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# Effective Hamiltonian and the properties of normal and superconductive phases of n-type cuprates

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**Abstract**

In the framework of the effective low-energy model for high-$T_c$ cuprates with account for three-center interaction terms and spin fluctuations the properties of normal and superconducting phases of n-type cuprates are investigated. Microscopic model parameters were obtained from ARPES data in undoped compounds. Obtained evolution of the chemical potential with doping, Fermi surface at optimal doping, and $T_c(x)$ phase diagram are in remarkably good agreement with the experiment.


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High-$T_c$ superconducting cuprates (HTSC) consist of two major classes—p-type class which stands for hole-doped ($La_{2-x}Sr_xCuO_4$—LSCO etc.) and n-type class which stands for electron-doped cuprates ($Nd_{2-x}Ce_xCuO_4$—NCCO, $Pr_{2-x}Ce_xCuO_4$—PCCO etc.). Despite the similar crystal structure and the presence of the common to all HTSC base element, the $CuO_2$-plane, experimentally observed properties of these two classes are quite different [1–3].

The adequate model for high-$T_c$ cuprates is the multiband p–d model [5]. Investigations of the normal phase of cuprates within this model in the framework of the generalized tight-binding (GTB) method with account for strong electron correlations gave results in quantitative agreement with ARPES data in LSCO [6] and NCCO [7]. In order to investigate the superconductive (SC) phase, the low-energy effective Hamiltonian for the

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multiband p–d model was obtained [8]. Effective Hamiltonian is asymmetric for electron and hole doping—for n-type system the usual t–J model takes place while for p-type systems with complicated band structure at the top of the valence band the proper model is the effective singlet-triplet model. In paper [9] it was shown that the influence of three-center interaction terms in the effective model could be crucial for the SC phase. Therefore, the effective Hamiltonian for n-type cuprates should have the form of the t–J model with the three-center interaction terms (t–J* model). All parameters of the effective Hamiltonian depend on microscopic parameters of the p–d model (see paper [10] where the set of microscopic and corresponding model parameters for n-type cuprates are presented). Microscopic parameters were obtained for undoped NCCO and in the further study they are fixed and considered doping independent. Since dependence of model parameters on distance is known from the explicit construction of Wannier states in the $CuO_2$ unit cell [7], the following calculations are performed with inclusion of the hoppings $t$ and exchanges $J$ up to the 5th coordination sphere. According to the recent experimental data [4] in the present work we will consider only $d_{x^2-y^2}$-pairing symmetry.

The effective model was investigated in the framework of the equation of motion method in the generalized Hartree–Fock approximation. To solve obtained equations we have used decoupling that includes short-range magnetic order beyond Hubbard I approximation: $\langle X_f^{\sigma\sigma} X_g^{\sigma'\sigma'}\rangle \to n_p^2 + \frac{\sigma}{\sigma'}\frac{1}{2} C_{fg}$, $\langle X_f^{\sigma\bar{\sigma}} X_g^{\bar{\sigma}\sigma}\rangle \to C_{fg}$. Here, $n_p$ is the occupation factors of the one-particle state, $C_{fg} = \langle X_f^{\sigma\bar{\sigma}} X_g^{\bar{\sigma}\sigma}\rangle = 2\langle S_f^z S_g^z\rangle$ are the spin correlation functions which were self-consistently calculated from the spin Green's functions in the 2D $t$–$J$ model of $CuO_2$-plane [11].

In the left inset in Fig. 1 the dependence $\mu(x)$ is shown. Our theoretical calculations are in very good agreement with experimental data [3] presented in the same figure. In particular, the $\mu(x)$

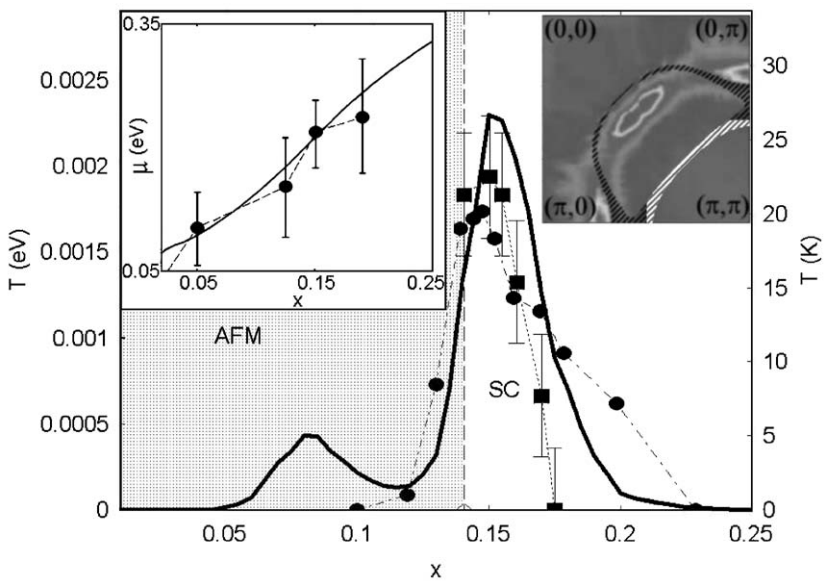


Fig. 1. The calculated dependence $T_c(x)$ (bold solid line), experimentally obtained dependences $T_N(x)$ (dashed line separates AFM phase on the left and paramagnetic phase on the right) and $T_c(x)$ for NCCO [1] (the dotted curve with filled squares) and $T_c(x)$ for PCCO [2] (the dash-dotted curve with filled circles) are presented. The left inset—the chemical potential $\mu$ vs. the doping $x$ in the t–J* model (the solid curve) and in the experiment [3] (filled circles with error bars connected by the dashed curve). The right inset—experimental [12] (the grayscale plot) and theoretically calculated (black and white dashed lines, white color is used where the quasiparticle decay rate is high) Fermi surfaces of $Nd_{1.85}Ce_{0.15}CuO_4$.

pinning is absent. In the right inset in Fig. 1 the experimental [12] (grayscale plot) and calculated (black and white dashed lines) Fermi surfaces are shown for optimally doped NCCO ($x_{opt} = 0.15$). In our theory there are two Fermi surface cuts, but due to the strong momentum dependence of the quasiparticle decay rate [11] the second cut falls into the area of large $\Gamma_k = -\mathrm{Im}\Sigma_k(\omega)$ (this part is shown in the inset by white dashed lines). That is why this second cut is not observed in the ARPES experiment. Thus, there is a good agreement between the calculated and experimental Fermi surfaces.

Interplay of spin fluctuations and three-center interaction terms gives tendency to restore antiferromagnetic (AFM) symmetry of the Brillouin zone—the local symmetry around $(\pi/2, \pi/2)$ and $(\pi, 0)$ appeared in dispersion due to the short-range order. This leads to the appearance of the saddle point around $(\pi, 0.4\pi)$, which gives an additional Van-Hove singularity. This singularity gives an additional "dome" of superconductivity at low doping with maximum $T_c(x)$ with $x_{opt} \approx 0.15$ (see Fig. 1). The well-known "dome" of superconductivity (which is not shown here) at higher concentrations with $x_{opt} \approx 0.53$ is due to another Van-Hove singularity corresponding to the saddle point at $(\pi, 0)$. These results could be qualitatively explained as follows. In the BCS theory $T_c \propto \exp(-1/N(\varepsilon_F)V)$, where $N(\varepsilon_F)$ is the density of states at the Fermi level $\varepsilon_F$, and $V$ is the effective attraction. If there is a singularity in the density of states then upon doping $\varepsilon_F$ will reach this singularity and there will be a maximum in $T_c(x)$. In the t–J* model with proper account for spin correlations, additional Van-Hove singularity appears due to saddle point around $(\pi, 0.4\pi)$. It is the singularity where the chemical potential is situated at optimal doping. Due to this fact the calculated distance between position of $\mu$ and Van-Hove singularity, corresponding to plateau around $(\pi, 0)$, is $\Delta E_{VH} = 0.27\,\mathrm{eV}$, that is very close to experimentally observed 0.25–0.35 eV in n-type cuprates [13]. Note that the weak maximum in $T_c(x)$ around $x = 0.08$ comes from minor details (shoulder) in the density of states. Moreover, this weak maximum and the part of $T_c(x)$ at concentrations $x < 0.14$ below the experimentally observed Néel temperature $T_N(x)$ must not be revealed in the experiment.

Summarizing, we have formulated a quantitative theory of high-$T_c$ superconductivity in electron-doped cuprates. This theory describes a number of properties of the n-type high-$T_c$ cuprates in the normal and superconducting states in good agreement with the experiment.

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