Abstract
Taking into account the real crystalline structure of the CuO_2 plane and the strong spin-fermion coupling, the influence of the on-site Coulomb repulsion of holes U_p and the intersite Coulomb repulsion V_2 between holes located at the next-nearest-neighbor oxygen ions on the formation of the superconducting gap with the d-wave symmetry of the order parameter of the spin-polaron quasiparticles is studied. It is shown that the formation of the resulting superconducting gap within the spin-fermion model is caused by three components. The dependence of the narrowing of the superconducting gap on the values U_p and V_2 is analyzed.

Keywords Cuprate superconductors · Unconventional superconductivity · Spin-charge correlations · Spin polarons · Intersite Coulomb interaction

1 Introduction

At the present time, the problem of influence of the interplay between the spin and charge degrees of freedom on the normal and superconducting properties of cuprate superconductors attracts a significant attention of researchers [1–4]. The strong spin-fermion coupling in these systems not only plays an important role, but determines a number of their low-temperature properties.

Recently, within the spin-fermion model (SFM), it was shown [5,6] that taking into account both the features of the real crystalline structure of the CuO_2 plane and the strong spin-fermion coupling resulting in an occurrence of the spin-polaron quasiparticles [7–9] allows one to solve the problem of stability of the superconducting

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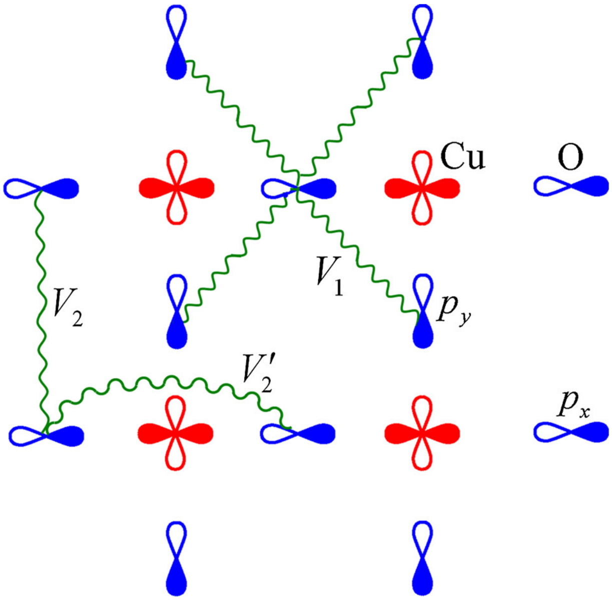

Fig. 1 The intersite Coulomb interactions on the CuO_2 plane (Color figure online)

d-wave pairing toward the intersite Coulomb repulsion in cuprates. It was demonstrated analytically [5] that the intersite Coulomb interaction V_1 of fermions located at the nearest oxygen ions of CuO_2 plane (Fig. 1) does not affect the superconducting d-wave pairing, because its Fourier transform $V_q = 4V_1 \cos(q_x/2)\cos(q_y/2)$ does not appear in the kernel of the corresponding integral equation. Taking into account both the intersite repulsion V_2 of fermions located at the next-nearest-neighbor oxygen ions (Fig. 1) and the Hubbard repulsion U_p leads to the decrease in the superconducting transition temperature; however, this temperature remains within the limits that are observed experimentally [6]. The subject of the present paper is to study the influence of the Coulomb interactions on the formation of the superconducting gap with the d-wave symmetry of the order parameter.

2 The Spin-Fermion Model

In the regime of strong electronic correlations, when the on-site Coulomb repulsion energy U_d of holes at one copper ion is large ($\Delta_{pd} = \varepsilon_p - \varepsilon_d$ is the charge transfer gap)

$$\Delta_{pd}, (U_d - \Delta_{pd}) \gg t_{pd} > 0, \tag{1}$$

the Emery model [10,11], which is one of the most realistic model for the CuO_2 plane, can be reduced to the SFM [12–17] with the Hamiltonian

$$
\begin{aligned}
\hat{H}_{sp-f} &= \hat{H}_h + \hat{U}_p + \hat{V}_{pp} + \hat{J} + \hat{I},\\
\hat{H}_h &= \sum_{k\alpha}\Big(\xi_{k_x} a^{\dagger}_{k\alpha} a_{k\alpha} + \xi_{k_y} b^{\dagger}_{k\alpha} b_{k\alpha} + t_k \left(a^{\dagger}_{k\alpha} b_{k\alpha} + b^{\dagger}_{k\alpha} a_{k\alpha}\right)\Big),\\
\hat{U}_p &= \frac{U_p}{N} \sum_{1,2,3,4} \left[a^{\dagger}_{1\uparrow} a^{\dagger}_{2\downarrow} a_{3\downarrow} a_{4\uparrow} + (a \to b)\right] \delta_{1+2-3-4},\\
\hat{V}_{pp} &= \frac{4V_1}{N} \sum_{\substack{1,2,3,4\\ \alpha\beta}} \phi_{3-2}\, a^{\dagger}_{1\alpha} b^{\dagger}_{2\beta} b_{3\beta} a_{4\alpha}\, \delta_{1+2-3-4}\\
&\quad + \frac{V_2}{N} \sum_{\substack{1,2,3,4\\ \alpha\beta}} \left[\theta^{xy}_{2-3}\, a^{\dagger}_{1\alpha} a^{\dagger}_{2\beta} a_{3\beta} a_{4\alpha} + \theta^{yx}_{2-3} (a \to b)\right] \delta_{1+2-3-4},\\
\hat{J} &= \frac{J}{N} \sum_{fkq\alpha\beta} e^{if(q-k)} u^{\dagger}_{k\alpha} (\mathbf{S}_f \boldsymbol{\sigma}_{\alpha\beta}) u_{q\beta}, \quad \hat{I} = \frac{I}{2} \sum_{f\delta} \mathbf{S}_f \mathbf{S}_{f+2\delta},
\end{aligned}
\tag{2}
$$

which describes the subsystem of oxygen holes interacting with the spins localized at copper ions. Here,

$$
\begin{aligned}
&\xi_{k_{x(y)}} = \varepsilon_p + 2V_{pd} + \tau(1 - \cos k_{x(y)}) - \mu, \quad t_k = (2\tau - 4t) s_{k,x} s_{k,y},\\
&s_{k,x} = \sin\frac{k_x}{2}, \quad \theta^{xy(yx)}_k = \frac{V_2'}{V_2} e^{ik_{x(y)}} + e^{-ik_{y(x)}}, \quad u_{k\beta} = s_{k,x} a_{k\beta} + s_{k,y} b_{k\beta},\\
&\tau = \frac{t^2_{pd}}{\Delta_{pd}}\left(1 - \frac{\Delta_{pd}}{U_d - \Delta_{pd} - 2V_{pd}}\right), \quad J = \frac{4t^2_{pd}}{\Delta_{pd}}\left(1 + \frac{\Delta_{pd}}{U_d - \Delta_{pd} - 2V_{pd}}\right).
\end{aligned}
\tag{3}
$$

In the Hamiltonian, $a^{\dagger}_{k\alpha}(a_{k\alpha})$ and $b^{\dagger}_{k\alpha}(b_{k\alpha})$ are the hole creation (annihilation) operators in the oxygen subsystem with the p_x- and p_y-orbitals (Fig. 1) in the momentum representation, $\alpha = \pm 1/2$ is the spin projection. The bare on-site energy of oxygen holes is ε_p, μ is the chemical potential, and t is the hopping integral of the oxygen holes. The intersite Coulomb interaction between holes (Fig. 1) is described by the operator V_{pp}. The operator $\hat{J}$ corresponds to the exchange interaction between the oxygen holes and the localized copper spins, where $\mathbf{S}_f$ is the operator of a spin at the site f and $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ is the vector of the Pauli matrices. The operator $\hat{I}$ describes the superexchange interaction between the neighboring copper spins arising in the fourth order in t_{pd} of the perturbation theory. For the sake of compactness, we denote momenta over which the summation is performed by numbers 1,...,4. The Dirac delta function $\delta_{1+2-3-4}$ takes into account the momentum conservation law.

Below, we use the commonly accepted set of parameters for the Emery model: $t_{pd} = 1.3$ eV, $\Delta_{pd} = 3.6$ eV, $U_d = 10.5$ eV, $V_{pd} = 1.2$ eV [18,19]. For the holes hopping integral, we use the value $t = 0.12$ eV [20] and suppose that the superexchange parameter $I = 0.136$ eV (1570 K) in accordance with experimental data on cuprate superconductors [19]. In the calculations, we put $V_2 = V_2'$ for simplicity.

3 Basis Set and Equations for Green's Functions

In order to describe the dynamics of oxygen holes, it is necessary to take into consideration the large exchange interaction ($J = 3.38\,\mathrm{eV} \gg \tau \approx 0.1$ eV) rigorously. This problem can be solved in the framework of the Zwanzig-Mori projection technique [21,22] using basis set of operators [20,23,24]

$$\left\{a_{k\uparrow}, b_{k\uparrow}, L_{k\uparrow}, a^{\dagger}_{-k\downarrow}, b^{\dagger}_{-k\downarrow}, L^{\dagger}_{-k\downarrow}\right\}, \tag{4}$$

where the operator $L_{k\alpha} = \frac{1}{N}\sum_{fq\beta} e^{if(q-k)}(\mathbf{S}_f \boldsymbol{\sigma}_{\alpha\beta})u_{q\beta}$ describes the strong spin-charge coupling. The system of equations for the normal G_{ij} and anomalous F_{ij} Green's functions can be represented in the form ($j = 1, 2, 3$)

$$\begin{aligned}
(\omega - \xi_{k_x})G_{1j} &= \delta_{1j} + t_k G_{2j} + J_x G_{3j} + \Delta_{1k}F_{1j} + \Delta_{2k}F_{2j},\\
(\omega - \xi_{k_y})G_{2j} &= \delta_{2j} + t_k G_{1j} + J_y G_{3j} + \Delta_{3k}F_{1j} + \Delta_{4k}F_{1j},\\
(\omega - \xi_L)G_{3j} &= \delta_{3j}K_k + (J_x G_{1j} + J_y G_{2j})K_k + \frac{\Delta_{5k}}{K_k}F_{3j},\\
(\omega + \xi_{k_x})F_{1j} &= \Delta^*_{1k}G_{1j} + \Delta^*_{3k}G_{2j} - t_k F_{2j} + J_x F_{3j},\\
(\omega + \xi_{k_y})F_{2j} &= \Delta^*_{2k}G_{1j} + \Delta^*_{4k}G_{2j} - t_k F_{1j} + J_y F_{3j},\\
(\omega + \xi_L)F_{3j} &= \frac{\Delta^*_{5k}}{K_k}G_{3j} + (J_x F_{1j} + J_y F_{2j})K_k.
\end{aligned} \tag{5}$$

Here, $G_{11} = \langle\langle a_{k\uparrow}|a^{\dagger}_{k\uparrow}\rangle\rangle$, $G_{21} = \langle\langle b_{k\uparrow}|a^{\dagger}_{k\uparrow}\rangle\rangle$, and $G_{31} = \langle\langle L_{k\uparrow}|a^{\dagger}_{k\uparrow}\rangle\rangle$. The functions G_{i2} and G_{i3} are determined in a similar way with the only difference that $a^{\dagger}_{k\uparrow}$ is replaced by $b^{\dagger}_{k\uparrow}$ and $L^{\dagger}_{k\uparrow}$, respectively. The anomalous Green's functions are defined as $F_{11} = \langle\langle a^{\dagger}_{-k\downarrow}|a^{\dagger}_{k\uparrow}\rangle\rangle$, $F_{21} = \langle\langle b^{\dagger}_{-k\downarrow}|a^{\dagger}_{k\uparrow}\rangle\rangle$, $F_{31} = \langle\langle L^{\dagger}_{-k\downarrow}|a^{\dagger}_{k\uparrow}\rangle\rangle$. For F_{i2} and F_{i3}, the same type of notation regarding the second index is used. The functions involved in the system (5) are given by the expressions

$$\begin{aligned}
J_{x(y)} &= Js_{k,x(y)}, \quad K_k = \langle\{L_{k\uparrow}, L^{\dagger}_{k\uparrow}\}\rangle = 3/4 - C_1\gamma_{1k},\\
\xi_L &= \varepsilon_p - \mu - 2t + 5\tau/2 - J + [(2t-\tau)(C_1\gamma_{1k} - C_2\gamma_{2k}) - (\tau/2)(C_1\gamma_{1k} - C_3\gamma_{3k})\\
&\quad + JC_1(1 + 4\gamma_{1k})/4 - IC_1(\gamma_{1k} + 4)]K_k^{-1},
\end{aligned} \tag{6}$$

where γ_{jk} are the square lattice invariants: $\gamma_{1k} = (\cos k_x + \cos k_y)/2$, $\gamma_{2k} = \cos k_x \cos k_y$, $\gamma_{3k} = (\cos 2k_x + \cos 2k_y)/2$.

The introduced superconducting order parameters $\Delta_{j,k}$ are related to the anomalous averages as follows

$$\Delta_{1k} = -\frac{2}{N}\sum_q \Big(\frac{U_p}{2} + V_2\cos(k_y - q_y) + V_2'\cos(k_x - q_x)\Big)\langle a_{q\uparrow}a_{-q\downarrow}\rangle,$$

$$\Delta_{2k} = -\frac{4V_1}{N}\sum_q \phi_{k-q}\langle a_{q\uparrow}b_{-q\downarrow}\rangle,$$

$$
\begin{aligned}
\Delta_{3k} &= -\frac{4V_1}{N}\sum_q \phi_{k-q}\langle b_{q\uparrow}a_{-q\downarrow}\rangle,\\
\Delta_{4k} &= -\frac{2}{N}\sum_q\Big(\frac{U_p}{2}+V_2\cos(k_x-q_x)+V_2'\cos(k_y-q_y)\Big)\langle b_{q\uparrow}b_{-q\downarrow}\rangle,\\
\Delta_{5k} &= \frac{1}{N}\sum_q\Big\{I_{k-q}\big(\langle L_{q\uparrow}L_{-q\downarrow}\rangle - C_1\langle u_{q\uparrow}u_{-q\downarrow}\rangle\big)+8IC_1\langle u_{q\uparrow}u_{-q\downarrow}\rangle\Big\}\\
&\quad+\frac{J}{N}\sum_q\Big\{-2\gamma_{1q}\langle L_{q\uparrow}L_{-q\downarrow}\rangle+\big(3/2-4C_1\gamma_{1k}\big)\langle u_{q\uparrow}u_{-q\downarrow}\rangle\Big\}\\
&\quad+\frac{2}{N}\sum_q\big(\xi(q_x)s_{q,x}+t_q s_{q,y}\big)\,\langle a_{q\uparrow}L_{-q\downarrow}\rangle\\
&\quad+\frac{2}{N}\sum_q\big(\xi(q_y)s_{q,y}+t_q s_{q,x}\big)\,\langle b_{q\uparrow}L_{-q\downarrow}\rangle\\
&\quad-\frac{U_p}{N}\sum_q\Big\{(3/8-\frac{C_1}{2}\cos k_x)\langle a_{q\uparrow}a_{-q\downarrow}\rangle+(3/8-\frac{C_1}{2}\cos k_y)\langle b_{q\uparrow}b_{-q\downarrow}\rangle\Big\}\\
&\quad-\frac{V_1}{N}\sum_q\Big\{(3/4-2C_1\gamma_{1k}+C_2\gamma_{2k})\psi_q+C_2\sin k_x\sin k_y\phi_q\Big\}\\
&\quad\times\big(\langle a_{q\uparrow}b_{-q\downarrow}\rangle+\langle b_{q\uparrow}a_{-q\downarrow}\rangle\big)\\
&\quad-\frac{1}{N}\sum_q\Big\{V_2(C_1\cos k_y-C_2\gamma_{2k})\cos q_y\\
&\quad+V_2'\Big(-\frac{3}{8}+C_1\cos k_x-\frac{C_3}{2}\cos 2k_x\Big)\cos q_x\Big\}\langle a_{q\uparrow}a_{-q\downarrow}\rangle\\
&\quad-\frac{1}{N}\sum_q\Big\{V_2(C_1\cos k_x-C_2\gamma_{2k})\cos q_x\\
&\quad+V_2'\Big(-\frac{3}{8}+C_1\cos k_y-\frac{C_3}{2}\cos 2k_y\Big)\cos q_y\Big\}\langle b_{q\uparrow}b_{-q\downarrow}\rangle.
\end{aligned}
\tag{7}
$$

Here $I_k = 4I\gamma_{1k}$, $\phi_k = \cos\frac{k_x}{2}\cos\frac{k_y}{2}$, $\psi_k = \sin\frac{k_x}{2}\sin\frac{k_y}{2}$, and the average

$$
\langle u_{q\uparrow}u_{-q\downarrow}\rangle = -s_{q,x}^2\langle a_{q\uparrow}a_{-q\downarrow}\rangle - s_{q,y}^2\langle b_{q\uparrow}b_{-q\downarrow}\rangle - \psi_q\big(\langle a_{q\uparrow}b_{-q\downarrow}\rangle+\langle b_{q\uparrow}a_{-q\downarrow}\rangle\big).
\tag{8}
$$

When deriving the system (5), we assume that the state of the localized momenta corresponds to the quantum spin liquid. In this case, the spin correlation functions $C_j = \langle \mathbf{S}_0\mathbf{S}_{r_j}\rangle$ arising in Eqs. (6) and (10) satisfy the relations

$$
C_j = 3\langle S_0^x S_{r_j}^x\rangle = 3\langle S_0^y S_{r_j}^y\rangle = 3\langle S_0^z S_{r_j}^z\rangle,
\tag{9}
$$

where r_j is the position of a copper ion within the coordination sphere j. Besides, $\langle S_f^x \rangle = \langle S_f^y \rangle = \langle S_f^z \rangle = 0$. The doping dependences of the correlation functions C_j were calculated within the spherical symmetric self-consistent approach for a frustrated antiferromagnet in Ref. [25]. Determination of the spin correlation functions with the use of the model considered here was described in detail in Ref. [20].

The role of the Coulomb repulsion V_1 between holes located at the nearest oxygen sites in superconducting pairing was clarified in Ref. [5]. It was shown that the Fourier transform of the Coulomb interaction $V_q = 4V_1 \cos(q_x/2)\cos(q_y/2)$ vanishes in the set of the integral self-consistency equations determining the superconducting order parameter with the $d_{x^2-y^2}$-wave symmetry. Therefore, the Coulomb repulsion of holes located at the neighboring oxygen sites V_1 has no influence on the Cooper pairing in the d-wave channel.

This result allows us to neglect all the contributions connected with V_1 in the system (7) and restrict ourselves to a treatment of the interactions V_2 and V_2' between the next-nearest neighbors. For the sake of simplicity, we rename $\Delta_{4k} \to \Delta_{2k}$ and $\Delta_{5k} \to \Delta_{3k}$ and, in view of the experimental data, we omit all the contributions in (7) which do not lead to the superconducting d-wave pairing. As a result, the relation between the introduced order parameters $\Delta_{j,k}$ and the anomalous averages becomes

$$
\begin{aligned}
\Delta_{1k} &= -\frac{2}{N}\sum_q \Big(V_2 \cos k_y \cos q_y + V_2' \cos k_x \cos q_x\Big)\langle a_{q\uparrow} a_{-q\downarrow}\rangle,\\
\Delta_{2k} &= -\frac{2}{N}\sum_q \Big(V_2 \cos k_x \cos q_x + V_2' \cos k_y \cos q_y\Big)\langle b_{q\uparrow} b_{-q\downarrow}\rangle,\\
\Delta_{3k} &= \frac{1}{N}\sum_q I_{k-q}\big(\langle L_{q\uparrow} L_{-q\downarrow}\rangle - C_1 \langle u_{q\uparrow} u_{-q\downarrow}\rangle\big)\\
&\quad - \frac{1}{N}\sum_q \Big\{V_2 C_1 \cos k_y \cos q_y - U_p \frac{C_1}{2}\cos k_x\\
&\quad + V_2' \Big(C_1 \cos k_x - \frac{C_3}{2}\cos 2k_x\Big)\cos q_x\Big\}\langle a_{q\uparrow} a_{-q\downarrow}\rangle\\
&\quad - \frac{1}{N}\sum_q \Big\{V_2 C_1 \cos k_x \cos q_x - U_p \frac{C_1}{2}\cos k_y\\
&\quad + V_2' \Big(C_1 \cos k_y - \frac{C_3}{2}\cos 2k_y\Big)\cos q_y\Big\}\langle b_{q\uparrow} b_{-q\downarrow}\rangle.
\end{aligned}
\tag{10}
$$

4 Self-Consistent Equations and Their Solutions

It follows from the analysis of the system (5) in the superconducting phase that the fermionic excitations spectrum of the quasiparticles within the SFM is determined by the solutions of the sextic equation in ω, which can be reduced to the bicubic equation. At low doping, the dynamics of holes is determined by the lower band E_{1k} which is caused by the strong spin-fermion coupling inducing both the exchange interaction between holes and the localized spins at the nearest copper ions and spin-correlated hoppings [24].

To analyze the Cooper instability, we express the anomalous Green's functions in terms of the Δ_{lk} parameters ($l = 1, 2, 3$). Then, using the spectral theorem [26], we find the expressions for the anomalous averages and obtain the closed system of integral equations for the superconducting order parameter components. The kernels of these equations appear to be split and this allows us to seek a solution of this system in the form

$$\Delta_{lk} = \Delta_{0l}(\cos k_x - \cos k_y). \tag{11}$$

Here, we neglect the contributions of harmonics $\cos 2k_x$ and $\cos 2k_y$ of the d-wave pairing because of their small contribution, according to our previous calculations [6]. Substituting Eq. (11) into the system of integral equations and equating the coefficients of the corresponding trigonometric functions, we finally arrive at the closed system of self-consistent equations

$$\begin{aligned}
\Delta_{01} &= -\frac{1}{N}\sum_q \left(V_2' \cos q_x - V_2 \cos q_y\right) A_{aa}(E_{1q}, \Delta_{01}, \Delta_{02}, \Delta_{03}) R_q, \\
\Delta_{02} &= -\frac{1}{N}\sum_q \left(V_2 \cos q_x - V_2' \cos q_y\right) A_{bb}(E_{1q}, \Delta_{01}, \Delta_{02}, \Delta_{03}) R_q, \\
\Delta_{03} &= \frac{I}{N}\sum_q \left(\cos q_x - \cos q_y\right) \Big[A_{LL}(E_{1q}, \Delta_{01}, \Delta_{02}, \Delta_{03}) \\
&\quad + C_1 \Big(s_{qx}^2 A_{aa}(E_{1q}, \Delta_{01}, \Delta_{02}, \Delta_{03}) + s_{qy}^2 A_{bb}(E_{1q}, \Delta_{01}, \Delta_{02}, \Delta_{03}) \\
&\quad + \psi_q (A_{ab}(E_{1q}, \Delta_{01}, \Delta_{02}, \Delta_{03}) + A_{ba}(E_{1q}, \Delta_{01}, \Delta_{02}, \Delta_{03})) \Big) \Big] R_q \\
&\quad - \frac{1}{N}\sum_q \frac{C_1}{2} \left(-U_p/2 + V_2' \cos q_x - V_2 \cos q_y\right) A_{aa}(E_{1q}, \Delta_{01}, \Delta_{02}, \Delta_{03}) R_q \\
&\quad - \frac{1}{N}\sum_q \frac{C_1}{2} \left(U_p/2 + V_2 \cos q_x - V_2' \cos q_y\right) A_{bb}(E_{1q}, \Delta_{01}, \Delta_{02}, \Delta_{03}) R_q,
\end{aligned} \tag{12}$$

where $R_q = \dfrac{\tanh\left(E_{1q}/2T\right)}{2E_{1q}(E_{1q}^2 - E_{2q}^2)(E_{1q}^2 - E_{3q}^2)}$ and E_{jq} are the solutions of the bicubic equation. Solving system (12) with regard to the equation for the doping dependence x of the chemical potential

$$\frac{x}{4} = \frac{1}{N}\sum_q \frac{\left(A_N(E_{1q}, \Delta_{01}, \Delta_{02}, \Delta_{03}) f(E_{1q}) - A_N(-E_{1q}, \Delta_{01}, \Delta_{02}, \Delta_{03}) f(-E_{1q})\right)}{2E_{1q}\left(E_{1q}^2 - E_{2q}^2\right)\left(E_{1q}^2 - E_{3q}^2\right)}, \tag{13}$$

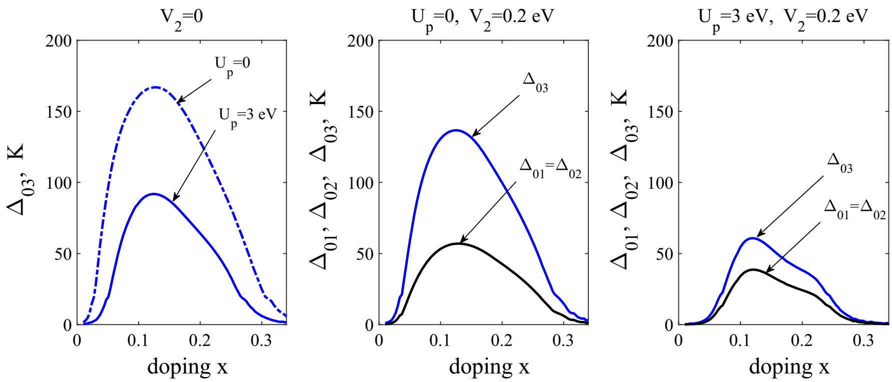

Fig. 2 Amplitudes of the superconducting order parameter components versus doping level (Color figure online)

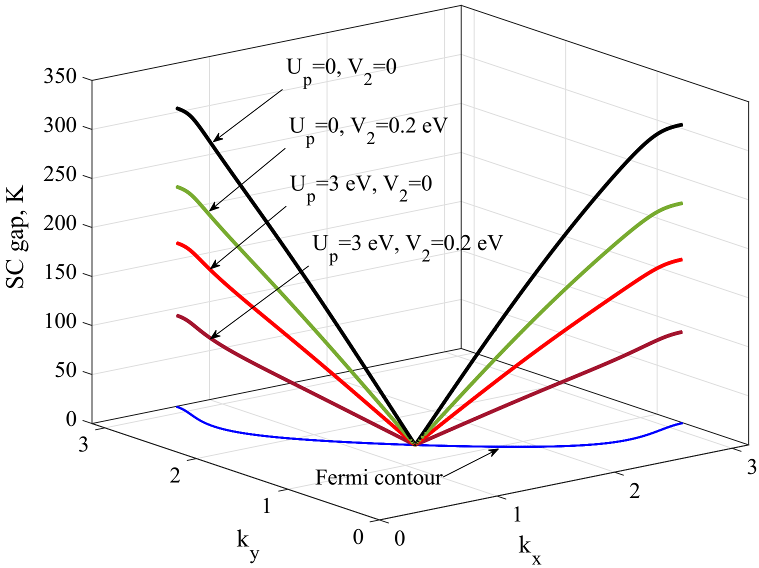

Fig. 3 Superconducting gap versus quasimomenta on the Fermi contour at $x = 0.125$, $I = 0.136\,\text{eV}$, $T = 0$ and the different values of the Coulomb interactions (Color figure online)

where $f(E_{1q}) = (e^{E_{1q}/T} + 1)^{-1}$ is the Fermi-Dirac distribution function, we find the dependence of amplitudes Δ_{01}, Δ_{02}, Δ_{03} of the superconducting order components on the doping (Fig. 2). The functions A_{aa}, A_{bb}, A_{ab}, A_{ba}, A_{LL}, A_N enter Eqs. (12) and (13) are found from Eq. (5) and listed in "Appendix."

Figure 3 shows the modifications of the gap in the excitations spectrum of the spin-polaron quasiparticles on the Fermi contour in the superconducting phase at the different values of the Coulomb interactions. It can be seen that the dependence of the gap on the quasimomentum in the first Brillouin zone is characterized by the d-wave symmetry. It follows from the plot that an increase in the intensity of interactions U_p

and V_2 results in the narrowing of the superconducting gap; however, as it was shown in Ref. [6], it determines the superconducting transition temperatures that are observed experimentally.

5 Conclusion

In conclusion, we have shown that the resulting gap in the excitation spectrum of the spin-polaron quasiparticles within the spin-fermion model with the on-site Coulomb repulsion of holes U_p and the intersite Coulomb repulsion V_2 of holes at the next-nearest-neighbor oxygen sites on the CuO_2 plane is formed by three components and determined by solutions of the system of self-consistency integral equations. It is shown that the inclusion of the realistic values of U_p and V_2 leads to the narrowing of the d-wave symmetry superconducting gap; however, it determines the superconducting transition temperatures remaining within the limits that are observed experimentally.

Acknowledgements The work was supported by the program of the Presidium of the Russian Academy of Sciences No. 12 "Fundamental problems of high-temperature superconductivity," the Russian Foundation for Basic Research (Projects Nos. 16-02-00304 and 18-02-00837) and partly by the Government of Krasnoyarsk Region and the Krasnoyarsk Region Science and Technology Support Fund (Projects Nos. 18-42-243002 "Manifestation of spin-nematic correlations in spectral characteristics of electronic structure and their influence on practical properties of cuprate superconductors" and 18-42-243018 "Contact phenomena and magnetic disorder in the problem of the formation and detection of topological edge states in semiconductor nanostructures"), and the grant of the President of the Russian Federation (Project MK-1398.2017.2).

Appendix

The functions $A_{aa}, A_{bb}, A_{ab}, A_{ba}, A_{LL}, A_N$ enter Eqs. (12) and (13) have the form

$$\begin{aligned}A_{aa}(E_{1k}) &= \Delta_{1k}E_{1k}^4 - (\Delta_{2k}t_k^2 + \Delta_{1k}\xi_L^2 + 2\Delta_{1k}K_kJ_y^2 + |\Delta_{2k}|^2\Delta_{1k} + \Delta_{1k}\xi_y^2 \\ &+ |\Delta_{3k}|^2\Delta_{1k}/K_k - J_x^2\Delta_{3k})E_{1k}^2 + \Delta_{2k}t_k^2\xi_L^2 + 2t_kJ_y\Delta_{3k}J_x\xi_y + J_y^4K_k^2\Delta_{1k} \\ &- 2t_k\Delta_{2k}K_k\xi_LJ_yJ_x - 2\xi_y\Delta_{1k}K_k\xi_LJ_y^2 - J_y^2\Delta_{3k}^*\Delta_{1k}\Delta_{2k} - |\Delta_{2k}|^2J_x^2\Delta_{3k} \\ &- \Delta_{2k}J_y^2\Delta_{1k}\Delta_{3k} + \Delta_{1k}\xi_y^2\xi_L^2 + |\Delta_{2k}|^2\Delta_{1k}\xi_L^2 + |\Delta_{2k}|^2|\Delta_{3k}|^2\Delta_{1k}/K_k^2 \\ &- J_y^2\Delta_{3k}t_k^2 + |\Delta_{3k}|^2t_k^2\Delta_{2k} - J_x^2\Delta_{3k}\xi_y^2 + |\Delta_{3k}|^2\Delta_{1k}\xi_y^2/K_k^2 + J_y^2K_k^2J_x^2\Delta_{2k},\end{aligned} \tag{14}$$

$$\begin{aligned}A_{bb}(E_{1k}) &= \Delta_{2k}E_{1k}^4 - (\Delta_{2k}\xi_x^2 + \Delta_{1k}t_k^2 + 2\Delta_{2k}K_kJ_x^2 + |\Delta_{1k}|^2\Delta_{2k} + \Delta_{2k}\xi_L^2 \\ &+ |\Delta_{3k}|^2\Delta_{2k}/K_k - J_y^2\Delta_{3k})E_{1k}^2 - 2\xi_x\Delta_{2k}K_k\xi_LJ_x^2 + 2\xi_xt_kJ_xJ_y\Delta_{3k} \\ &- 2t_k\Delta_{1k}K_k\xi_LJ_xJ_y - J_y^2\Delta_{3k}\xi_x^2 + J_x^4K_k^2\Delta_{2k} - J_x^2\Delta_{3k}^*\Delta_{1k}\Delta_{2k} - J_x^2\Delta_{1k}^*\Delta_{2k}\Delta_{3k} \\ &- J_x^2\Delta_{3k}t_k^2 - |\Delta_{1k}|^2\Delta_{3k}J_y^2 + \Delta_{2k}\xi_x^2\xi_L^2 + |\Delta_{3k}|^2\Delta_{2k}\xi_x^2 + J_x^2J_y^2K_k^2\Delta_{1k} \\ &+ \Delta_{1k}t_k^2\xi_L^2 + |\Delta_{3k}|^2\Delta_{1k}t_k^2/K_k^2 + |\Delta_{1k}|^2|\Delta_{3k}|^2\Delta_{2k}/K_k^2 + |\Delta_{1k}|^2\Delta_{2k}\xi_L^2,\end{aligned} \tag{15}$$

$$A_{LL}(E_{1k}) = \Delta_{3k}E_{1k}^4/K_k + (J_y^2K_k^2\Delta_{2k} - (|\Delta_{2k}|^2 + |\Delta_{1k}|^2)\Delta_{3k} - 2t_k^2\Delta_{3k} - \Delta_{3k}(\xi_x^2 + \xi_y^2) + J_x^2K_k^2\Delta_{1k})E_{1k}^2/K_k + (2\xi_x J_y K_k^2\Delta_{2k}t_k J_x + 2t_k J_y K_k^2\Delta_{1k}J_x\xi_y + |\Delta_{2k}|^2\Delta_{3k}\xi_x^2 - J_y^2K_k^2\Delta_{1k}t_k^2 - 2\xi_x\Delta_{3k}\xi_y t_k^2 - J_y^2K_k^2\Delta_{2k}\xi_x^2 + t_k^4\Delta_{3k} - J_x^2K_k^2\Delta_{1k}\xi_y^2 + \Delta_{2k}^*\Delta_{1k}t_k^2\Delta_{3k} - J_x^2K_k^2t_k^2\Delta_{2k} + |\Delta_{1k}|^2\Delta_{3k}\xi_y^2 - J_x^2K_k^2|\Delta_{2k}|^2\Delta_{1k} + \Delta_{1k}^*t_k^2\Delta_{2k}\Delta_{3k} + |\Delta_{1k}|^2|\Delta_{2k}|^2\Delta_{3k} + \Delta_{3k}\xi_x^2\xi_y^2 - |\Delta_{1k}|^2J_y^2K_k^2\Delta_{2k})/K_k, \quad (16)$$

$$A_{ab}(E_{1k}) = A_{1k}E_{1k}^3 + A_{2k}E_{1k}^2 + A_{3k}E_{1k} + A_{4k}, \quad (17)$$

$$A_{1k} = t_k(\Delta_{2k} - \Delta_{1k}),$$
$$A_{2k} = t_k(\xi_x\Delta_{2k} + \xi_y\Delta_{1k}) + J_xJ_y(\Delta_{1k}K_k + \Delta_{2k}K_k + \Delta_{3k}),$$
$$A_{3k} = J_xJ_y\xi_x(\Delta_{2k}K_k + \Delta_{3k}) - \Delta_{3k}J_xJ_y\xi_y + \Delta_{3k}t_k(J_y^2 - J_x^2) + |\Delta_{3k}|^2t_k(\Delta_{1k} - \Delta_{2k})/K_k^2 - \xi_y\Delta_{1k}K_kJ_yJ_x + \Delta_{1k}t_k\xi_L^2 + \xi_LJ_xJ_yK_k(\Delta_{2k} - \Delta_{1k}) - \Delta_{2k}t_k\xi_L^2 + J_y^2K_k\Delta_{1k}t_k - t_k\Delta_{2k}K_kJ_x^2,$$
$$A_{4k} = t_k\Delta_{2k}K_k\xi_LJ_x^2 - \xi_y\Delta_{1k}t_k\xi_L^2 - \xi_y|\Delta_{3k}|^2\Delta_{1k}t_k/K_k^2 - \xi_yJ_x\Delta_{3k}J_y\xi_x + J_yK_kJ_x\Delta_{2k}\xi_x\xi_L + \xi_y\Delta_{1k}K_k\xi_LJ_yJ_x - t_k|\Delta_{3k}|^2\Delta_{2k}\xi_x/K_k^2 + t_kJ_y^2\Delta_{3k}\xi_x - J_y\Delta_{3k}t_k^2J_x + J_y\Delta_{3k}^*\Delta_{1k}\Delta_{2k}J_x + J_y^2K_k\Delta_{1k}t_k\xi_L - t_k\Delta_{2k}\xi_x\xi_L^2 - J_yK_k^2J_x^3\Delta_{2k} - J_y^3K_k^2\Delta_{1k}J_x + \xi_yJ_x^2\Delta_{3k}t_k,$$

$$A_{ba}(E_{1k}) = -A_{1k}E_{1k}^3 + A_{2k}E_{1k}^2 - A_{3k}E_{1k} + A_{4k}, \quad (18)$$

$$A_N(E_{1k}) = E_{1k}^5 + \xi_xE_{1k}^4 - (t_k^2 + |\Delta_{3k}|^2/K_k^2 + 2K_kJ_y^2 + K_kJ_x^2 + \xi_L^2 + \xi_y^2 + |\Delta_{2k}|^2/K_k^2)E_{1k}^3 + (2K_kt_kJ_yJ_x - \xi_x\xi_L^2 - \xi_x\xi_y^2 - (|\Delta_{2k}|^2 + |\Delta_{3k}|^2/K_k^2)\xi_x - 2K_k\xi_xJ_y^2 + K_k\xi_LJ_x^2 + \xi_yt_k^2)E_{1k}^2 + (|\Delta_{3k}|^2\xi_y^2/K_k^2 - 2\xi_yK_k\xi_LJ_y^2 + J_y^4K_k^2 + |\Delta_{3k}|^2t_k^2/K_k^2 - 2K_k\xi_Lt_kJ_yJ_x + \xi_y^2\xi_L^2 + K_kJ_x^2\xi_y^2 + J_y^2K_kt_k^2 + t_k^2\xi_L^2 - \Delta_{2k}^*J_y^2\Delta_{3k} + J_y^2K_k^2J_x^2 - J_y^2\Delta_{3k}^*\Delta_{2k} + |\Delta_{2k}|^2K_kJ_x^2 + |\Delta_{2k}|^2\xi_L^2 + J_y^4K_k^2\xi_x + |\Delta_{2k}|^2|\Delta_{3k}|^2/K_k^2 - 2\xi_yK_kt_kJ_yJ_x)E_{1k} + J_y^2K_kt_k^2\xi_L - K_k\xi_LJ_x^2\xi_y^2 + J_y^2K_k^2J_x^2\xi_y + |\Delta_{3k}|^2\xi_x\xi_y^2/K_k^2 + J_y\Delta_{3k}^*\Delta_{2k}t_kJ_x + \Delta_{3k}\Delta_{2k}^*J_yt_kJ_x - \xi_yt_k^2\xi_L^2 - 2J_y^3K_k^2t_kJ_x - \xi_y|\Delta_{3k}|^2t_k^2/K_k^2 - J_y^2\Delta_{3k}^*\Delta_{2k}\xi_x + |\Delta_{2k}|^2|\Delta_{3k}|^2\xi_x/K_k^2 + \xi_x\xi_y^2\xi_L^2 + 2\xi_yK_k\xi_Lt_kJ_yJ_x - \Delta_{3k}\Delta_{2k}^*J_y^2\xi_x - 2\xi_yK_k\xi_L\xi_xJ_y^2 - |\Delta_{2k}|^2K_k\xi_LJ_x^2 + |\Delta_{2k}|^2\xi_x\xi_L^2. \quad (19)$$

The functions Δ_{1k}, Δ_{2k} and Δ_{3k} are defined in Eq. (11).

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