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LDA + GTB (generalized tight-binding) method for the electronic structure calculations of strongly correlated electron systems: Application for the band structure calculations of p-type cuprates

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Abstract

Mean-field theory of the non-superconducting phase of the high-T_c cuprates is formulated within the effective t–t'–t''–J model with three-site correlated hoppings. This model with the *ab initio* calculated parameters results from the LDA + GTB method. The static spin and kinematical correlation functions beyond Hubbard I approximation are calculated self-consistently taking into account hoppings to the first, the second, and the third neighboring sites, as well as the three-site correlated hoppings. The obtained Fermi surface evolves from hole-pockets at low-doping to large hole-type Fermi surface at higher doping concentrations. Calculated doping dependence of the nodal Fermi velocity, the effective mass and the chemical potential shift are in good agreement with experimental data.

Keywords: Strongly correlated electron systems; Superconductivity; p-Type cuprates; Spin fluctuations; Fermi surface

Recent significant improvements of experimental techniques, especially of the angle-resolved photoemission spectroscopy (ARPES) and the scanning tunneling microscopy (STM), revealed new exciting facts on the low-energy features of the high-T_c copper oxides. First of all, the evolution of the Fermi surface with doping has been measured [1]. Then, the dependence of the chemical potential shift $\Delta\mu$ on doping x shows pinning at $x < x_{opt}$ with $x_{opt} = 0.15$ [2]. The measured nodal Fermi velocity v_F is almost doping-independent within experimental error of 20% [3], together with the effective electron mass $m^*/m = 3.8 \pm 2$ in $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_y$ [4].

Since high-T_c cuprates belong to a class of strongly correlated systems, the standard LDA-like schemes and weak-coupling perturbation theories lead to inappropriate results. To overcome this difficulty recently we have formulated an LDA + GTB method [5]. In this method the *ab initio* LDA calculation is used to construct the Wannier functions and to obtain the single electron and Coulomb parameters of the multiband Hubbard-type model. Within this multiband Hubbard model the electronic structure in the strong correlation regime is calculated by the generalized tight-binding (GTB) method that combines the exact diagonalization of the model Hamiltonian for a small cluster (unit cell) with perturbative treatment of the intercluster hopping and interactions. For undoped La_2CuO_4 and Nd_2CuO_4 this scheme results in charge transfer insulator with a correct value of the gap and the dispersion of bands in agreement with the experimental ARPES data.

Then the multiband Hamiltonian for the real crystal structure was mapped onto low-energy model. Parameters of this effective model were obtained directly from the *ab initio* multiband model parameters. The low-energy model appears to be the t–t'–t''–J^* model (t–t'–t''–J model with three-cite correlated hoppings) for n-type cuprates and

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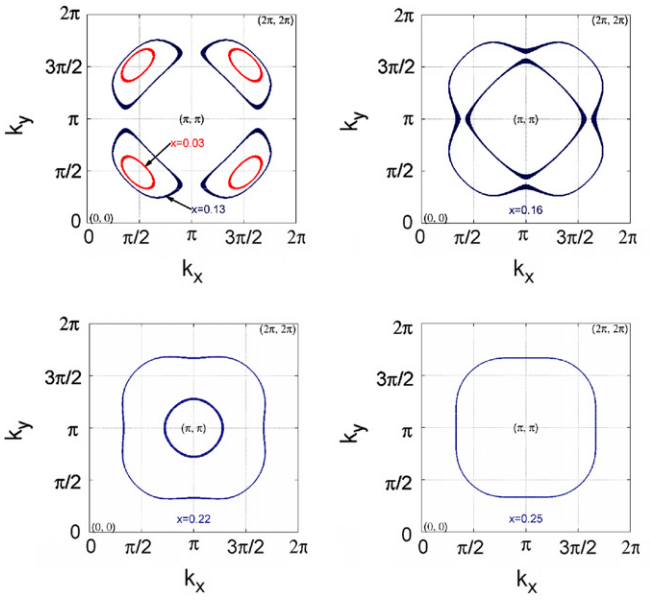

Fig. 1. Fermi surface evolution with doping (hole concentration) x.

the singlet–triplet t–t'–t''–J^* model for p-type systems. But for $x < 0.7$ in a phase without long-range order the role of triplet state and singlet–triplet hybridization is negligible [6]. Therefore the triplet could be omitted, and in the present paper we will describe low-energy excitations in the single-layer p-type cuprates within t–t'–t''–J^* model with LDA + GTB calculated parameters (in eV): $t = 0.93$, $t' = -0.12$, $t'' = 0.15$, $J = 0.295$, $J' = 0.003$, $J'' = 0.007$.

To go beyond the Hubbard I approximation we will calculate electronic Green function using equation of motion method and retain [7] static spin correlation functions $C_{fg} = 2\left\langle S_f^z S_g^z \right\rangle = \left\langle X_f^{\uparrow\downarrow} X_g^{\downarrow\uparrow} \right\rangle$ and kinematical correlation functions $K_{fg} = \left\langle X_f^{\uparrow 0} X_g^{0\downarrow} \right\rangle$.

The importance of the three-cite correlated hoppings in the normal and superconducting phases has been demonstrated in Refs. [7,8]. To take them into account we use method [9] to self-consistently calculate all C_n and K_n correlation functions. In the latter method the spin-liquid phase is considered and static spin correlation functions calculated using bosonic Green functions similar to [10].

Calculated evolution of the Fermi surface (FS) is presented in Fig. 1. At low dopings FS has the form of the hole pockets centered around $(\pm\pi/2, \pm\pi/2)$. At higher dopings these pockets merge together and become one large hole-type FS.

Also, we have calculated v_F, m^*/m and $\Delta\mu$ vs. doping x (see Fig. 2). Nodal Fermi velocity and chemical potential reveals only slight doping dependence in good agreement with the experiments [2,3]. Effective mass m^* increase with decreasing x reveals tendency to the localization in the vicinity of the metal-insulator transition. But this increase is not very large and overall m^* doping dependence agrees very well with experimentally observed one [4].

To summarize, we have investigated the doping-dependent evolution of the low-energy quantities for p-type

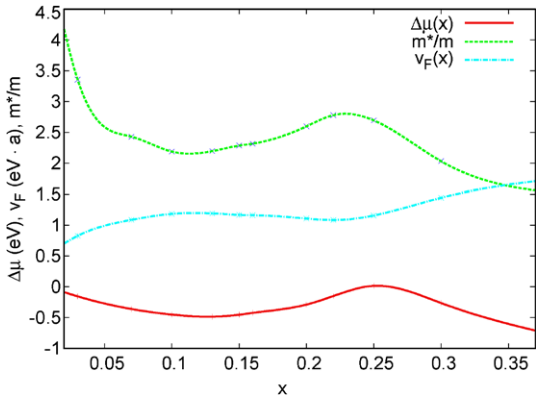

Fig. 2. Doping-dependent evolution of the chemical potential shift, nodal Fermi velocity, and effective mass.

high-T_c cuprates in the regime of strong electron correlations within sequentially derived effective model with *ab initio* parameters. Although our approach is a mean-field theory, the calculations within t–t'–J model including finite quasiparticle lifetime [11] shows that the results of the mean-field-like approximation is qualitatively correct. Quantitatively, at low doping the imaginary part of the self-energy leads to the hiding of the FS portions above the antiferromagnetic Brillouin zone ($(\pi,0)$–$(0,\pi)$ line). This results in Fermi arc rather than hole pockets at $x < x_{opt}$ (see Fig. 1).

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