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ORIGINAL PAPER

Quantum Phase Transitions and Superconductivity in Single- and Two-Layer Cuprates in the Multiband Theory of Hubbard Fermions

S.G. Ovchinnikov · M.M. Korshunov · I.A. Makarov · E.I. Shneyder

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Abstract We consider the doping dependence of the normal and superconducting properties of $La_2Sr_{2-x}CuO_2$ and $YBa_2Cu_3O_7$ in the low energy effective model based on the ab initio LDA+GTB calculations. With doping we have found a concentration region with electronic instability of the uniform state. We have shown that two quantum phase transitions (QPT) of the Lifshitz type correspond well to the experimental phase diagram. For superconducting state we have considered both magnetic and phonon mechanisms of pairing.

Keywords Strong electron correlations · Fermi surface reconstruction

1 Introduction

A complexity of the high-temperature superconductivity materials stems from several reasons. Among them there are strong electron correlations (SEC), strong electron–phonon interaction, strong fluctuations of different possible order parameters due to low dimension, strong *p-d* hybridization of copper and oxygen orbitals. In the normal phase the mystery of the pseudogap state is still unsolved. Fluctuations of spin density wave, charge density wave, orbital current state and superconducting gap are competing mechanisms to form the pseudogap state. Here we discuss one more mechanism of the electron instability. It is of pure electronic origin and results from a non-rigid band behavior of the electronic structure calculated by LDA+GTB method designed in our group to study band structure of materials with SEC [1]. The short range antiferromagnetic correlation functions determine the self-energy of the Hubbard fermions band within the LDA+GTB approach. A self-consistent calculation of the electronic structure and spin correlation functions in a spin liquid regime [2] results in the doping dependent band structure of $La_2Sr_{2-x}CuO_2$ and $YBa_2Cu_3O_{7-y}$. A transformation of the Fermi surface with doping from weakly doped Mott insulator to Fermi liquid normal metal occurs via two (for single CuO_2 layer LaSrCuO) or three (for two-layer cuprates like YBCO or Bi2212) Lifshitz type quantum phase transitions. There relation to the electronic instability will be discussed in this paper.

2 Electronic Structure of High-T_c Cuprates in the LDA+GTB Approach

Due to effects of SEC the conventional LDA calculations failed for undoped and underdoped region of the phase diagram. Our LDA+GTB is the hybrid method. It starts with the LDA calculations, then Wannier functions are constructed for some set of orbitals and the parameters of the multiband tight binding *p-d* model are calculated. The second step is the multielectron cluster perturbation (generalized tight binding) approach with the exact diagonalization of all intracell interactions and perturbation treatment of the intercell hopping and interactions [3]. The Hubbard

S.G. Ovchinnikov (✉) · M.M. Korshunov · I.A. Makarov · E.I. Shneyder
L.V. Kirensky Institute of Physics, Siberian Branch of Russian Academy of Sciences, 660036 Krasnoyarsk, Russia
e-mail: sgo@iph.krasn.ru

S.G. Ovchinnikov · M.M. Korshunov
Siberian Federal University, 660041 Krasnoyarsk, Russia

S.G. Ovchinnikov · I.A. Makarov · E.I. Shneyder
Reshetnev Siberian State Aerospace University, 660014 Krasnoyarsk, Russia

X-operators constructed with the help of the cell exact multielectron eigenstates are very useful tool for the cluster perturbation theory. The minimal realistic model for high-T_c cuprates should incorporate both $d_{x^2-y^2}$- and $d_{3z^2-r^2}$-orbitals and hybridization with b_{1g}, a_{1g} and p_z oxygen molecular orbitals to get both in-plane and out-of-plane polarized states in the Fermi energy density of states (DOS) found by XAS [4]. These orbitals were involved in the LDA+GTB calculations [1]. The effective Hamiltonian depends on the energy scale. To study ARPES with the binding energy $1 \div 2$ eV the two-band singlet–triplet t–J model is required, while to study the Fermi surface the effective t–t'–t''–J^* model has been derived and its parameters calculated from the ab initio approach [1, 2]. For the two-layer cuprates additional interplane hopping parameter $t_\perp$ is incorporated [5]. We have used the Mori–Zwanzig projection method (see [6, 7]) to calculate electronic Green function in the Hubbard X-operator representation. A self-energy has been obtained in the non-crossing approximation, and at low temperature we have neglected the time dynamics $\Sigma(k,\omega) \to \Sigma(k)$. Finally, for the two-layer cuprate we get the electron dispersion [8]. The spin correlation functions have been calculated self-consistently following [2, 9]. The evolution of the Fermi surface in $La_2Sr_{2-x}CuO_2$ has been discussed in [2]. It appears that transformation from underdoped to overdoped cuprates requires two Lifshitz type quantum phase transitions (QPT) [10]. The first one at $x_{c1} = 0.15$ results in a log singularity in the DOS at ε_F and determined the maximum in the $T_c(x)$ (optimal doping). The second one at $x_{c2} = 0.24$ separate the non-Fermi liquid region (pseudogap state) at $x < x_{c2}$ from the Fermi liquid normal metal at $x > x_{c2}$.

3 Doping Dependence of the Electronic Structure

Effect of the bilayer splitting for the two-layer cuprates makes the Fermi surface evolution with doping more complicate (Fig. 1). The bilayer splitting of small hole pockets in Fig. 1a results in two similar QPT at $x'_{c1} = 0.135$ (Fig. 1b) and $x''_{c1} = 0.165$ (Fig. 1d). At these QPT small hole pockets centered near $(\pi/2, \pi/2)$ transform into two large pockets centered in (π, π). The larger one is a hole pocket while the smaller one is the electron pocket. With doping increase the electronic pocket has collapsed at the critical point $x_{c2} \approx 0.25$. The effect of the bilayer splitting on the QPT at x_{c2} is negligible small due to the doping dependence of $t_\perp$ and $C_\perp$. The dependence of the chemical potential on the hole concentration is shown in Fig. 2. Electronic concentration $n = 1 - x$, so the region $0.135 < x < 0.25$ where $\partial\mu/\partial x > 0$ corresponds to condition of the electronic instability $\partial n/\partial x < 0$. Thus we have obtained the result that the existence of both hole and electron's Fermi surfaces and electronic instability take place in the same doping region.

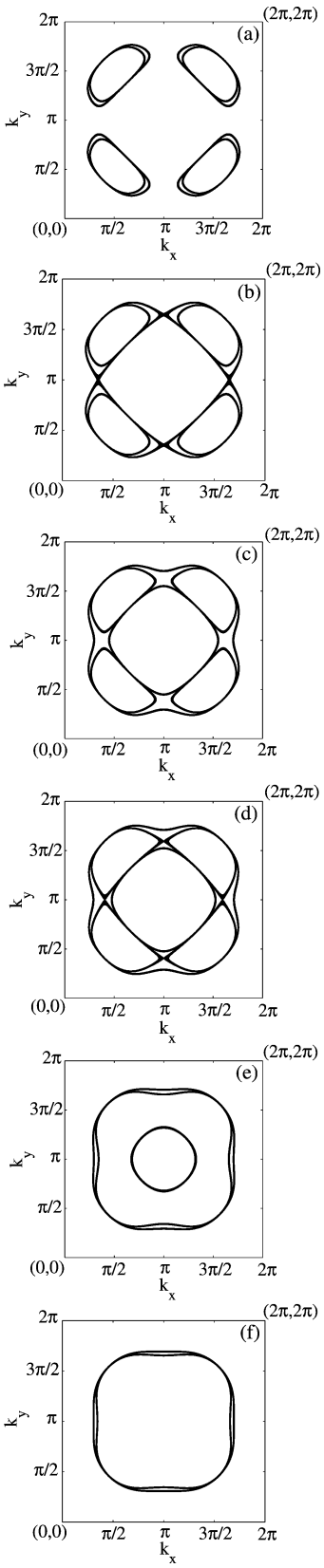

Fig. 1 Evolution of Fermi surface of two-layer cuprates with doping (**a**) $x = 0.11$; (**b**) $x = 0.135$; (**c**) $x = 0.155$; (**d**) $x = 0.165$; (**e**) $x = 0.22$; (**f**) $x = 0.26$

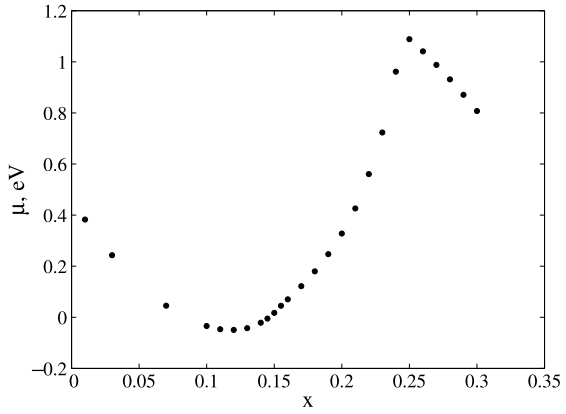

Fig. 2 Dependence of electronic chemical potential on the number of holes for $La_2Sr_{2-x}CuO_2$

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