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The Strong Effect of Three-Center Interactions on the Formation of Superconductivity with $d_{x^2-y^2}$ Symmetry in the *t–J** Model

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The effect of three-center interactions on the formation of a superconducting phase with $d_{x^2-y^2}$ symmetry is considered using the diagram technique for Hubbard operators and irreducible Green's functions. It is shown that these interactions lead to a decrease in T_c by a factor of several tens.© *2002 MAIK "Nauka/Interperiodica".*

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1. It is known that, in spite of its relative simplicity, the Hubbard model [1] reflects the most essential feature of the behavior of an ensemble of strongly correlated electrons and is frequently used as a base model for constructing the effective Hamiltonian H_{eff} acting in a truncated Hilbert space. The expedience of constructing H_{eff} is determined by the possibility of explicitly obtaining interactions that open, for example, additional ways for Cooper instability. Thus, when the *t–J* model is derived [2, 3], an interaction leading to the magnetic mechanism of Cooper pairing is distinguished.

In this work, it is shown that the three-center interactions arising in constructing H_{eff} and having the same parametric smallness as exchange interactions radically affect the properties of the superconducting phase, decreasing (*by more than an order of magnitude*) T_c with model parameters remaining unchanged.

2. Using an atomic representation, let us write the Hamiltonian in the Hubbard model

$$H = H_0 + V,$$
$$H_0 = \sum_f \left\{ \sum_\sigma (\epsilon - \mu) X_f^{\sigma\sigma} + (2\epsilon + U - 2\mu) X_f^{22} \right\},$$
$$V = \sum_{fm\sigma} t_{fm} \{ X_f^{\sigma 0} X_m^{0\sigma} + X_f^{2\bar{\sigma}} X_m^{\bar{\sigma}2} + \sigma (X_f^{\sigma 0} X_m^{\bar{\sigma}2} + X_m^{2\bar{\sigma}} X_f^{0\sigma}) \}, \quad (1)$$

where H_0 takes into account contributions of one- and two-electron states on one site with energies ϵ and $2\epsilon + U$, respectively; U is the Coulomb interaction parameter between two electrons located on one site; and μ is the chemical potential of the system. The operator V describes the hopping of electrons within the lower and the upper Hubbard subbands and also hopping from one subband to another; X_f^{nm} are the Hubbard operators

$$X_f^{nm} \equiv |n, f\rangle\langle f, m|, \quad X_f^{nm}|p, f\rangle = \delta_{mp}|n, f\rangle. \quad (2)$$

The symbol σ in Eq. (1) designates the quantity that takes values ± 1 and corresponds to two possible projections of the electron spin moment $\bar{\sigma} = -\sigma$.

In addition to the energy parameters of the model, an essential factor is the electron concentration on a per-site basis $n = N_e/N$ (N_e is the total number of electrons in the system, N is the number of sites in the lattice). At $n < 1$ and large Coulomb repulsion $U \gg |t_{fm}|$, electrons will tend to fill the lower Hubbard subband. The effect of states with two electrons on one site can be taken into account by perturbation theory based on the use of the small parameter $|t_{fm}|/U \ll 1$. An elegant implementation of such a program is provided, for example, by perturbation theory in the operator form [4] indicating a particular algorithm for constructing the effective Hamiltonian.

In the case under consideration, H_{eff} acts in the Hilbert subspace containing no doubles. The contributions of double states are reflected in H_{eff} as additional terms that represent an operator series in increasing order of the smallness parameter. With an accuracy quadratic in

t_{fm}/U, the effective Hamiltonian is determined by the equation [4]

$$H_{\text{eff}} = PH_0P + PVP + PV(H_0 - E_0)^{-1}(PV - V)P, \quad (3)$$

where P is the operator of projection onto the Hilbert subspace without doubles. Using the multiplication rules for Hubbard operators $X_f^{nm}X_f^{lq} = \delta_{ml}X_f^{nq}$, we obtain

$$P = \Pi_f(X_f^{00} + X_f^{\uparrow\uparrow} + X_f^{\downarrow\downarrow}),$$
$$PVP - VP = -\sum_{fm\sigma} t_{mf}\sigma X_m^{2\bar{\sigma}}X_f^{0\sigma}P. \quad (4)$$

With regard to these relationships, we find the form of the third term in H_{eff},

$$PV(H_0 - E_0)^{-1}(PV - V)P$$
$$= P\sum_{fmg\sigma}\left(\frac{t_{fm}t_{mg}}{U}\right)(X_f^{\sigma 0}X_m^{\bar{\sigma}\sigma}X_g^{0\bar{\sigma}} - X_f^{\sigma 0}X_m^{\bar{\sigma}\bar{\sigma}}X_g^{0\sigma})P. \quad (5)$$

Addition of the first two terms from Eq. (3) leads to the following structure of H_{eff}:

$$H_{\text{eff}} = \sum_{f\sigma}(\epsilon - \mu)X_f^{\sigma\sigma} + \sum_{fm\sigma} t_{fm}X_f^{\sigma 0}X_m^{0\sigma}$$
$$+ \sum_{fmg\sigma}\left(\frac{t_{fm}t_{mg}}{U}\right)(X_f^{\sigma 0}X_m^{\bar{\sigma}\sigma}X_g^{0\bar{\sigma}} - X_f^{\sigma 0}X_m^{\bar{\sigma}\bar{\sigma}}X_g^{0\sigma}).$$

In this equation, the projection operator is omitted, because the Hilbert subspace of states without doubles is invariant with respect to the action of H_{eff}. Among others, the last summand in H_{eff} contains terms with $f = g$, which, taken together with the two first terms of H_{eff}, give the Hamiltonian of the t–J model

$$H_{t-J} = \sum_{f\sigma}(\epsilon - \mu)X_f^{\sigma\sigma} + \sum_{fm\sigma} t_{fm}X_f^{\sigma 0}X_m^{0\sigma}$$
$$+ \frac{1}{2}\sum_{fm\sigma} J_{fm}(X_f^{\sigma\bar{\sigma}}X_m^{\bar{\sigma}\sigma} - X_f^{\sigma\sigma}X_m^{\bar{\sigma}\bar{\sigma}}). \quad (6)$$

Thus, H_{eff} (thereafter H_{t-J^*}) can be written as

$$H_{t-J^*} = H_{t-J} + H_{(3)},$$
$$H_{(3)} = \sum_{\substack{fmg\sigma \\ f\neq g}}\left(\frac{t_{fm}t_{mg}}{U}\right)(X_f^{\sigma 0}X_m^{\bar{\sigma}\bar{\sigma}}X_g^{0\bar{\sigma}} - X_f^{\sigma 0}X_m^{\bar{\sigma}\bar{\sigma}}X_g^{0\sigma}). \quad (7)$$

Let us discuss the differences between H_{t-J^*} for the metallic phase and for the case of half-filling. At $n = 1$, each site is occupied by one electron. Therefore, the Hilbert subspace for H_{t-J^*} represents a set of homopolar states, when not only doubles but holes as well are absent. In this case, the projection operator can be written as $P = \Pi_f(X_f^{\uparrow\uparrow} + X_f^{\downarrow\downarrow})$, and, to a given accuracy, H_{t-J^*} is reduced to the Heisenberg model [5]. On the other hand, if $n < 1$, holes are present in the system. Therefore, electron hopping processes (the second term in Eq. (6)) and three-center interactions $H_{(3)}$ are included in H_{t-J^*}.

It is evident from Eq. (7) that the parametric smallness of three-center interactions $H_{(3)}$ is the same as for the exchange part of the t–J model, but it is considerably lower than for the kinetic part. This fact explains the smallness of the effect of $H_{(3)}$ on the spectral properties of the system in the normal phase [2, 3].

The situation is different when a superconducting state with the d-type symmetry of the order parameter (OP) is formed. In this case, the coupling constant in the superconducting phase $J \sim t^2/U$ is of the same order of magnitude as three-center interactions. This is why one should expect that $H_{(3)}$ will strongly affect superconductivity with the d-type symmetry of OP. Below, the truth of this statement will be confirmed by numerical calculations.

3. Two methods were used in the solution of the problem. In the first case, the diagram technique for the Hubbard operators [6, 7] was generalized to the case where three-center interaction is taken into account. In the second approach, the apparatus of two-time irreducible Green's functions was used in the same way as in the consideration of the t–J in [8, 9]. Self-consistent equations obtained within the above methods coincide completely.

The linearized system of equations for normal and anomalous Green's functions is reduced to the standard form of the Gor'kov equations:

$$(E - \tilde{\epsilon}_{\mathbf{k}} + \mu)\langle\langle X_{\mathbf{k}\sigma}|X_{\mathbf{k}\sigma}^+\rangle\rangle$$
$$- \Delta_{\mathbf{k}}\langle\langle X_{-\mathbf{k}\bar{\sigma}}^+|X_{\mathbf{k}\sigma}^+\rangle\rangle = 1 - n/2,$$
$$-(\Delta_{\mathbf{K}})^*\langle\langle X_{\mathbf{k}\sigma}|X_{\mathbf{k}\sigma}^+\rangle\rangle$$
$$+ (E + \tilde{\epsilon}_{\mathbf{k}} - \mu)\langle\langle X_{-\mathbf{k}\bar{\sigma}}^+|X_{\mathbf{k}\sigma}^+\rangle\rangle = 0. \quad (8)$$

In Eq. (8), the renormalized electron spectrum $\tilde{\epsilon}_{\mathbf{k}}$ is described by the equation

$$\tilde{\epsilon}_{\mathbf{k}} = \epsilon - \frac{n^2}{4}\frac{1 - n/4}{1 - n/2}J_0 + \left(1 - \frac{n}{2}\right)t_{\mathbf{k}} - \frac{n}{2}\left(1 - \frac{n}{2}\right)\frac{t_{\mathbf{k}}^2}{U}$$
$$- \frac{1}{N}\sum_{\mathbf{q}}\left\{t_{\mathbf{q}} + \frac{n}{2}J_{\mathbf{k}-\mathbf{q}} + [(2-n)t_{\mathbf{k}} + (1-n)t_{\mathbf{q}}]\frac{t_{\mathbf{q}}}{U}\right\}n_{\mathbf{q}\sigma}, \quad (9)$$

where the Fourier transform of the hopping integral $t_{\mathbf{q}} = 2t(\cos q_x + \cos q_y)$ is written in the nearest neighbor

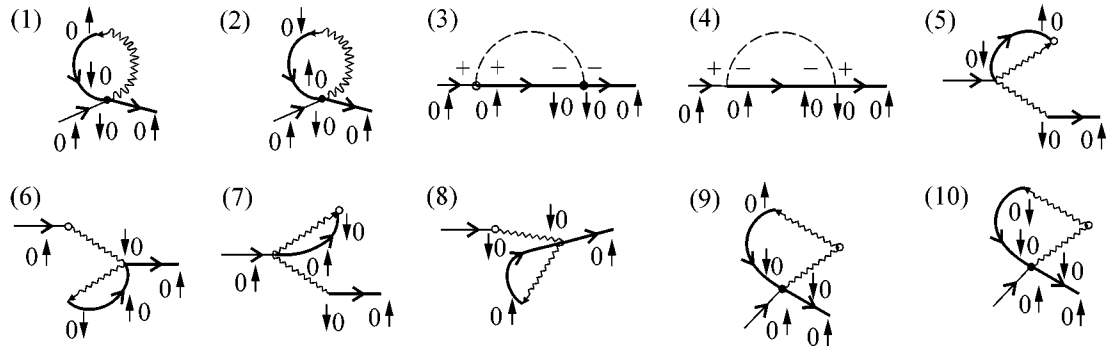

Fig. 1. Diagrams for the anomalous component of the mass operator in the *t–J** model.

approximation, $J_{\mathbf{q}} = (2t/U)t_{\mathbf{q}}$, and $n_{\mathbf{q}\sigma}$ is determined by the equation

$$n_{\mathbf{q}\sigma} = \frac{E_{\mathbf{q}} - \xi_{\mathbf{q}}}{2E_{\mathbf{q}}} + \frac{\xi_{\mathbf{q}}}{E_{\mathbf{q}}}(\exp(E_{\mathbf{q}}/T) + 1)^{-1}, \qquad \xi_{\mathbf{q}} = \tilde{\varepsilon}_{\mathbf{q}} - \mu. \tag{10}$$

Here, $E_{\mathbf{q}} = \sqrt{(\tilde{\varepsilon}_{\mathbf{q}} - \mu)^2 + |\Delta_{\mathbf{q}}|^2}$ is the spectrum of quasiparticle excitations, and $\Delta_{\mathbf{q}}$ designates the OP of the superconducting state.

To demonstrate the relative role of three-center interactions, the contributions of the mass operator $\Sigma_{0\uparrow,\downarrow 0}(\mathbf{p}, \omega_n)$ to the component are given. This contribution determines the superconducting order parameter. Ten graphs are shown in Fig. 1, whose analytical expressions in total determine

$$\Sigma_{0\uparrow,\downarrow 0}(\mathbf{p}, \omega_n) = -\frac{T}{N} \times \sum_{\mathbf{q}\omega_m} [2t_{\mathbf{q}} + (J_{\mathbf{p}+\mathbf{q}} + J_{\mathbf{p}-\mathbf{q}}) + A_{\mathbf{q}}^{(3)}] G_{0\uparrow,\downarrow 0}(\mathbf{p}, \omega_m), \tag{11}$$

$$A_{\mathbf{q}}^{(3)} = \left(1 - \frac{n}{2}\right)\frac{4t_{\mathbf{p}}t_{\mathbf{q}}}{U} - n\left(\frac{t_{\mathbf{q}}^2}{U} - \frac{J_0}{2}\right) - \left(1 - \frac{n}{2}\right)(J_{\mathbf{p}+\mathbf{q}} + J_{\mathbf{p}-\mathbf{q}}).$$

In Eq. (11), the contribution $\sim 2t_{\mathbf{q}}$ originates from the first two graphs and determines the kinematic mechanism [10]; the term in round brackets reflects the contribution determined by the third and fourth graphs [7] and is responsible for the magnetic mechanism of the *t–J* model. Finally, the term $\sim A_{\mathbf{q}}^{(3)}$ is induced by three-center interactions $H_{(3)}$ and is determined by the last six graphs in Fig. 1.

The last term in $\sim A_{\mathbf{q}}^{(3)}$ is the most significant factor for the *d*-symmetry OP. It leads in the total $\Sigma_{0\uparrow,\downarrow 0}$ to the renormalization of the coupling constant by the scenario $J \longrightarrow J[1 - (1 - n/2)] = (n/2)J$. It is this renormalization that determines the strong effect of $H_{(3)}$ on the formation of superconductivity with the *d* symmetry of OP. The self-consistent equation for OP can be found in the conventional way:

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

There are two things distinguishing this equation from the corresponding equation for the *t–J* model. First, additional terms appear, which can be easily distinguished by the explicit dependence on the parameter *U*. The second distinction is more important and is associated with the renormalization of the coefficient before the terms $J_{\mathbf{k}\pm\mathbf{q}}$ indicated above.

4. Within the nearest neighbor approximation, the equation for OP possesses solutions differing in the symmetry types of the order parameter $\Delta_{\mathbf{k}}$. The solution with the *s* type of symmetry $\Delta_{\mathbf{k}} = \Delta_0$ does not obey the sum rule [9] and is not considered here. The solution with the *d* symmetry of OP $\Delta_{\mathbf{k}} = \Delta_0(\cos k_x - \cos k_y)$ is of prime interest. In this case, the equations for determining the temperature dependence $\Delta_0(T)$ and for calculating the critical temperature T_c can be written as follows:

$$1 = \frac{nJ}{2N}\sum_{\mathbf{q}}\frac{(\cos q_x - \cos q_y)^2}{E_{\mathbf{q}}}\tanh\left(\frac{E_{\mathbf{q}}}{2T}\right), \qquad 1 = \frac{nJ}{2N}\sum_{\mathbf{q}}\frac{(\cos q_x - \cos q_y)^2}{\tilde{\varepsilon}_{\mathbf{q}} - \mu}\tanh\left(\frac{\tilde{\varepsilon}_{\mathbf{q}} - \mu}{2T_c}\right). \tag{12}$$

The results of the numerical solution of the equation for T_c are given in Fig. 2 at various *n* for the *t–J** model (curve *2*). For comparison, the dependence of T_c on the electron concentration obtained without regard for $H_{(3)}$ is also given in this figure (curve *1*). The numerical cal-

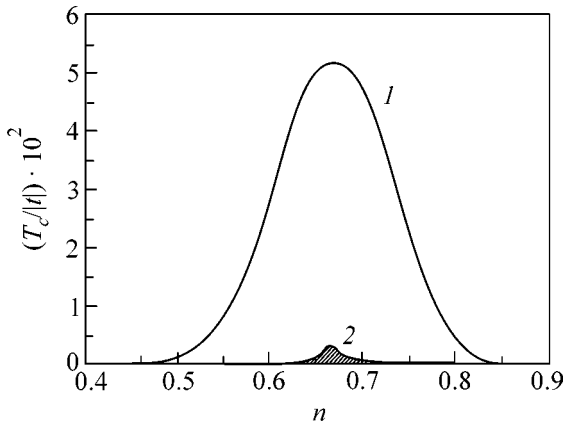

Fig. 2. Regions of the superconducting state in the (*1*) *t–J* and (*2*) *t–J** models.

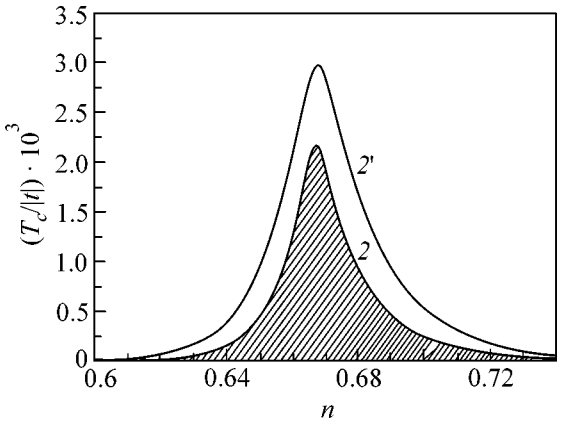

Fig. 3. Variations of T_c caused by the renormalization of the spectrum due to $H_{(3)}$.

culations were performed under the assumption that the ratio $2|t|/U$ equals 0.25. It is evident that the inclusion of $H_{(3)}$ leads to a significant decrease in the superconducting transition temperature (hatched region).

The decrease in the critical temperature caused by $H_{(3)}$ is due to two factors. The first (and the main) factor is in the renormalization of the coupling constant. The second factor is the additional renormalization of the electron energy spectrum. In order to demonstrate the role of the second factor, Fig. 3 displays (on an enlarged scale as compared with Fig. 2) the critical temperature in the *t–J** model as a function of electron concentration both with regard for the contributions of $H_{(3)}$ to the renormalization of the electron spectrum (curve *2*) and without these contributions (curve *2*'). It is evident that the second factor affects T_c much more weakly.

Figure 4 shows the dependence of T_c on the ratio $2|t|/U$ obtained without regard for three-center interactions (curve *1*) and with regard for these interactions (curve *2*). The electron concentration in the plots corresponds to the optimal doping level ($n = 0.665$). It is evident that, at $2|t|/U = 0.25$ (dashed lines), T_c obtained taking into account the effect of $H_{(3)}$ is 25 times smaller than T_c calculated without taking the three-center interactions into account.

5. In order to demonstrate clearly the physical nature of the renormalization of the coupling constant by three-center interactions obtained in this work, consider the action of the H_{t-J} and $H_{(3)}$ operators on a singlet pair. If there are no other electrons, the state of a system with this pair is described by the ket vector

$$|\psi(f, f+\Delta)\rangle = \frac{1}{\sqrt{2}}(X_f^{\uparrow 0}X_{f+\Delta}^{\downarrow 0} - X_f^{\downarrow 0}X_{f+\Delta}^{\uparrow 0})|0\rangle,$$

where $|0\rangle$ is the state without electrons. This pair corresponds to an eigenvector of H_{t-J}

$$H_{t-J}|\psi(f, f+\Delta)\rangle = (2\epsilon - 4t^2/U)|\psi(f, f+\Delta)\rangle.$$

After the action of $H_{(3)}$ on the singlet pair, a superposition of states is obtained:

$$H_{(3)}|\psi(f, f+\Delta)\rangle = (-2t^2/U)$$

$$\times \sum_{\Delta_1 \neq -\Delta} \{|\psi(f, f+\Delta_1)\rangle + |\psi(f+\Delta+\Delta_1, f+\Delta)\rangle\}.$$

It is evident that the effect of $H_{(3)}$ is reduced to rotations through the angles $\pi/2$, π, and $3\pi/2$ of the singlet pair under consideration around sites f and $f+\Delta$. It is essential that the energy parameter in this case equals $-2t^2/U$. Because of this, when the right-hand side of the last equation is written in the form that does not contain the restriction $\Delta_1 \neq \Delta$ (one has to make an operation of this

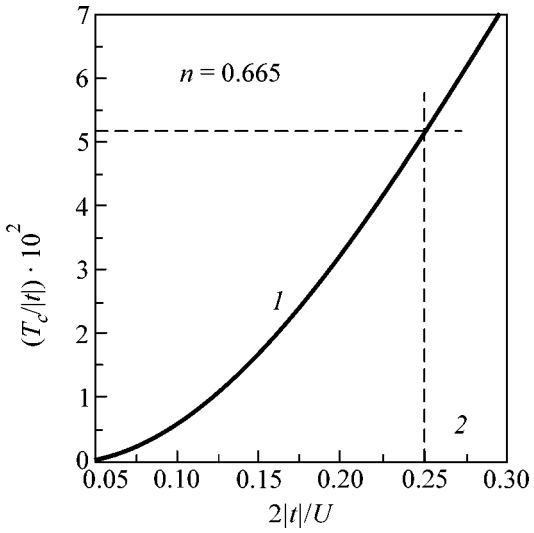

Fig. 4. Effect of $H_{(3)}$ on the dependence of T_c on the parameter $2t/U$.

kind when passing on to the Fourier representation), the term $(+4t^2/U)|\psi(f, f + \Delta)\rangle$ should be added, and this term fully compensates the action of the exchange part of the Hamiltonian H_{t-J}. Thus, it can be seen that three-center interactions make a significant contribution to the dynamics of singlet pairs, whose formation underlies the mechanism of superconducting pairing. Therefore, in the case where the system contains only one singlet pair, one can talk about the full compensation of the corresponding two-center terms of the effective Hamiltonian. If the system contains other electrons, three-center terms act in such a way that the states arising because of changes in the lattice sites adjacent to the singlet pair under consideration start to make a contribution to the resulting superposition. These additional contributions increase as electrons fill the sites adjacent to the pair. These circumstances explain the appearance of the concentration factor, which leads to the renormalization of the coupling constant mentioned above.

We note in conclusion that the analysis performed unambiguously points to the essential role of three-center interactions in the formation of a superconducting state with the *d*-type symmetry of OP. Since it was found that without $H_{(3)}$ $T_c \sim 100$ K at typical values of parameters [2], we found, with regard to these terms, that $T_c \sim 4$ K for the same parameters.

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