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Modification of the Superconducting Order Parameter Δ(k) by Long-Range Interactions

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It is demonstrated that the inclusion of long-range intersite interactions qualitatively modifies the dependence of a superconducting gap on quasimomentum for both *s*- and *d*-symmetry types. In particular, the order parameter of a superconducting phase with the $d_{x^2-y^2}$ symmetry type depends on two amplitudes and has the form $\Delta(\mathbf{k}) = \Delta_1(\cos k_x - \cos k_y) + \Delta_2(\cos 2k_x - \cos 2k_y)$. In this case, the theoretical dependence of the critical temperature on the degree of doping agrees with the experimental dependence. *© 2003 MAIK "Nauka/Interperiodica".*

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1. It is known that the (t–J) model [1] properly describes, on a qualitative level, the magnetic pairing mechanism in high-temperature superconductors (see, e.g., review [2]). If this model is developed on the basis of the Hubbard model in the strong-correlation regime, the effective Hamiltonian H_{eff} includes so-called three-center terms [3, 4]. In [5], it was shown that the three-center terms $H_{(3)}$make a weak contribution to the dispersion curves of energy spectrum. This result is quite natural, because the corrections $H_{(3)}$ to the hopping parameters contain the additional smallness. A different situation appears in the analysis of a superconducting phase. In the case of the magnetic pairing mechanism, the exchange interaction plays the role of coupling constant. The energy parameters in the three-center terms are of the same order of magnitude. For this reason, the contribution $H_{(3)}$ to the self-consistent equation for the superconducting gap becomes appreciable. The influence of three-center terms on the formation of superconductivity was studied in [6, 7]. It was shown in [7] that the inclusion of three-center terms results in the renormalization of the coupling constant. This substantially reduces the region of a superconducting phase with the $d_{x^2-y^2}$ symmetry type of order parameter [8].

Beyond the nearest-neighbor approximation, the effective Hamiltonian includes the exchange interaction between the spins of quasiparticles separated by a distance larger than the lattice parameter. The important role of quasiparticle hopping between the sites from the distant coordination spheres and the exchange interactions between the non-nearest-neighboring spins was demonstrated in many works dealing with the quasiparticle energy spectrum (see, e.g., [9–13]). In these cases, the theoretical positions agreed satisfactorily with the APRES data. In particular, it was pointed out that the inclusion of frustrated bonds ($J_2 > 0$) is important for the description of the evolution of spectral dependence in the presence of doping [12]. Since, as was mentioned above, the exchange interaction parameters play the role of coupling constants in the magnetic mechanism of superconducting pairing, one can expect that J_2 and J_3 may influence both the functional form of the order parameter and the conditions for the appearance of superconducting state.

Below, the effective Hamiltonian based on the strong-correlation Hubbard model (extended (t–J) model with three-center interactions) is used to demonstrate that the exchange interactions between the spins of non-nearest neighbors have an appreciable effect both on the quasimomentum dependence of the order parameter and on the form of the equation for the superconducting gap and critical temperature T_c.

2. The Hubbard Hamiltonian

$$H = \sum_{f\sigma}(\varepsilon - \mu)a^{+}_{f\sigma}a_{f\sigma} + \sum_{fm\sigma} t_{fm}a^{+}_{f\sigma}a_{m\sigma} + U\sum_{f\sigma}\hat{n}_{f\uparrow}\hat{n}_{f\downarrow} \quad (1)$$

is chosen as the initial model, and it is assumed that three hopping parameters are nonzero: $t_{f,\, f+\delta_1} = -t_1$,

$t_{f,\,f+\delta_2} = -t_2$, and $t_{f,\,f+\delta_3} = -t_3$, where δ_i are the radius vectors of the sites from the ith coordination sphere.

It is well known that, in the regime of strong electron correlations ($U \gg |t_{fm}|$) and for concentrations $n < 1$, one can pass, in the Hubbard operator representation, to the effective Hamiltonian of the form

$$H = \sum_{f\sigma}(\varepsilon - \mu)X_f^{\sigma\sigma} + \sum_{fm\sigma} t_{fm} X_f^{\sigma 0} X_m^{0\sigma}$$
$$+ \sum_{fm\sigma}\left(\frac{t_{fm}t_{mf}}{U}\right)(X_f^{\sigma\bar{\sigma}}X_m^{\bar{\sigma}\sigma} - X_f^{\sigma\sigma}X_m^{\bar{\sigma}\bar{\sigma}}) \tag{2}$$
$$+ \sum_{\substack{fmg\sigma \\ (f \neq g)}}\left(\frac{t_{fm}t_{mg}}{U}\right)(X_f^{\sigma 0}X_m^{\bar{\sigma}\sigma}X_g^{0\bar{\sigma}} - X_f^{\sigma 0}X_m^{\bar{\sigma}\bar{\sigma}}X_g^{0\sigma})$$

with a quadratic accuracy in $|t_{fm}|/U$ [7, 2, 8]. The notation is standard, and its meaning can be found in the cited works and in review [2]. Note, nevertheless, that the last term in the Hamiltonian depends on three sites and describes the correlated hopping.

By using the diagram technique for the Hubbard operators [14, 15] or the method of irreducible Green's functions in the atomic representation with anomalous means [16], one arrives at the self-consistency equation for the superconducting order parameter (SOP) $\Delta_{\mathbf{q}}$ with allowance made for the three-center terms [8]:

$$\Delta_{\mathbf{k}} = \frac{1}{N}\sum_{\mathbf{q}}\left\{2t_{\mathbf{q}} + \frac{n}{2}(J_{\mathbf{k}+\mathbf{q}} + J_{\mathbf{k}-\mathbf{q}}) + 4\left(1 - \frac{n}{2}\right)\frac{t_{\mathbf{k}}t_{\mathbf{q}}}{U}\right.$$
$$\left. - n\left(\frac{t_{\mathbf{q}}^2}{U} - \frac{J_0}{2}\right)\right\}\left(\frac{\Delta_{\mathbf{q}}}{2E_{\mathbf{q}}}\right)\tanh\left(\frac{E_{\mathbf{q}}}{2T}\right). \tag{3}$$

In this equation, t_k and J_k are the Fourier transforms of the parameters t_{fm} and $2t_{fm}^2/U$. The energy of Bogoliubov quasiparticles is denoted by $E_k = \sqrt{(\tilde{\varepsilon}_{\mathbf{k}} - \mu)^2 + |\Delta_{\mathbf{k}}|^2}$, and the renormalized electronic spectrum is

$$\tilde{\varepsilon}_{\mathbf{k}} = (1 - n/2)\left(1 - \frac{n}{2}\frac{t_{\mathbf{k}}}{U}\right)t_{\mathbf{k}} - \frac{1}{N}$$
$$\times \sum_{\mathbf{q}}\left\{t_{\mathbf{q}} + \frac{n}{2}J_{\mathbf{k}-\mathbf{q}} + [(2-n)t_{\mathbf{k}} + (1-n)t_{\mathbf{q}}]\frac{t_{\mathbf{q}}}{U}\right\}n_{\mathbf{q}\sigma},$$
$$n_{\mathbf{q}\sigma} = (1 - \vartheta_{\mathbf{q}})/2 + \vartheta_{\mathbf{q}}(\exp(E_{\mathbf{q}}/T) + 1)^{-1},$$
$$\vartheta_{\mathbf{q}} = \xi_{\mathbf{q}}/E_{\mathbf{q}}, \quad \xi_{\mathbf{q}} = \tilde{\varepsilon}_{\mathbf{q}} - \mu. \tag{4}$$

Note that, when deriving Eq. (3) from H_{eff}, only $\langle X_f^{0\downarrow}X_m^{0\uparrow}\rangle$ anomalous means appear. If, however, one starts from the Hamiltonian (1) written in the atomic representation, then, as was shown by Zaĭtsev *et al.* in [17], the anomalous means $\langle X_f^{0\sigma}X_m^{\sigma 2}\rangle$ and $\langle X_f^{\sigma 2}X_m^{\bar{\sigma}2}\rangle$ also appear, which are caused by the transitions from the lower to the upper Hubbard subband and the transitions inside the upper subband that make contribution at finite U. The formal absence of these anomalous means in our approach does not mean that we ignore these processes. The matter is that, when passing to H_{eff}, all calculations are carried out in the new representation, for which the indicated processes are taken into account by different operator structures. This statement can be clarified as follows.

We first consider the $\langle X_f^{02}\rangle$ and $\langle X_f^{0\sigma}X_m^{02}\rangle$ means that are associated with the transitions from the lower to upper Hubbard subband (in this case, it is tacitly assumed that the representation is induced by the original Hamiltonian). The transition to H_{eff} implies the unitary transformation ($S^+ = -S$)

$$H \longrightarrow H_{\text{eff}} = \exp(S)H\exp(-S); \quad H|\Psi_n\rangle = E_n|\Psi_n\rangle,$$
$$H_{\text{eff}}|\Phi_n\rangle = E_n|\Phi_n\rangle, \quad |\Phi_n\rangle = \exp(S)|\Psi_n\rangle,$$

after which the Hamiltonian, the basis functions, and all operators, whose averaging gives the physical quantities of interest, change their form. For example, the operators X_f^{02} and $X_f^{0\sigma}X_m^{\sigma 2}$ are transformed as

$$X_f^{02} \longrightarrow \tilde{X}_f^{02}$$
$$= -\sum_g (t_{fg}/U)(X_f^{0\downarrow}X_g^{0\uparrow} - X_f^{0\uparrow}X_g^{0\downarrow}) + O\{(t_{fg}/U)^3\},$$

$$X_f^{0\sigma}X_m^{\sigma 2} \longrightarrow \tilde{X}_f^{0\sigma}\tilde{X}_m^{\sigma 2} = -\sum_g (t_{mg}/U)\eta(\sigma)$$
$$\times (X_f^{0\sigma}X_m^{\sigma\bar{\sigma}}X_g^{0\sigma} - X_f^{0\sigma}X_m^{\sigma\sigma}X_g^{0\bar{\sigma}}) + O\{(t_{fm}/U)^3\}.$$

The transformation laws clearly demonstrate that, in the new representation, the above-mentioned anomalous means are not ignored within the linear accuracy in (t_{fm}/U), and their contribution is determined by the means of operators which are responsible only for the transitions between the states without pairs. In essence, this is a particular case that follows from the general statement made in [18]. As for the anomalous means associated with the transitions inside the upper Hubbard band, one can readily verify that the corresponding contribution is nonzero only in the quadratic (and not linear) approximation in (t_{fm}/U). For this reason, these means make no contribution to our theory.

As known, Eq. (3) has solutions differing in the type of $\Delta_{\mathbf{k}}$ symmetry. We will consider the influence of long-range hopping separately on the type of SOP symmetry and on the $\mathbf{k}$ dependence for a given symmetry.

(a) s Symmetry; due to the presence of three nonzero t_1, t_2, $t_3 \neq 0$, the solution to Eq. (3) for this symmetry type is given by $\Delta_\mathbf{k}$, which is expressed as

$$\Delta_\mathbf{k} = \Delta_0 + \Delta_1 S_1(\mathbf{k}) + \Delta_2 S_2(\mathbf{k}) + \Delta_3 S_3(\mathbf{k}). \quad (5)$$

Hereafter, the following invariants are used for brevity:

$$S_1(\mathbf{k}) = (\cos k_x a + \cos k_y a)/2,$$
$$S_2(\mathbf{k}) = \cos(k_x a)\cos(k_y a),$$
$$S_3(\mathbf{k}) = (\cos 2k_x a + \cos 2k_y a)/2.$$

The order parameter in the form of Eq. (5) is the solution to the integral Eq. (3), if the unknown coefficients Δ_i satisfy the set of four equations

$$\Delta_0 = \sum_{l=0}^{3}\left\{\sum_{j=1}^{3} 2G_{lj}T_j + \left(\frac{n}{2}\right)J_0 G_l - \frac{n}{U}\sum_{i,j=1}^{3} G_{lij}T_i T_j\right\}\Delta_l$$
$$(T_j = -4t_j, \quad j = 1, 2, 3),$$
$$\Delta_m = 4\sum_{l=0}^{3}\left\{nJ_m G_{ml} + (1-n/2)T_m \sum_{i=1}^{3} G_{li}T_i/U\right\}\Delta_l, \quad (6)$$
$$J_m = 2t_m^2/U, \quad m = 1, 2, 3,$$

where

$$G_i = G_{i00}, \quad G_{ij} = G_{ij0},$$

$$G_{ijl} = \frac{1}{N}\sum_\mathbf{q} S_i(\mathbf{q})S_j(\mathbf{q})S_l(\mathbf{q})\Psi_\mathbf{q},$$

$$\Psi_\mathbf{q} = \frac{\tanh(E_\mathbf{q}/2T)}{2E_\mathbf{q}}, \quad S_0(\mathbf{k}) = 1.$$

From the set of Eqs. (6) it follows that, in the limit of infinitely strong repulsion, for which the superconducting pairing is governed only by the Zaĭtsev kinematic mechanism, the order parameter includes only the contributions linear in t;

(b) d_{xy} symmetry; $\Delta_\mathbf{k} = \Delta_1\sin(k_x a)\sin(k_y a)$ This symmetry type is absent for the SOP in the nearest-neighbor approximation and appears only if $t_2 \neq 0$. The corresponding SOP amplitude Δ_1 is found from the transcendental equation

$$1 = (4nJ_2/N)\sum_\mathbf{q} \sin^2 q_x \sin^2 q_y \Psi_\mathbf{q}\,; \quad (7)$$

(c) $d_{x^2-y^2}$ symmetry. Due to the distant hopping (t_2, $t_3 \neq 0$), the well-known SOP $\Delta_\mathbf{k} = \Delta_0(\cos(k_x a) - \cos(k_y a))$ is impossible, because it does not satisfy the integral Eq. (3). The solution to this equation can be represented in a two-parameter form

$$\Delta_\mathbf{k} = \Delta_1\varphi_1(\mathbf{k}) + \Delta_2\varphi_2(\mathbf{k}),$$
$$\varphi_l(\mathbf{k}) = (\cos(lk_x a) - \cos(lk_y a)), \quad l = 1, 2, \quad (8)$$

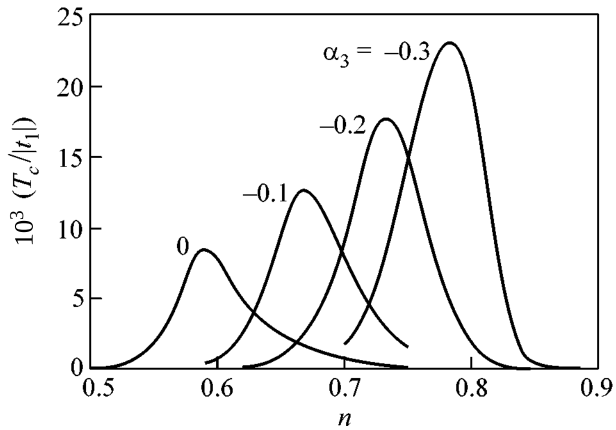

Fig. 1. Effect of hopping to the third coordination sphere on the concentration dependence of T_c for different $\alpha_3 = t_3/t_1$. Parameters: $t_2/t_1 = -0.2$ and $|t_1|/U = 0.2$.

if the amplitudes Δ_1 and Δ_2 are the solutions to the following two equations:

$$\Delta_i = \lambda_i \sum_{j=1}^{j=2}\Phi_{ij}\Delta_j; \quad \lambda_1 = n\left(\frac{t_1^2}{U}\right), \quad \lambda_2 = n\left(\frac{t_3^2}{U}\right),$$
$$\Phi_{nm} = \frac{1}{N}\sum_\mathbf{q}\varphi_n(\mathbf{q})\varphi_m(\mathbf{q})\tanh\left(\frac{E_\mathbf{q}}{2T}\right). \quad (9)$$

It follows that, for $t_3 \neq 0$, $\Delta_1$is always nonzero. The condition for the compatibility of this set of equations leads to the equation

$$(1-\lambda_1\Phi_{11})(1-\lambda_2\Phi_{22}) = \lambda_1\lambda_2\Phi_{12}^2, \quad (10)$$

which determines, in particular, the critical temperature. One can see that the well-known equation for the critical temperature in the (t–J*) model is obtained only for $t_3 = 0$.

3. Because of the lack of volume, we only present the results of numerical analysis for the influence of distant hopping on the characteristics of superconducting state for $\Delta_\mathbf{k}$ of the $d_{x^2-y^2}$-type symmetry. Figure 1 shows the concentration dependence of the transition temperature to the $d_{x^2-y^2}$ phase with inclusion of the parameter t_3. One can see that the electron hopping from the third coordination sphere exerts a substantial effect on the position of the maximum of the $T_c(n)$ curve. It is notable that the experimentally observed situation with a T_c maximum at $n \sim 0.8$ can easily be realized. Curves *1* and *2* in Fig. 2 demonstrate the effect of modified Eq. (10) with long-range interactions on the critical temperature. Curve *1* is constructed using the solution to the complete Eq. (10), and curve *2* is obtained on the assumption that $\lambda_2 = 0$.

In the superconducting phase ($T < T_c$), the amplitudes Δ_1 and Δ_2 are nonzero and change synchronously

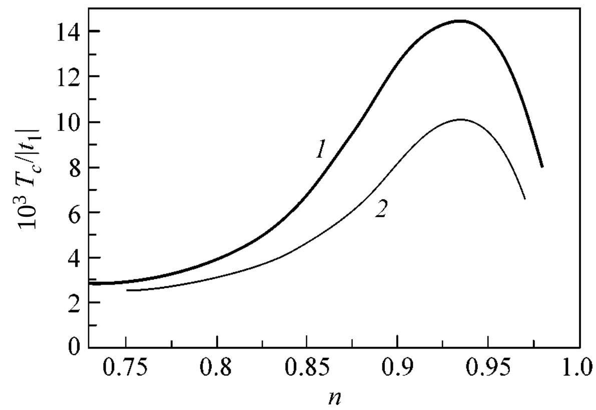

Fig. 2. Concentration dependence $T_c(n)$: $t_2/t_1 = 0.4$, $t_3/t_1 = 0.3$, and $|t_1|/U = 0.2$. For the values for curves *1* and *2*, see the text.

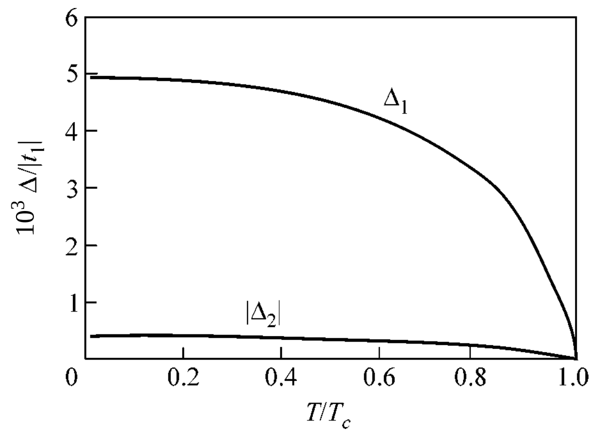

Fig. 3. Temperature dependence of the amplitudes Δ_1 and $|\Delta_2|$ for $n = 0.84$. Parameters are as in Fig. 2.

with temperature. An example of the behavior of this type is demonstrated in Fig. 3. One can see that, over the entire temperature range where the superconducting solution occurs, the temperature of $|\Delta_2|$ ($\Delta_2 < 0$) is the same as for Δ_1.

Note in conclusion that the effect of long-range hopping both on the occurrence of superconducting state and on the momentum dependence of the order parameter has been demonstrated in this work by the example of effective Hamiltonian obtained from the Hubbard model in the strong electron-correlation regime. In this case, there is a correspondence between t_3 and exchange parameter J_3. Nevertheless, a situation is often considered where the hopping parameters and the exchange constants are thought to be independent. In this case, a situation can in principle be realized where the magnitude of long-range exchange interactions will not be related to the hopping amplitudes.

It is worth noting that the more general results could be obtained using the original Hamiltonian (1), if the set of four equations is written in the form as it was done by Zaĭtsev *et al.* in [17]. However, if one is interested in the leading approximation with respect to (t_{fm}/U), the variant presented in this work is simpler. It is this fact that allows the influence of the long-range hopping on the possible symmetry type of order parameter and on the modification of the quasimomentum dependence to be analyzed for any symmetry type.

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