

Cooper Instability of Nonlocal Spin Polarons in the CuO_2 Plane of High-Temperature Superconductors

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The energy structure of nonlocal spin polarons has been obtained for the real structure of the CuO_2 plane of cuprate superconductors in the ensemble of such Fermi quasiparticles. A nonlocal spin polaron is formed due to the exchange interaction of the spin of an oxygen hole with the spins of the two nearest copper ions. The scattering amplitude of nonlocal spin polarons in the cooper channel calculated using the diagrammatic technique indicates that the spin and charge degrees of freedom are strongly correlated.

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1. After the discovery of the high-temperature superconductivity, it has been found that the physical properties of the normal and superconducting phases of copper oxides are primarily determined by the features of the electronic structure of the CuO_2 plane and the copper instability is formed because of strong correlations between the charge and spin degrees of freedom [1–4]. To describe these correlations in the tight binding regime between the spin and electron subsystems, the spin-polaron concept of the electronic structure of the CuO_2 plane was developed [5]. A number of features of variation of the physical properties of cuprates with an increase in the doping degree (e.g., the pseudogap behavior of the spectral intensity [6] and the concentration dependence of the transition temperature to the superconducting phase [7]) were described in this approach.

In the mentioned work, the theory was developed with the Hamiltonian of the 2D Kondo lattice, under the assumption that the spin of a hole is exchange-coupled with only one localized spin.

In reality, the hole located on an oxygen ion in the CuO_2 plane interacts with two copper ions through the p - d exchange (see Fig. 1). This fact was mentioned in [8] and was taken into account in [9], where the evolution of the Fermi surface in the normal phase was described. In this work, we analyze the appearance of the Cooper instability under the conditions when Fermi quasiparticles are nonlocal spin polarons.

It is known that the Hamiltonian of the Emery model describing the electronic structure of the CuO_2 plane is reduced in the regime of strong electron cor-

relations to the Hamiltonian, in which copper ions are described by homopolar states with the spin $S = 1/2$. These states are represented in Fig. 1 as thick arrows in the circles. The configuration of the arrows corresponds to the Néel phase. The upper electronic states of the oxygen subsystem are shown in the form of p_x and p_y orbitals. A hole in such an orbital interacts with the two spins of the nearest copper ions through the p -

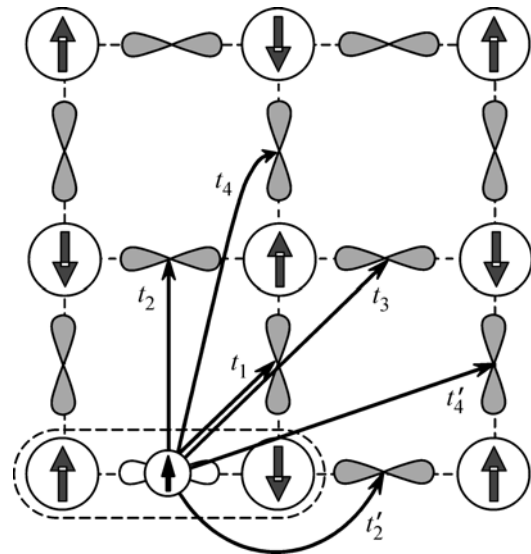


Fig. 1. Role of the structure of the CuO_2 plane in the formation of the nonlocal spin polaron. The arrows indicate used hops of holes over the oxygen subsystem.

d exchange. The position of this hole is shown in the lower left corner of Fig. 1. It is important that the mean-field contribution to the energy of the hole from the interaction with the neighboring spins of copper atoms is zero, because of the antiferromagnetic coupling between the spins of copper ions in the nonlocal spin polaron. For this reason, quantum fluctuations in the spin subsystem are of particular importance from the very beginning of the construction of nonlocal spin polarons.

2. In the atomic representation, the effective Hamiltonian of the spin-fermion system of the CuO_2 plane can be represented in the form

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{T} + \hat{V}, \quad (1)$$

where

$$\begin{aligned} \hat{\mathcal{H}}_0 &= \sum_f (\varepsilon - \mu) X_f^{22} + \sum_g (\varepsilon - \mu) Y_g^{22} \\ &+ A \sum_{f\Delta_f} (\mathbf{S}_{f+\Delta_f} \cdot \boldsymbol{\sigma}_f) + A \sum_{g\Delta_g} (\mathbf{S}_{g+\Delta_g} \cdot \boldsymbol{\sigma}_g), \\ \hat{T} &= \sum_{ff'\gamma} t_{ff'} X_f^{2\gamma} X_{f'}^{\gamma 2} + \sum_{gg'\gamma} t_{gg'} Y_g^{2\gamma} Y_{g'}^{\gamma 2} \\ &+ \sum_{fg\gamma} t_{fg} (X_f^{2\gamma} Y_g^{\gamma 2} + Y_g^{2\gamma} X_f^{\gamma 2}), \\ \hat{V} &= \frac{1}{2} \sum_{l,l'} I_{ll'} (\mathbf{S}_l \cdot \mathbf{S}_{l'}) + \frac{J}{2} \sum_{\langle fg \rangle \gamma} (X_f^{\gamma \bar{\gamma}} Y_g^{\bar{\gamma} \gamma} - X_f^{\gamma \gamma} Y_g^{\bar{\gamma} \bar{\gamma}}). \end{aligned}$$

Here, $\hat{\mathcal{H}}_0$ includes the diagonal part of the energy of the oxygen subsystem in the Vanier representation and the p - d exchange interaction of oxygen holes with the spin of copper ions, ε , corresponds to a change in the energy of the oxygen ion in the transition from the p^5 configuration to the p^6 configuration, and μ is the chemical potential of the system. From here on, we use the two-sublattice description of the oxygen subsystem, where ions the p_x and p_y orbitals refer to the F sublattice with sites f, f' , and f'' and to the G sublattice with sites g, g' , and g'' , respectively. The Hubbard operators $X^{\alpha\beta} = |\alpha\rangle\langle\beta|$ and $Y^{\alpha\beta} = |\alpha\rangle\langle\beta|$ ($\alpha, \beta = \uparrow, \downarrow, 2$) refer to the F and G oxygen subsystems, respectively. Each of such operators describes the transition of the ion from the $|\beta\rangle$ state to the $|\alpha\rangle$ state. The parameter A in $\hat{\mathcal{H}}_0$ specifies the energy of the p - d exchange interaction of the spin of the hole with the spins of neighboring copper atoms and $\boldsymbol{\sigma}_f(\boldsymbol{\sigma}_g)$ is the vector operator of the spin of the hole at site $f(g)$. The vector operators of the spins of the copper ions are denoted as $\mathbf{S}_{f+\Delta_f}$ and $\mathbf{S}_{g+\Delta_g}$, where the vector $\Delta_f = \pm a_x/2$ couples

site f with one of the nearest sites, where a copper ion is located. Similarly, the vector $\Delta_g = \pm a_y/2$ couples site g (the oxygen ion with the p_y orbital) with the nearest of two copper sites. The kinetic energy operator \hat{T} describes the hops of electrons over the oxygen ions both within the $F(G)$ sublattices with the tunneling integrals $t_{ff'}$ ($t_{gg'}$) and between sublattices with the integrals t_{fg} . The first term in \hat{V} corresponds to the energy of the exchange interaction between the spins of the nearest copper ions located at the l th and l' th sites. The second term presents the exchange coupling between the nearest oxygen ions, such as the exchange interaction in the t - J model. The exchange coupling constants are denoted as $I_{ll'}$ and J , respectively.

3. According to the spin-polaron concept, the parameter A of the p - d exchange interaction is the largest energy parameter of the system. For this reason, single-site energies of holes on oxygen ions should be calculated with the exact inclusion of quantum spin fluctuations caused by the strong p - d exchange interaction of the spin of the hole with the two spins of the nearest two copper atoms. Such an inclusion leads to the renormalization of the local Green's function $G(i\omega_n)$. The calculation of the renormalized function $\tilde{G}(i\omega_n)$ is reduced to the calculation of the local mass and force operators in the zeroth approximation in the hopping parameters and J .

For simplicity, we present below the solution of this problem on the basis of the exact solution of the equations of motion. The first exact equation of motion for the operator $X^{\gamma 2}$ has the form

$$\begin{aligned} (\omega - \varepsilon + \mu) X^{\gamma 2} &= -(A/2) d_\gamma, \\ d_\gamma &\equiv S^\alpha \sigma_{v\gamma}^\alpha X^{\gamma 2}. \end{aligned} \quad (2)$$

Here, repeated indices imply summation; $\sigma_{v\gamma}^\alpha$ are the components of the Pauli matrix σ^α , where $\alpha = x, y, z$; and the site index is omitted (it remains unchanged in the problem under consideration and, hence, it can be temporarily omitted). For the same reason, it is convenient to introduce the vector operator of the total spin $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$, which is the sum of the spins of the two copper ions nearest to the given oxygen ion.

The second exact equation of motion for the operator d_γ has the form

$$(\omega - \varepsilon - A/2 + \mu) d_\gamma = -(3A/4) X^{\gamma 2} - A \Lambda_\gamma, \quad (3)$$

where $\Lambda_\gamma = (\mathbf{S}_1 \cdot \mathbf{S}_2) X^{\gamma 2}$. The operator Λ_γ satisfies the third exact equation of motion

$$(\omega - \varepsilon + \mu) \Lambda_\gamma = -(A/8) d_\gamma. \quad (4)$$

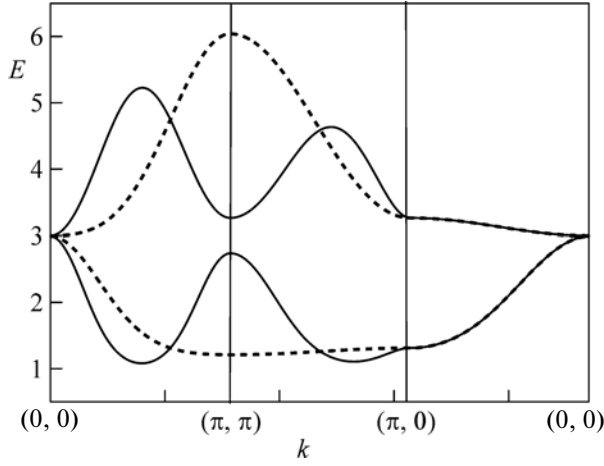


Fig. 2. Spectrum of the upper bands of polaron excitations ($\varepsilon = 0$). The solid and dashed lines are obtained with $t_4 = 0.45$ and 0 , respectively.

With the use of the resulting system of three equations, it is easy to represent the following explicit expression for the renormalized function $\tilde{G}(i\omega_n)$:

$$\tilde{G}(i\omega_n) = P_0(i\omega_n)/(i\omega_n - \varepsilon + \mu - \Sigma_0(i\omega_n)). \quad (5)$$

Here, the local force and mass operators have the form

$$P_0(i\omega_n) = C_h + A \frac{AC_1^{dd}C_h/2 - C_1^{dp}(i\omega_n - \varepsilon + \mu)}{\varphi(i\omega_n)},$$

$$\Sigma_0(i\omega_n) = (3/8)A^2(i\omega_n - \varepsilon + \mu)/\varphi(i\omega_n),$$

where

$$\varphi(i\omega_n) = (\omega_n - \varepsilon + \mu)(i\omega_n - \varepsilon + \mu - A/2) - A^2/8.$$

Here, $C_h = 1 - h/2$, where h is the number of holes per oxygen ion; $C_1^{dd} = \langle (\mathbf{S}_1 \cdot \mathbf{S}_2) \rangle$ and $C_1^{dp} = \langle (\mathbf{S}_1 \cdot \boldsymbol{\sigma}) \rangle$ are the spherically symmetric spin correlation functions between the nearest copper–copper and copper–oxygen sites, respectively.

After the analytic continuation of Eq. (5), the spectrum of localized Fermi excitations degenerate in the spin projection and ordinal number of the oxygen orbital is obtained in the form

$$E_1 = \varepsilon - A/2, \quad E_2 = \varepsilon, \quad E_3 = \varepsilon + A. \quad (6)$$

4. The inclusion of hops leads to the formation of energy bands, which can be calculated by the diagrammatic technique for the Hubbard operators [10, 11]. Since the concentration of holes h per oxygen ion in the weak doping region is low, the spin-polaron spectrum can be calculated in the approximation of independent quasiparticles. In view of the presence of two sublattices in the oxygen subsystem, we write the Dyson equation in the matrix form

$$\hat{G}(k) = \hat{g}(k) + \hat{g}(k)\hat{\Sigma}(k)\hat{G}(k), \quad (7)$$

where $k = (\mathbf{k}, i\omega_n)$,

$$\hat{G}(k) = \begin{pmatrix} G^{(11)}(k) & G^{(12)}(k) \\ G^{(21)}(k) & G^{(22)}(k) \end{pmatrix},$$

$$\hat{g}^{-1}(k) = \text{diag}(i\omega_n - \varepsilon + \mu, i\omega_n - \varepsilon + \mu),$$

and the mass operator irreducible in Dyson's sense in the Hubbard-I approximation has the form

$$\hat{\Sigma}(k) = \begin{pmatrix} \Sigma_0 + P_0 t_{\mathbf{k}}^{(1)} & P_0 \Gamma_{\mathbf{k}} \\ P_0 \Gamma_{\mathbf{k}} & \Sigma_0 + P_0 t_{\mathbf{k}}^{(2)} \end{pmatrix}. \quad (8)$$

Here, $t_{\mathbf{k}}^{(1)}$, $t_{\mathbf{k}}^{(2)}$, and $\Gamma_{\mathbf{k}}$ are the Fourier transforms of the hopping integrals t_{ff} , t_{gg} , and t_{fg} , respectively; and Σ_0 and P_0 are functions of $i\omega_n$.

Solving Eq. (7), we obtain the components of the matrix Green's function

$$G^{(11)}(k) = (i\omega_n - \varepsilon + \mu - \Sigma_0 - P_0 t_{\mathbf{k}}^{(2)})/\det(k),$$

$$G^{(22)}(k) = (i\omega_n - \varepsilon + \mu - \Sigma_0 - P_0 t_{\mathbf{k}}^{(1)})/\det(k), \quad (9)$$

$$G^{(12)}(k) = G^{(21)}(k) = P_0 \Gamma_{\mathbf{k}}/\det(k),$$

where

$$\det(k) = (i\omega_n - \varepsilon + \mu - \Sigma_0 - P_0 \tilde{t}_{\mathbf{k}}^+) \quad (10)$$

$$\times (i\omega_n - \varepsilon + \mu - \Sigma_0 - P_0 \tilde{t}_{\mathbf{k}}^-),$$

$$\tilde{t}_{\mathbf{k}}^{\pm} = \frac{t_{\mathbf{k}}^{(1)} + t_{\mathbf{k}}^{(2)}}{2} \pm \frac{1}{2} \sqrt{(t_{\mathbf{k}}^{(1)} - t_{\mathbf{k}}^{(2)})^2 + 4\Gamma_{\mathbf{k}}}. \quad (11)$$

Therefore, the six branches of the spectrum of collective excitations $E_{j,\mathbf{k}}^{\pm}$ ($j = 1, 2, 3$) are obtained as the solutions of two third-order dispersion equations

$$\omega - \varepsilon + \mu - \Sigma_0(\omega) - P_0(\omega) \tilde{t}_{\mathbf{k}}^{\pm} = 0. \quad (12)$$

Two upper branches of the electron spectrum of the spin-polaron states are shown in Fig. 2, which demonstrates the strong effect of the hopping integral t_4 on these branches. The choice of the model parameters for the CuO_2 plane is ambiguous. This important problem was discussed, e.g., in [6]. We performed calculations with the exchange parameters $A = 2.5$ and $J = 2$. From here on, energies are measured in the units of the hopping integral t_1 . To obtain the dispersion relations corresponding to the ARPES data, we took into account three more hopping parameters $t_2 = -0.5$, $t_3 = -0.2$, and $t_4 = 0.45$, in addition to t_1 (see Fig. 1). For simplicity, we set $t_2' = t_2$ and $t_4' = t_4$. The

correlation functions were chosen as $C_1^{dd} = 0.23$ and $C_1^{dp} = -0.43$, which are different from the respective nominal values $C_1^{dd} = 1/4$ and $C_1^{dp} = -1/2$ for an individual nonlocal polaron, because hops weaken magnetic correlations.

The upper part of Fig. 3 shows the density of states of spin-polaron fermions calculated for the aforementioned model parameters and $h = 0.2$. The dotted line shows the chemical potential. The comparison with the bare density of states obtained at $A = 0$ (the lower part of Fig. 3) shows that six rather than two bands appear when the p - d exchange interaction is taken into account. The fractions of the spectral weight that correspond to three bands, which are broadened local levels, are given in the figure.

5. To determine the Cooper instability, we calculated the scattering amplitude of charge carriers owing to the exchange interaction in the oxygen subsystem (the second term in the operator \hat{V}).

Figure 4 graphically presents the system of equations for this amplitude in the Cooper channel. Symbols m , n , and l mark sublattices 1 and 2 and an overbar means a change in the ordinary number of the sublattice; i.e., if $n = 1$ (2), then $\bar{n} = 2$ (1). Closed squares correspond to the vertex functions $\Gamma^{(21)}(\mathbf{k}|\mathbf{p})$ and $\Gamma^{(12)}(\mathbf{k}|\mathbf{p})$, which are specified by the sequence of the propagators referring to different sublattices: the first and second propagators in the vertex with superscript (21) correspond to the second and first sublattices, respectively, whereas this sequence for the vertex with superscript (12) is opposite. The lines with the arrows present the Green's functions with the corresponding indices given by Eqs. (9). The open and closed arrows correspond to the propagators of the quasiparticles with up and down spins, respectively. The bare vertices are defined in Fig. 5.

The system of equations graphically shown in Fig. 4 has the form ($q = (\mathbf{q}, i\omega_m)$)

$$\Gamma^{(\bar{n}n)}(\mathbf{k}|\mathbf{p}) = -\frac{1}{2}\Gamma_{\bar{n}n; 12}^{(0)}(\mathbf{k}|\mathbf{p}) + \frac{T}{2N} \sum_{q, m, l} \Gamma_{\bar{n}n; m\bar{m}}^{(0)}(\mathbf{k}|\mathbf{q}) G^{(\bar{m}l)}(-q) G^{(ml)}(q) \Gamma^{(l)}(\mathbf{q}|\mathbf{p}). \quad (13)$$

Here, $\Gamma_{\bar{n}n; m\bar{m}}^{(0)}(\mathbf{k}|\mathbf{q}) = \delta_{nm} J_{\mathbf{k}-\mathbf{q}} + \delta_{n\bar{m}} J_{\mathbf{k}+\mathbf{q}}$. In other words, if $m = n$, the function $\Gamma^{(0)}$ is the first bare vertex in Fig. 5; otherwise, this function is the second bare vertex. Since the Fourier transform of the exchange interaction $J_{\mathbf{k}}$ is independent of the frequency ω_n , $\Gamma^{(\bar{n}n)}$ are also independent of the frequency. To solve system (13), it is convenient to define the symmetric

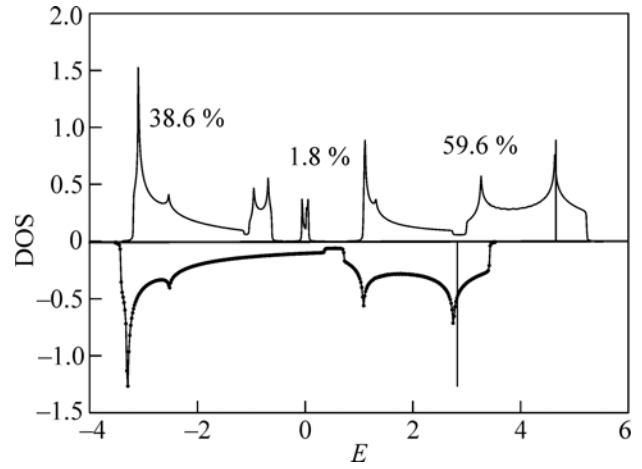


Fig. 3. Densities of states for (upper part) polarons and (lower part) strongly correlated holes at $A = 0$.

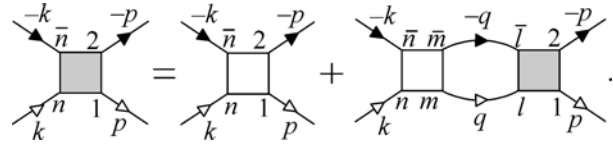


Fig. 4. Diagrams of the system of equations of the scattering amplitude of quasiparticles in the Cooper channel.

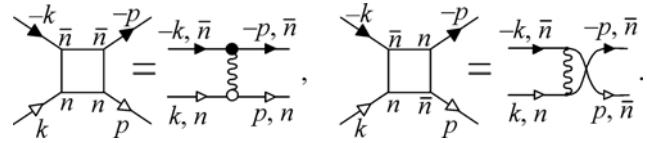


Fig. 5. Diagrams for the bare vertices.

and antisymmetric combinations of the vertices $\Gamma^{(\pm)} = \Gamma^{(21)} \pm \Gamma^{(12)}$. For these vertices, Eq. (13) yields

$$\Gamma^{(\pm)}(\mathbf{k}|\mathbf{p}) = -J^{(\pm)}(\mathbf{k}, \mathbf{p}) + \frac{1}{N} \sum_{\mathbf{q}} J^{(\pm)}(\mathbf{k}, \mathbf{q}) L^{(\pm)}(\mathbf{q}) \Gamma^{(\pm)}(\mathbf{q}|\mathbf{p}). \quad (14)$$

Here, $J^{(\pm)}(\mathbf{k}, \mathbf{p}) = (J_{\mathbf{k}-\mathbf{p}} \pm J_{\mathbf{k}+\mathbf{p}})/2$ and, following [12], we introduced the function

$$L^{(\pm)}(\mathbf{q}) = T \sum_{\omega_m} (G^{(11)}(q) G^{(22)}(-q) \pm G^{(12)}(-q) G^{(21)}(q)), \quad (15)$$

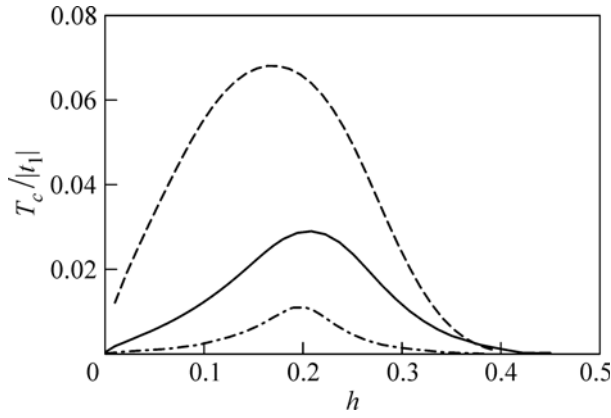


Fig. 6. Concentration dependences of the critical temperature for the d -type symmetry of the order parameter.

after the summation over the Matsubaru frequencies, this function is given by the expression

$$L^{(\pm)}(\mathbf{q}) = \sum_{l=1, s=\pm}^3 \frac{\tanh(E_{lq}^s/2T_c)}{\prod_{j=1, (j \neq l)}^3 ((E_{lq}^s)^2 - (E_{jq}^s)^2)} \times \frac{\Phi^{(\pm)}(E_{lq}^s)}{2E_{lq}^s \prod_{r=1}^3 ((E_{lq}^s)^2 - (E_{rq}^s)^2)}, \quad (16)$$

where

$$\begin{aligned} \Phi^{(\pm)}(\omega) &= -\varphi(\omega)\varphi(-\omega) \{ \pm a(\omega)a(-\omega)\Gamma_{\mathbf{q}}^2 \\ &+ [(\omega - \varepsilon - \mu)(\varphi(\omega) - 3A^2/8) - a(\omega)t_{\mathbf{q}}^{(1)}] \\ &\times [(-\omega - \varepsilon - \mu)(\varphi(-\omega) - 3A^2/8) - a(-\omega)t_{\mathbf{q}}^{(2)}] \}, \\ a(\omega) &= C_h(\varphi(\omega) + C_1^{dd}A^2/2) - AC_1^{dp}(\omega - \varepsilon - \mu). \end{aligned}$$

Since $J(\mathbf{q}) = 4J\cos(\mathbf{q}_x/2)\cos(\mathbf{q}_y/2)$, then

$$\begin{aligned} J^{(+)}(\mathbf{k}, \mathbf{p}) &= 4J \{ \cos(k_x/2)\cos(k_y/2)\cos(p_x/2)\cos(p_y/2) \\ &+ \sin(k_x/2)\sin(k_y/2)\sin(p_x/2)\sin(p_y/2) \}, \\ J^{(-)}(\mathbf{k}, \mathbf{p}) &= 4J \{ \cos(k_x/2)\sin(k_y/2)\cos(p_x/2)\sin(p_y/2) \\ &+ \sin(k_x/2)\cos(k_y/2)\sin(p_x/2)\cos(p_y/2) \}. \end{aligned} \quad (17)$$

Thus, the kernels of Eqs. (14) are split and the solutions of these equations are written in the form

$$\Gamma^{(+)}(\mathbf{k}|\mathbf{p}) = \cos(k_x/2)\cos(k_y/2)C^{(+)}(\mathbf{p})$$

$$+ \sin(k_x/2)\sin(k_y/2)S^{(+)}(\mathbf{p}), \quad (18)$$

$$\begin{aligned} \Gamma^{(-)}(\mathbf{k}|\mathbf{p}) &= \cos(k_x/2)\sin(k_y/2)C^{(-)}(\mathbf{p}) \\ &+ \sin(k_x/2)\cos(k_y/2)S^{(-)}(\mathbf{p}). \end{aligned}$$

Here, the functions $C^{(\pm)}$ and $S^{(\pm)}$ satisfy a simple system of algebraic equations.

The substitution of solutions in the form of Eqs. (18) into Eqs. (14) provides the expressions determining the poles of the scattering amplitude and giving the following three independent equations for the critical temperature of the superconducting transition corresponding to various types of the symmetry of the superconducting order parameter:

$$1 = 4J \frac{1}{N} \sum_{\mathbf{q}} \sin^2\left(\frac{q_x}{2}\right) \sin^2\left(\frac{q_y}{2}\right) L^{(+)}(\mathbf{q}),$$

$$1 = 4J \frac{1}{N} \sum_{\mathbf{q}} \cos^2\left(\frac{q_x}{2}\right) \cos^2\left(\frac{q_y}{2}\right) L^{(+)}(\mathbf{q}), \quad (19)$$

$$1 = 4J \frac{1}{N} \sum_{\mathbf{q}} \cos^2\left(\frac{q_x}{2}\right) \sin^2\left(\frac{q_y}{2}\right) L^{(-)}(\mathbf{q}).$$

The solid line in Fig. 6 shows the $T_c(n)$ dependence for the d -type symmetry (the first equation in Eqs. (19)), which was obtained by solving the equation for T_c for the same parameters as those in the calculation of the spectrum of Fermi excitations. It is seen that the concentration dependence of the critical temperature corresponds to the experimental data for cuprate superconductors. To demonstrate the effect of spin correlation functions, the concentration dependence of T_c calculated at $C_1^{dd} = C_1^{dp} = 0$ is shown by the dashed line in Fig. 6. The comparison with the solid line indicates that the inclusion of correlation functions leads to a strong decrease in the maximum T_c value and a shift of the position of the maximum. The dash-dotted line was calculated with a change only in the parameter of the p - d exchange interaction, $A = 4$. It is seen that an increase in A is accompanied by a decrease in T_c .

6. The results reported above indicate that the presence of the strong coupling between the spins of copper ions and oxygen holes leads to the strong rearrangement of the energy spectrum of Fermi quasiparticles. When two oxygen orbitals in one cell are taken into account, the total spectrum includes six bands. When the total spectral weight of all bands remains unchanged, the spin weight of each band depends on the spin state of the localized subsystem. Such a dependence is manifested through the magnetic correlation functions C_1^{dd} and C_1^{dp} . The calculations were performed with a positive C_1^{dd} value, since the appear-

ance of the nonlocal spin polaron at $A \gg I$ is accompanied by a change in the sign of C_1^{dd} , because the energy minimum corresponds to the case where the spins of copper ions have the same orientation opposite to the spin of the hole. Without the hole on the oxygen ion, the correlation function C_1^{dd} between the spins of copper ions nearest to this oxygen ion is negative. Therefore, the appearance of the hole on the oxygen ion qualitatively changes the spin configuration of the nearest copper ions. Such a change in the configuration in the process of the formation of the nonlocal spin polaron is an important mechanism of the destruction of the Néel phase under doping.

The possibility of a doping-induced change in the spin state of copper ions was mentioned in the first works on the theory of the electronic structure of cuprates. The change in the spin configuration of the copper ion was attributed to the formation of the Zhang–Rice singlet, because of the effective exchange interaction of the spins of one copper ion and the hole located on the nearest four oxygen ions [13].

In our case, the situation is significantly different and involves the simultaneous inclusion of the exchange coupling of the spin of the oxygen hole with the spins of two copper ions in the nearest vicinity of this hole. This is responsible for the formation of the nonlocal spin polaron. As a result, there is a significant difference in the action on the spin state of copper ions: the appearance of the nonlocal spin polaron is accompanied by the induction of strong correlations both between the spin of the oxygen hole and two spins of copper ions and between the spins of these copper ions, leading to the destruction of the antiferromagnetic coupling and to the formation of the ferromagnetic coupling between them. In the case of the formation of the Zhang–Rice singlet, correlation appears only between the spin of one copper ion and the spin of the oxygen hole. Correlation between the spins of copper ions is absent.

Since the superconducting transition temperature was determined from the analysis of the scattering amplitude in the Cooper channel for a normal phase, the relation important in applications between the critical temperature and the superconducting order parameter at zero temperature cannot be found from the equations obtained. To determine this parameter, it is necessary to use the equations describing the superconducting phase. The derivation of such equa-

tions taking into account nonlocal spin polarons will be performed elsewhere.

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