

Effective Hamiltonian and Properties of the Normal and Superconducting Phases of n -Type Cuprates

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Received March 11, 2004; in final form, May 24, 2004

An effective low-energy Hamiltonian is derived from a microscopic multiband p - d model in the regime of strong electron correlations. The parameters of the p - d model are determined by comparison with the ARPES data for undoped Nd_2CuO_4 . The Hamiltonian is the t - J^* model in which hopping and exchange slowly decay with distance and are taken into account up to the fifth coordination sphere. The quasiparticle band structure is calculated as a function of the doping concentration with regard to short-range magnetic order, and the superconductivity theory with the spin-fluctuation pairing mechanism is constructed. Assuming that the parameters of the model do not depend on the doping level, we obtained quantitative agreement with the properties observed experimentally for the normal and superconducting phases without introducing fitting parameters.
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PACS numbers: 74.20.Mn; 74.72.Jt; 74.25.-q

1. There exist two types of high- T_c superconductors: the p type, that is, hole-doped cuprates ($\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (LSCO), etc.) and the n type, that is, electron-doped cuprates ($\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$ (NCCO), $\text{Pr}_{2-x}\text{Ce}_x\text{CuO}_4$ (PCCO), etc.). Though cuprates of these two types contain the base element of high- T_c superconductors, namely, the CuO_2 plane, their properties differ substantially (see, for example, [1, 2]). In this work, a quantitative theory has been constructed to describe the dependence of the properties of the normal phase and the critical temperature $T_c(x)$ on the electron concentration x in n -type superconductors. The theory contains no fitting parameters. The effective Hamiltonian in the form of the t - J^* model has been derived from the microscopic multiband p - d model in the regime of strong electron correlations (SECs). The parameters of the model have been determined from experimental data for undoped Nd_2CuO_4 . The spin-fluctuation mechanism of superconductivity in the t - J model has long been known. However, details of the effective Hamiltonian such as the slow decrease of interatomic hoppings and exchange interaction with distance (five coordination spheres have been taken into account) and the occurrence of weakly correlated hoppings (three-center interactions, whose importance for determining T_c was noted in [3]) have proved to be of fundamental importance in obtaining quantitative agreement for $T_c(x)$ and for the properties of the normal phase. Taking into account short-range antiferromagnetic (AFM) order has also been found to be critical for determining the quasiparticle dispersion law, leading to the appearance

of additional Van Hove singularities. Agreement with experimental data for the electronic structure of the normal phase and for $T_c(x)$ has been obtained only with allowance made simultaneously for all these details.

As for the symmetry of the order parameter, recent experimental data (phase-sensitive experiments [4] and resistance measurements in magnetic fields [5] in NCCO, measurements of the penetration depth in PCCO [6, 7], and angular-resolved photoemission spectroscopy (ARPES) measurements [8]) point to the d type of the order parameter (most likely, $d_{x^2-y^2}$). Therefore, we will further investigate the superconducting state only with the $d_{x^2-y^2}$ symmetry type.

2. The multiband p - d model [9] is an adequate model for the description of high- T_c superconductivity in cuprates [9]. The use of this model with strong electron correlations taken into account within the framework of the generalized tight-binding method made it possible to achieve quantitative agreement with the ARPES data for undoped LSCO [10–12], to describe the pinning of $\mu(x)$ in the p -type superconductors and its absence in the n -type superconductors [13], and to obtain an indirect optical gap in NCCO [14]. To consider the superconducting phase, an effective low-energy Hamiltonian for the multiband p - d model was obtained in [15] using operator perturbation theory. The effective Hamiltonian is asymmetric with respect to electron and hole doping: the conventional t - J model is appropriate for p -type systems, whereas the effective singlet–triplet model is an adequate model for p -type

systems with a complex band structure at the valence band top. It was shown in [3] that the inclusion of the three-center terms in the effective Hamiltonian plays a very significant part in the consideration of the superconducting phase. With regard to the aforesaid, the effective Hamiltonian for n -type superconductors including three-center terms can be written using the Hubbard operators as follows:

$$H_{t-J^*} = H_{t-J} + H_3,$$

$$H_{t-J} = \sum_{f,\sigma} (\varepsilon_1 - \mu) X_f^{\sigma\sigma} + \sum_{\langle f,g \rangle, \sigma} t_{fg}^{00} X_f^{\sigma 0} X_g^{0\sigma} + \sum_{\langle f,g \rangle} J_{fg} \left(\mathbf{S}_f \mathbf{S}_g - \frac{1}{4} n_f n_g \right), \quad (1)$$

$$H_3 = \sum_{\langle f,g,m \rangle, \sigma} \frac{t_{fm}^{0S} t_{mg}^{0S}}{E_{ct}} (X_f^{\sigma 0} X_m^{\bar{\sigma}\sigma} X_g^{0\bar{\sigma}} - X_f^{\sigma 0} X_m^{\bar{\sigma}\sigma} X_g^{0\bar{\sigma}}).$$

Here, $J_{fg} = 2(t_{fg}^{0S})^2/E_{ct}$ is the exchange integral, $E_{ct} \approx 2$ eV is the charge-transfer gap (an analogue of the Hubbard term U), and t_{fg}^{NM} are the hopping integrals corresponding to the annihilation of a quasiparticle in the state M and its creation in the state N . The Hamiltonian parameters in Eq. (1) are expressed through microscopic parameters of the p - d model (see [16], where a set of microscopic parameters and the corresponding model parameters for n -type cuprates are also given). The distance dependence of the exchange and hopping integrals is known, and the subsequent calculations in this work were performed with the inclusion of all the integrals up to the fifth coordination sphere. The parameters were obtained by comparison with the ARPES data for undoped NCCO. Subsequently, they were considered fixed and independent of the doping level.

When the model given by Eq. (1) was applied to the nonmagnetic phase, the equations-of-motion method was used within the generalized Hartree-Fock approximation [17]. In this case, correlators of the $\langle X_f^{\sigma\sigma} X_g^{\sigma'\sigma'} \rangle$ and $\langle X_f^{\sigma\bar{\sigma}} X_g^{\bar{\sigma}\sigma} \rangle$ types arise. Decoupling of the Hubbard I type would lead to the following results:

$$\langle X_f^{\sigma\sigma} X_g^{\sigma'\sigma'} \rangle \longrightarrow \langle X_f^{\sigma\sigma} \rangle \langle X_g^{\sigma'\sigma'} \rangle = n_p^2,$$

$$\langle X_f^{\sigma\bar{\sigma}} X_g^{\bar{\sigma}\sigma} \rangle \longrightarrow \langle X_f^{\sigma\bar{\sigma}} \rangle \langle X_g^{\bar{\sigma}\sigma} \rangle = 0,$$

where n_p are the occupation numbers of the single-particle state. However, spin fluctuations are completely neglected in the case of such decoupling, whereas their consideration crucially affects the calculated properties of both the superconducting and normal phases (see, for example, [18, 19]). Therefore, we will use the fol-

lowing decoupling scheme that takes into account spin fluctuations beyond the Hubbard I approximation:

$$\langle X_f^{\sigma\sigma} X_g^{\sigma'\sigma'} \rangle \longrightarrow n_p^2 + \frac{\sigma}{\sigma'} \frac{1}{2} C_{fg},$$

$$\langle X_f^{\sigma\bar{\sigma}} X_g^{\bar{\sigma}\sigma} \rangle \longrightarrow C_{fg}.$$

Here, $C_{fg} = \langle X_f^{\sigma\sigma} X_g^{\bar{\sigma}\sigma} \rangle = 2 \langle S_f^z S_g^z \rangle$ are spin correlation functions.

The spin correlators C_{fg} were calculated using the two-dimensional t - J model of the CuO_2 plane. The self-energy equations with Green's functions constructed on Hubbard operators were obtained using the Mori formalism, which allows these functions to be represented as continuous fractions. The elements of the fractions for the electron and spin Green's functions contain correlators for close sites, and residual members of the fractions are many-particle Green's functions. The latter are approximated by decoupling corrected by the introduction of a vertex correction [20, 21]. This correction is determined from the condition that the site magnetization is zero in the paramagnetic state under consideration. This condition, the self-energy equations for the electron and spin Green's functions, and the self-consistency conditions for correlators form a closed system, which was solved by iterations at a fixed chemical potential and a fixed temperature. For small clusters and in the undoped case, the results of calculations [22, 23] are in good agreement with the data of the exact diagonalization and the Monte Carlo method. The spin correlators used in this work were obtained from the spin Green's function calculated within this self-consistent approach on a 20×20 lattice.

It was shown in [23] that the damping of quasiparticles $\Gamma_k = -\text{Im} \Sigma_k(\omega = 0)$, where $\Sigma_k(\omega)$ is the self-energy part, is large in the vicinity of points $(0, 0)$ and (π, π) . In the subsequent calculations, we broadened the spectral peaks in the vicinity of these points by artificially introducing Γ_k . The value of Γ_k itself was taken from [24]. It should be noted that, as calculations showed, the damping of quasiparticles introduced in this way weakly affect such integral characteristics as chemical potential $\mu(x)$ and superconducting transition temperature $T_c(x)$.

3. The dispersion curves and corresponding densities of states calculated for the paramagnetic nonsuperconducting phase are shown in Fig. 1 for the t - J and t - J^* models with and without regard for spin correlators. It is evident that the inclusion of three-center terms leads to a strong change at the conduction band top, that is, will have an effect at low doping levels x . In the AFM phase, there is a symmetry in the spectrum of the t - J model in the vicinity of the $(\pi/2, \pi/2)$ and $(\pi, 0)$ points (see Fig. 1). Such a symmetry does not exist in the paramagnetic phase. However, the inclusion of spin

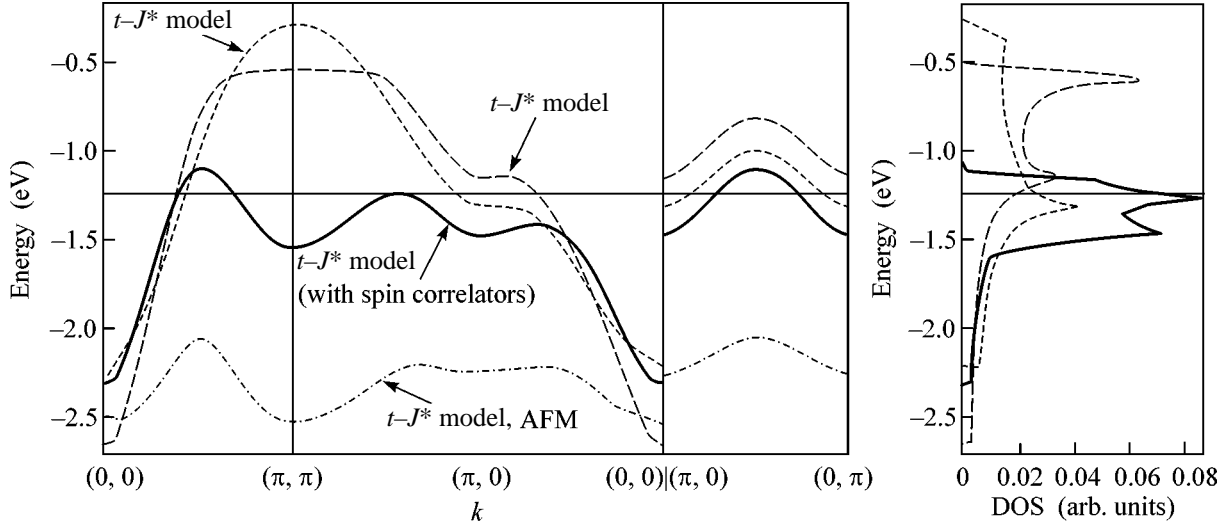


Fig. 1. Dispersion curves along the principal directions of the Brillouin zone and the density of states in the paramagnetic phase in the t - J (dotted line) and t - J^* (dashed line) models in the Hubbard I approximation and in the t - J^* model with the inclusion of spin correlators (heavy solid line). The solid horizontal line indicates the chemical potential calculated self-consistently for the latter model. The spectrum of the t - J model in the AFM phase is also shown (dash-dot line).

correlators C_{fg} results in a tendency toward the restoration of symmetry in the points mentioned above.

The dependence $\mu(x)$ is shown in Fig. 2. It is seen that the theoretical calculation is in perfect agreement with the experimental data [13] shown in the same figure; in particular, the pinning of the chemical potential is absent. The experimental [25] and calculated Fermi surfaces (black heavy shading and light solid line) for optimally doped ($x_{\text{opt}} = 0.15$) NCCO are shown in the inset in the same figure. Only one cross section is observed experimentally. Because of the occurrence of a pseudogap, spectral peaks differ in intensity along this section. In the theory considered here, there are two cross sections of the Fermi surface. However, because the damping of quasiparticles strongly depends on the momentum, the second section falls in the region of large Γ_k (this region is shown by a light solid line in the figure). This is why the second section should virtually not be observed experimentally. In light of the above, it may be argued that the calculated and experimental Fermi surfaces are in good agreement.

4. Now, when we see that the t - J^* model with the approximation considered above gives good agreement with the experimental data for the nonsuperconducting phase, we pass to the consideration of the superconducting phase. The equations for the superconducting order parameter Δ_k obtained in this work are completely similar to those given in [3, 26]; therefore, we will not write them here. Note only that, first, the coupling constant of the superconducting phase is substantially renormalized as a result of taking into account three-center terms [3]. Second, because we take into account the hopping and exchange integrals up to the fifth coordi-

nation sphere, the order parameter in the case of the $d_{x^2-y^2}$ symmetry type takes the form [26]

$$\Delta_k = \sum_{m=1}^2 \Delta_m (\cos(mk_x a) - \cos(mk_y a)). \quad (2)$$

The experimental data for NCCO and PCCO [1, 2] and the theoretical dependences of the superconducting

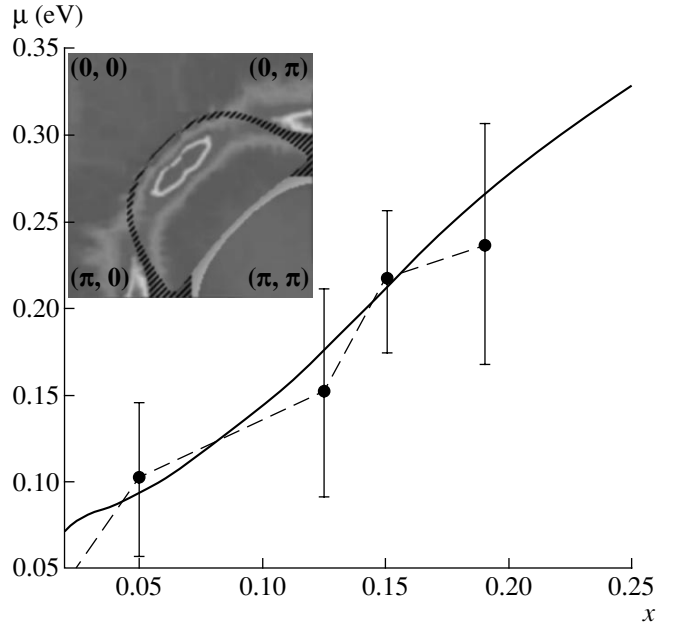


Fig. 2. Chemical potential μ as a function of the doping level x in the t - J^* model with the inclusion of spin correlators (solid line); the dashed line connects experimental points [13]. The inset shows the experimental [25] and calculated Fermi surfaces for $\text{Nd}_{1.85}\text{Ce}_{0.15}\text{CuO}_4$.

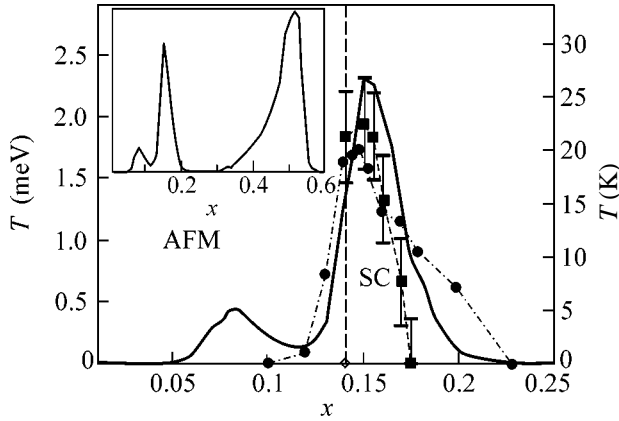


Fig. 3. Phase diagram for n -type cuprates: the theoretically calculated dependence $T_c(x)$ (heavy solid line) and experimental dependences $T_N(x)$ for NCCO (dashed line; the AFM and paramagnetic phases are on the left and on the right of this line), $T_c(x)$ for NCCO (dashed line with black squares), and $T_c(x)$ for PCCO (dash-dot line with black circles). The inset shows the theoretically calculated dependence $T_c(x)$ for a wider concentration range.

transition temperature $T_c(x)$ obtained in this work are compared in Fig. 3. Note that the experimental errors shown in the figure are associated with differences in sample quality rather than the accuracy of the determination of the superconducting transition temperature. The inset shows the same theoretical dependence $T_c(x)$ but for a wider concentration range. Two pronounced maxima of T_c at $x = 0.15$ and $x = 0.53$, as well as a weak maximum at $x = 0.08$, are quite evident. The additional maximum at small x in the t - J^* model with self-consistently calculated spin correlators was first obtained in [27].

The observed dependence is easily understood from simple physical considerations. In the superconductivity theory of the BCS type, there exists the relationship $T_c \propto \exp(-1/N(\epsilon_F)V)$, where $N(\epsilon_F)$ is the density of states at the Fermi level ϵ_F and V is the effective attraction. It is evident that a maximum in $T_c(x)$ will be reached when the chemical potential falls on a Van Hove singularity. In the case of neglecting spin correlators in the t - J model, only one Van Hove singularity associated with the flat portion of the dispersion curve at the $(\pi, 0)$ point. As is known, in this case in the nearest neighbor approximation, $x_{\text{opt}} = 0.33$, and, with regard for more than three coordination spheres, $x_{\text{opt}} = 0.53$ —a maximum in $T_c(x)$ is also seen at this concentration in the inset in Fig. 3. With the inclusion of three-center terms (t - J^* model), an additional singularity appears because of the flat dispersion in the region of the (π, π) point. However, this point corresponds to the conduction band bottom. Therefore, the chemical potential falls on this singularity only at very small $x \leq 0.07$, that is, in the region where the carrier mobility is low and the short-range AFM order is still high. This

leads to the fact that the superconducting state becomes energetically unfavorable. However, in the t - J^* model with the inclusion of spin correlators, an additional singularity arises at -1.25 eV because of the saddle point at $(\pi, 0.4\pi)$ (see Fig. 1). This singularity is responsible for the maximum in $T_c(x)$ at $x \approx 0.15$. It is on this singularity that the chemical potential falls at the optimal doping level. This is the reason why the distance between the position of μ and the Van Hove singularity corresponding to the plateau in the dispersion curve at the $(\pi, 0)$ point equals $\Delta E_{\text{VH}} = 0.27$ eV. This is in good agreement with the experimental value ≈ 0.25 – 0.35 eV [14, 28]. In contrast to the n type, ΔE_{VH} in all the p -type cuprates is small and less than 0.03 eV. Note that the weak maximum in $T_c(x)$ at $x = 0.08$ is associated with the shoulder (kink) in the density of states at -1.2 eV (see Fig. 1). Moreover, because the energy of the AFM phase is lower than the energy of the normal and superconducting phases, this weak maximum and the entire part of $T_c(x)$ lying in the region of $x < 0.14$ below the experimentally observed Neel temperature $T_N(x)$ will not be revealed in the experiment.

5. Thus, in the framework of an effective model for n -type high- T_c superconductivity and simple physical approximations based on the inclusion of spin fluctuations beyond the Hubbard I approach, we obtained quantitative agreement with such experimental data as the evolution of the chemical potential with the doping level, the Fermi surface for optimally doped NCCO, and the dependence $T_c(x)$. Though analogous results for the dependence $T_c(x)$ were obtained previously in the framework of the FLEX approximation [29], the approach used in this work is characterized by physical transparency and by the fact that it explicitly takes into account the effects of strong electron correlations, which play a very important role in high- T_c superconductors. It is shown that the physical mechanisms responsible for the concentration dependence $T_c(x)$ in n -type cuprates are different from those in the p -type cuprates. Namely, because of spin fluctuations, the system tends to restore AFM ordering. In this case, the dispersion curve is transformed in such a way that it forms flat portions in the vicinity of the $(\pi, 0.4\pi)$ point (and points symmetrical with respect to it). This leads to the formation of an additional Van Hove singularity. Because of this transformation of the density of states, an additional superconducting “dome” arises at x of order 0.15 in good agreement with experimental results. Note once again that this study was free of fitting parameters: all the parameters of the effective model are unambiguously connected with the microscopic parameters of the multiband p - d model. These microscopic parameters were determined in our previous studies by comparison with the ARPES data for undoped AFM cuprates.

As for the electron-phonon interaction, which was not taken into account in this work, there are indications that this interaction is weak in n -type high- T_c

superconductors. The first indication is that the isotope effect is almost completely absent [30]. The second indication is the absence of a kink in the $(0, 0) \rightarrow (\pi, \pi)$ direction [31]. This is in sharp contrast with p -type high- T_c superconductors, where the appearance of a kink is considered as the manifestation of strong electron–phonon interaction.

We are grateful to V.V. Val'kov, V.F. Gantmakher, D.M. Dzebisashvili, E.G. Maksimov, and G.M. Éliashberg for discussions of the results of this study. This work was supported by INTAS (project no. 01-0654), ETF (project no. 5548), the Russian Foundation for Basic Research (project no. 03-02-16124), Federal Target Program Integration (project no. B0017), the Quantum Macrophysics Program of the Siberian Branch of the Russian Academy of Science (Lavrent'ev competition of young researchers' projects), Dynasty Foundation, and The International Centre for Fundamental Physics in Moscow.

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Translated by A. Bagatur'yants