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INFLUENCE OF ORTHORHOMBIC DEFORMATIONS IN CuO_2 PLANE ON THE ELECTRONIC STRUCTURE OF HIGH-TC CUPRATE FAMILY

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It is widespread believed that all hole-doped high-temperature superconducting cuprates have a common generic phase diagram in the plane (concentration of doped holes x per Cu site, temperature T). In fact, the phase diagram of cuprates is determined not only by doping degree x but also by the strain of CuO_2 lattice [1]. In this work we theoretically investigate effect of CuO_2 lattice parameter variation on the electronic structure of HTSC cuprate $La_{2-x}Sr_xCuO_4$ in the orthogonal phase at different concentration of doped holes. This work is direct continuation our previous work [2], where we were investigating tetragonal phase of mentioned system.

$La_{2-x}Sr_xCuO_4$ compound is modelled by CuO_2 plane, where lattice constant b is more then constant a. Electronic system is described in the framework of three-band $p-d$ model, including copper $d_{x^2-y^2}$ and oxygen p_x and p_y orbitals. For getting realistic parameters of Hamiltonian and taking into account strong electronic correlations we are using LDA+GTB method [3].

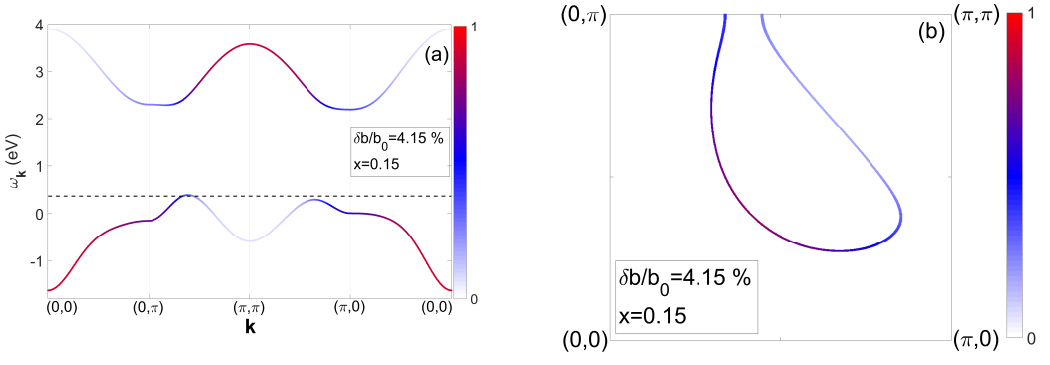

Figure 1. Band structure (left) and Fermi surface (right) with orthorhombic deformations ($b > a$, $\delta b = b-a$, a, $b-$ lattice parameters along axis x and y accordingly) with doping level $x = 0.15$. Dotted line indicates the level of chemical potential. Color of each k-point indicates quasiparticle spectral weight

On-site energies and hopping integrals are obtained by LDA calculation and next by projection onto Wannier functions basis of the chosen model for the undoped La_2CuO_4 for the set of lattice deformations $\delta a/a_0$: −1.6, −1.1, 0, 0.86, 1.85, 2.85, 3.49%. We chose such values of deformations according to our previous work with the condition that the volume of CuO_6 octahedron remains unchanged. Generalized tight-binding (GTB) method [4] is cluster form of perturbation theory in the terms of Hubbard operators, it provides representation of electron as set of quasiparticle excitations between multiparticle eigenstates of finite cluster. Electronic structure of quasiparticle excitations in the effective two-band

Hubbard model is obtained with equation of motion method for the matrix Green function. System of equations of motion is decoupled within generalized Hartri-Fock approximation by applying the Mori-type projection technique with taking into account spin-spin and kinematic correlation functions.

Using the LDA+GTB method we obtained electronic structure (bands structure, Fermi surface, density of states) for different values of orthorhombic deformations and hole doping. The main effect of orthorhombic deformations is asymmetric Fermi surface about the nodal direction; the reason of that is nonequal hopping value along the axis x and y between the clusters (fig.). Thanks to such asymmetry changing of FS topology — from four hole pockets to large electronic and hole contours — is going through two quantum phase transitions and then not like one in tetragonal phase. At first hole pockets are closing in the direction $(\pi, 0) - (\pi, \pi)$, then at $(0, \pi) - (\pi, \pi)$. So there is two Van Hove singularities. It is believed when chemical potential matches maximum in density of states we can get maximum value of critical temperature of superconducting transition. So we hope that presence of two maximums in density of states in orthorhombic phase will improve theoretical results for T_C comparing to ones for tetragonal phase.

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