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Spin fluctuations influence on quasiparticle spectrum of realistic p–d model

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Abstract

In the present work the multiband p–d model for CuO_2-layer is treated. It was shown that for the realistic set of parameters besides Zhang–Rice two-particle singlet state there is non-negligible contribution of two-particle triplet state to the top of the valence band. Also shown, that to gain quantitative agreement with experimental data the minimal approximation should include the spin fluctuations beyond the Hubbard-I scheme. Quasiparticle spectrum, obtained in this approximation, is in fairly good agreement with ARPES data on Bi2212 High—T_c compound.

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Since the ab initio band theories still have problems in calculations of strongly correlated electron systems (SCES) properties, the model approach is still valuable and preferable in this field. One of the most interesting SCES phenomena is high-T_c superconductivity (HTSC). To explain superconductive phase of the cuprates we should start with a model that properly describes normal paramagnetic phase. Good candidate is a 3-band p–d model [1,2] but this model omits d(z^2)–orbitals on Cu and p(z)–orbitals on apical oxygen; importance of these orbitals is shown experimentally [3–5]. This lack is absent in the multiband p–d model of transition metal oxides [6]. Calculations [7,8] of the quasiparticle dispersion and spectral intensities in the framework of this model with use of generalized tight binding method (GTBM) [9] are in very good agreement with ARPES data on insulating compound $Sr_2CuO_2Cl_2$ [10].

Other fascinating feature of multiband p–d model is that the difference $\varepsilon_T - \varepsilon_S$ between energy of two-particle Zhang–Rice-type singlet A_{1g} and two-particle triplet $^3B_{1g}$ depends strongly on various model parameters, particularly on distance of apical oxygen from planar oxygen, energy of apical oxygen, difference between energy of d(z^2)-orbitals and d($x^2 - y^2$)-orbitals [11]. For the realistic values of model parameters $\varepsilon_T - \varepsilon_S$ is less or equal to 0.5 eV [7,8] contrary to the 3-band model with this value being about 2 eV. Latter case was considered in Refs. [12,13] but due to the large singlet–triplet splitting the contribution of singlet–triplet excitations in low-energy physics was negligible. The former case will be considered in this paper.

To take into account triplet states we have derived an effective Hamiltonian for CuO_2-layer [14]. Hamiltonian of this effective singlet–triplet model has the form of the generalized t–t′–J model, but has several important features: (i) the account of a triplet leads to renormalization of exchange integral J, (ii) the model is asymmetric for n- and p-type systems (for n-type systems the usual t–J model takes place while for p-type superconductors with complicated structure on the top of the valence band the singlet–triplet excitations plays an important role; the asymmetry of p- and n-type systems is known experimentally [15]), (iii) evolution of the system with doping is described only by changes in band structure

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while all parameters are fitted in undoped case and therefore fixed for all doping levels [7,8].

The paramagnetic non-superconductive phase was investigated in Hubbard-I approximation both in the singlet–triplet and t–t′–J models. Results for optimal doping (concentration of holes $x = 0.15$) are presented in Fig. 1.

As one can see the mixture of triplet state (dotted line) and singlet state (straight line) is significant along $(0,0) - (\pi,\pi)$ and $(\pi,0) - (0,0)$ directions. Meanwhile singlet sub-band is rather wide, near 2 eV, that contradicts to experimental ARPES data [16]. It is a consequence of neglecting spin fluctuations in Hubbard-I approximation [17,18]. Because spin part of the effective singlet–triplet model is the same as in the usual t–J model, we can use in our calculations the spin correlators self-consistently obtained in the framework of t–J model. By exploiting this approach, we were able to calculate dispersion in paramagnetic non-superconductive phase of effective singlet–triplet model for square lattice beyond the Hubbard-I approximation similar to t–J model [17]. Spin correlations in t–J model was calculated in rotationally invariant approximation [18], which gives close agreement between calculated and experimental data on temperature and concentration dependencies of magnetic susceptibility [19].

Obtained dispersion for $x = 0.15$ in this approximation together with ARPES data on high-T_c optimally doped compound Bi2212 [16] is presented in Fig. 2. The line-shape of dispersion now is in good agreement with experimental data while the positions of chemical potentials (and, consequently, Fermi surfaces) quite differ. To reconcile our calculations and the Fermi surface we have to shift the whole band by about 0.5 eV (at optimal doping the position of flat region near $(\pi,0)$ and chemical potential should be nearly the same).

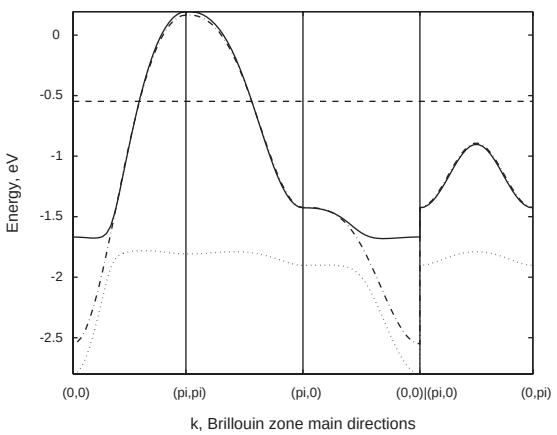

Fig. 1. Comparison of dispersion curves on top of the valence band for effective singlet–triplet model (straight and dotted lines) and t–t′–J model (dash–dotted line), dashed line denotes self-consistently obtained chemical potential.

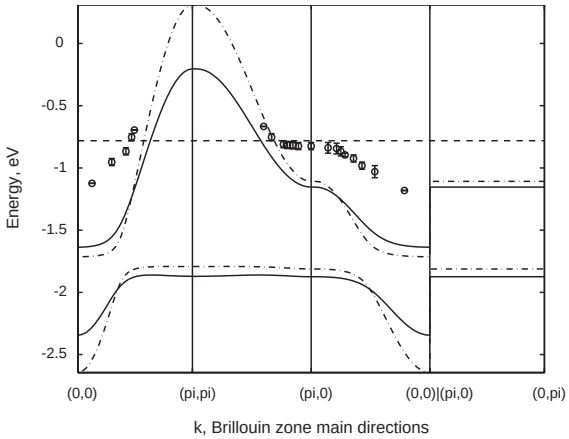

Fig. 2. Quasiparticle dispersion on top of the valence band for effective singlet–triplet model in Hubbard-I approximation (dash–dotted line), beyond the Hubbard-I approximation (straight lines), chemical potential position (dashed line) and experimental ARPES data (circles with error bars) [16].

There are few reasons why this shift appears. One of the most important is the neglecting of 3-centers terms during formulation of effective singlet–triplet model. While these terms are very important for superconductive phase [20], their influence on chemical potential renormalization in normal phase may be significant too. Another necessary but yet not used in this approach ingredient is the second and third nearest neighbors. The importance of these hopping terms was pointed out in work [21], where the LDA bands for 8-band, 3- and 1-band Hamiltonians were compared.

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