Single hole dispersion relation for the real CuO$_2$ plane.

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Dispersion relation for the CuO$_2$ hole is calculated basing on the generalized $t$-$t'$-$J$ model, recently derived from the three-band one. Numerical ranges for all model parameters, $t/J = 2.4..2.7$, $t'/t = 0..-0.25$, $t''/t = 0.1..0.15$, and three-site terms $2t_N \sim t_S \sim J'/4$, have been strongly justified previously. Physical reasons for their values are also discussed. Self-consistent Born approximation is used for the calculation of the hole dispersion. An excellent agreement between calculated $E_k$ and one obtained from the angle-resolved photoemission experiments is found.

Recent angle-resolved photoemission experiments (ARPES) on insulating copper oxide Sr$_2$CuO$_2$Cl$_2$ [1] can be considered as a direct test for low-energy models describing holes (holes) in the CuO$_2$ plane. Experimentally observed dispersion relation $E_k$ for a single hole has the following characteristic features: (i) bandwidth about $2J$, (ii) band minimum at the $(\pi/2, \pi/2)$ point, (iii) isotropic dispersion near the band minimum, and (iv) almost flat dispersion along the line $(0, 0) \to (\pi/2, 0) \to (\pi, 0)$.

The first result agrees with $t$-$J$ model prediction as well as with ones of all possible $t$-$J$ model generalizations in the region of parameters when $t \gg J$. Following the physical arguments by Kane, Lee and Read [2] it seems to be rather general that in presence of the strong spin fluctuations there are no stable quasiparticles at higher energies ($> 2J$). It is of no importance whether the 'bare' dispersion of the hole exists ($t$-$t'$-$J$ model) or not ($t$-$J$ model), since the basic arguments are the absence of the hole–magnon scattering near the bottom of the band and its domination at higher energies. Roughly, it looks like some kind of the Cherenkov effect: a massive quasiparticle cannot create an excitation with linear dispersion up to the threshold energy.

Experimental observation of the band minimum at $(\pi/2, \pi/2)$ point also agrees with the quasiparticle (spin-polaron) dispersion calculated in the framework of $t$-$J$-like models. It is well established by now that the almost degenerate dispersion along the magnetic Brillouin zone (MBZ) boundary $((\pi, 0) - (0, \pi) \text{ line})$ is an intrinsic property of the pure $t$-$J$ model, and that it is lifted out by any small (compared to $t$, not $J$) additional hopping integral, for example the next-nearest-neighbor hopping $t'$. Moreover, including $t'$-term in the low-energy model of the real CuO$_2$ plane is strongly supported by the first principle calculations, which show that the direct O-O hopping provide large enough transfer amplitude to the next-nearest-neighbor site [3].

Thus, it is not much surprising that the masses in the directions along and perpendicular to the MBZ boundary were found close to each other. To be considered as the experimental constraint on the parameters of the $t$-$t'$-$J$ model at $J/t = 0.4$ it fixes $t'$ near $-0.3t$ [4].

Returning to the experimental results, note that theoretical description of the last feature, i.e., flat band along $(0, 0) \to (\pi, 0)$ line presents a problem. This flat region is absent in the $t$-$J$ model quasiparticle band. Simple $t'$-term adds the 'bare' hole dispersion in the form: $E_k^t = 4t' \cos k_x \cos k_y$. Considering this term as the correction to the pure $t$-$J$ model dispersion one can see that it does not lift $(\pi/2, 0)$ point from its $t$-$J$ model position, and so it cannot provide the flat dispersion.

Disagreement between experimental band shape and theoretical one based on the $t$-$t'$-$J$ model returns us to the problem of the correct low-energy model of the real CuO$_2$ plane. There were some recent works devoted to this problem, which consider CuO$_2$ holes in the framework of the three-band model in the strong-coupling limit [5], [6]. These calculations reproduce the experimental bandstructure much better than the $t$-$t'$-$J$ ones, but some of the fitting parameters differ from those proposed in the cluster analysis of the spectroscopic data and [7] electronic structure works [7].

From our point of view the experimental and pure $t$-$t'$-$J$ model discrepancy is the reason to revise approximations were made in obtaining this model for the CuO$_2$ plane, not to deny it.

In our previous works [8] we developed ideas of the three-band model low-energy reduction, firstly proposed by Zhang and Rice [9]. We performed the consistent quantitative mapping of the initial model to the single-band one using Vannier-ortogonalized basis of the oxygen states and canonical transformation approach [10]. It allowed us to obtain the low-energy generalized $t$-$t'$-$J$ model and to calculate the ranges of its parameters for the real CuO$_2$ plane [11].

Our general statement [11] is that there are physical reasons for including some other terms except $t'$ one, namely hopping term to the next-next-nearest neighbors and the so-called 'three-site' terms, into low-energy model. We also should stress that the simple addition of the $t'$-term alone to the $t$-$J$ model is too naive to give the correct description of the subtle details of the hole spectrum.

In this paper we show that the generalized $t$-$t'$-$J$ model with the set of parameters, which presented in our recent work [11], reproduces the experimental bandshape at all $k$-points quite well.
Hamiltonian of the generalized $t$-$t'$-$J$ model has the form [11]:

$$H = H_{t-J} + H_{t'},$$

$$H_{t-J} = t \sum_{\langle ij \rangle, \alpha} \tilde{c}_{i,\alpha}^\dagger \tilde{c}_{j,\alpha} + J \sum_i S_i S_j,$$

$$H_{t'} = t' \sum_{\langle ij \rangle, \alpha} \tilde{c}_{i,\alpha}^\dagger \tilde{c}_{j,\alpha} + t'' \sum_{\langle ij \rangle, \alpha} \tilde{c}_{i,\alpha}^\dagger \tilde{c}_{j,\alpha} + t N \sum_{\langle ij \rangle, \alpha, \beta} \sigma_{\beta\alpha} \tilde{c}_{i,\alpha}^\dagger \tilde{c}_{j,\sigma} S_l$$

in standard notations of the constrained Fermi operators, brackets denote first ($\langle \rangle$), second and third ($\langle \rangle_{2,3}$) neighbor sites, respectively. Three-site terms are written in the rotationally invariant form, $N_l$, $S_i$ are the number of fermion and spin operators, respectively. $t_N$ and $t_S$ obtained for the usual Hubbard model are $2t_N = -t_S = t^2 / U = J / 4$, their ‘three-band’ values are not so simply related to the other parameters due to the presence of triplet state.

Ranges for the parameters of the model [11] are [11]: $t / J = 2.4 \ldots 2.7$, $t' = 0.01 \ldots -0.25$, $t'' = 0.12 \ldots 0.16$, $t_N = 0.01 \ldots 0.07$, $t_S = -0.07 \ldots -0.16$. It is worth to note that the $t'$ amplitude is smaller than it follows from the cluster calculation [8] and $t''$ is not small compared to $t'$. As it was discussed in Ref. [12] and in the work by Jefferson et al. [13], the main reason for the difference between Cu$_2$O$_8$ cluster and infinite plane $t'$ hopping parameters is the Vannier nature of the latter. It was shown [11, 12] that the Cu-O and O-O hopping amplitudes tend to cancel each other for $t''$, and sum up for $t''$-term. This is the cause of not small and weakly varied $t''$, whereas $t''_{Cu-O} \approx t''_{O-O}$ ($t''_{Cu-O} \approx t''_{O-O}$).

Previously [11] we have calculated spin-polaron dispersion for the parameters discussed above using the simple variational ansatz [13], which is quite good for the pure $t$-$J$ model. It consists of the ‘bare’ hole and four ‘one-string’ holes, that is, it is clear by now, not enough for the correct treating of the $t''$-terms.

In this paper we treat the energy calculation problem using the self-consistent Born approximation (SCBA). First of all, one should turn to the well known spinless-fermion Schwinger-boson representation for the Hubbard (constrained fermion) operators [14]. In that case constraint on the fermion degrees of freedom fulfilled exactly [15], and the only approximation is the spin-wave one. Hamiltonian of the model [13] becomes:

$$H \simeq \sum_{k} \epsilon_k h_k^\dagger h_k + \sum_{q} \omega_q a_q^\dagger a_q$$

$$+ \sum_{k, q} \left( M_{k, q} h_k^\dagger h_{k-q}^\dagger a_q^\dagger + \text{H.c.} \right) + H^{(2)}$$

where $h^\dagger(h), a^\dagger(a)$, are the spinless hole and magnon operators, respectively, $\epsilon_k$ is the ‘bare’ hole dispersion, $\omega_q = 2J(1 - \gamma_q)^{1/2}$ is the spin-wave energy, $M_{k, q} = 4t(\gamma_{k-q} U_q + \gamma_{k} V_q)$. $U_q, V_q$ are the Bogolubov canonical transformation parameters. $H^{(2)}$ includes the higher-order magnon terms. Bare hole dispersion has the form:

$$\epsilon_k = \epsilon_k^0 + \delta \epsilon_k$$

$$\epsilon_k^0 = 4(t' + 2t_N - t_S)(\gamma_k^2 - (\gamma_k^-)^2)$$

$$+ 8(t'' + t_N - t_S / 2)(\gamma_k^2 + (\gamma_k^-)^2 - 0.5)$$

where we used shorthand notations $\gamma_k = \frac{1}{2}(\cos(k_x) + \cos(k_y))$, $\gamma^-_k = \frac{1}{2}(\cos(k_x) - \cos(k_y))$. $\delta \epsilon_k$ is the addition from zero-point fluctuations:

$$\delta \epsilon_k = 4\alpha_1(t' + 2t_N + t_S)(\gamma_k^2 - (\gamma_k^-)^2)$$

$$+ 8\alpha_2(t'' + t_N + t_S / 2)(\gamma_k^2 + (\gamma_k^-)^2 - 0.5)$$

$$+ 4\beta t_S (4\gamma_k^2 - 1)$$

where $\alpha_1 = 0.138, \alpha_2 = 0.107, \beta = -0.347$. One can see from Eqs. (3), (4) that in contrast to $t'$ (first terms), $t''$ (second terms) lift $(\pi / 2, 0)$ point to the higher energy.

Using SCBA we find the Green function of the hole as $G(k, \omega) = (\omega - \epsilon_k - \Sigma(k, \omega - \omega_q)^{-1}$ with the self-energy

$$\Sigma(k, \omega - \omega_q) = \frac{1}{N} \sum_{q} M_{k, q}^2 G(k - q, \omega - \omega_q)$$

It was proved earlier [16] that the first order correction to the hole-magnon vertex is absent and the highest are very small.

Recently Bala, Oles and Zaanen [17] showed that the higher-order vertices ($H^{(2)}$) do not change the SCBA results and confirmed that one-magnon coupling are accurate enough to reproduce the realistic properties of the $t$-$J$-like models.

Equation (3) was solved numerically by the simple iteration procedure. We found no significant changes of the results for $16 \times 16 k$-points (in MBZ) and 1000 $\omega$-points, and for $24 \times 24 \times 3000$ points. Also, we checked our procedure for the pure $t$-$J$ model and found very close agreement with earlier results [18]. Results of our generalized $t$-$t'$-$J$ model calculations together with the experimental points are presented on Fig. 1. It is important to stress that it is not the ‘best fit’, we simply used the average values of parameters from their ‘realistic range’. In the main term of the bare dispersion $\epsilon_k^0 \equiv \epsilon_k^0(t_N$ and $t_S$ terms enter in a combination $2(t_N - t_S)$, which realistic range is $[1.5, 0.5 J]$, so we simply take its Hubbard value $(2t_N - t_S) = J / 2 = 0.2t$. We used $t / J = 2.5, t_N = 7 / 8, t_S = -J / 4, J = 0.14$ eV (from Ref. [19]). For $t'$ and $t''$ we used $t' = -0.2t, t'' = 0.15t$. Note, that the bare dispersion (3) consist of two terms, which can be considered as the $t'_{eff}$ ($= t' + 2t_N - t_S$) and $t''_{eff} (= t'' + t_N - t_S / 2)$, and since $t'$ and $(2t_N - t_S)$ have the opposite signs, $t'_{eff}$ becomes very small at all realistic values of parameters.

Figure 1 shows an excellent agreement with experiment along $(\pi, 0) - (0, \pi)$ as well as along $(0, 0) - (\pi, 0)$ lines. Notice, that another feature of the ARPES can be
explained in the spin-polaron approach. Lower intensity of the photoemission peaks at the top of the hole band (bottom in the electron language) easily connected to the lower quasiparticle residue at $(0, 0) \to (\pi, 0)$ points. The last is due to importance of multi-magnon scattering processes for the ‘cutting’ of the wide initial (‘bare’) band.

We also found an important feature of the energy spectrum of the proposed model: if the values of $t'', t_S$, $t_N$ are not small (average and larger), the shape of the bandwidth is fully insensitive to the $t'$ changes. Changes of $t'$ only shift the energy of ground state and change the quasiparticle residue at the top of the band. Opposite to it, $t''$ strongly varies the $(\pi/2, 0)$ position. These results are shown in Fig. 3. They are easily understood remembering that the higher energy states are unstable. When $t''$ and three-site terms are not very small, they already form the band up to the characteristic energy $2J$, and further changes of $t'$ (even in a broad region) touch only the higher states, which are unstable. It is interesting that the further increasing of $t'' (> 0.15t)$ also do not change the shape of the band.

Summarizing, we showed that the generalized version of the $t$-$t'$-$J$ model accurately derived from the three-band model describe very well the experimental results of ARPES on Sr$_2$CuO$_2$Cl$_2$ system. Parameters of the model, at which good agreement are achieved, are from realistic regions and so they are strongly justified. Hopping integral to the next-nearest neighbor site ($t''$) as well as three-site hopping terms ($t_S, t_N$) is found to be the key parameters for the description of the flat region along $(0, 0) - (\pi, 0)$ line. It is argued that the isotropy of the spectra around the minimum $(\pi/2, \pi/2)$ easily arise at any (not very small) $t'$, $t''$, $t_S$, $t_N$ parameters of the definite sign. In addition we found that the shape of the spectrum is insensitive to varying of $t'$ if the other parameters are not small. Thus, the model has some rigidity to parameter changes. Smaller intensity of the photoemission peaks at the top of the band can be directly related to the small quasiparticle residues at these points.

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Figure captions

FIG. 1. Dispersion curve of a hole in the generalized $t$-$t'$-$J$ model along the main directions $(0, 0) \to (\pi, \pi)$, $(\pi, 0) \to (0, 0)$, and $(\pi, 0) \to (0, \pi)$ (solid curve). Model parameters that provide this $E_k$ are: $t/\sqrt{J} = 2.5$, $t'' = -0.2t$, $t''' = 0.15t$, $t_S = -2t_N = -J/4$, $J = 0.14$ eV. Experimental results from Ref. [3] are also shown (open circles).

FIG. 2. Dispersion relation of a hole in the generalized $t$-$t'$-$J$ model for the different sets of parameters: $t' = -0.2t$, $t'' = 0.15t$ (solid curve), $t' = -0.5t$, $t'' = 0.15t$ (dashed curve), $t' = -0.2t$, $t'' = 0$ (dotted-dashed curve). Other parameters are: $t/J = 2.5$, $t_S = -2t_N = -J/4$. 
Figure 1
Figure 2