

Single-hole dispersion relation for the real CuO_2 plane

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Dispersion relation for the CuO_2 hole is calculated based 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 , $t'/t=0.0$ to -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. A self-consistent Born approximation is used for the calculation of the hole dispersion. Good agreement between calculated $E_{\mathbf{k}}$ and one obtained from the angle-resolved photoemission experiments is found. A possible explanation of the broad peaks in the experimental energy distribution curves at the top of the hole band is presented. [S0163-1829(96)04345-7]

Recent angle-resolved photoemission experiments (ARPES) on insulating copper oxide $\text{Sr}_2\text{CuO}_2\text{Cl}_2$ (Ref. 1) can be considered as a direct test for low-energy models describing carriers (holes) in the CuO_2 plane. The experimentally observed dispersion relation $E_{\mathbf{k}}$ 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 $(0,0) \rightarrow (\pi/2,0) \rightarrow (\pi,0)$.

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 $t > J$. Following the physical arguments by Kane, Lee, and Read² it seems to be rather general that in the presence of 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 [$(\pi,0) - (0,\pi)$ 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 the t' term in the low-energy model of the real CuO_2 plane is strongly supported by first principles calculations, which show that direct O-O hopping provides a large enough transfer amplitude to the next-nearest-neighbor site.³

Thus, it is not very surprising that 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 self-consistent Born approximation studies of the t - t' - J model performed in Ref. 4 show a very good fitting of

features (i)–(iii), but a theoretical description of the last feature, i.e., a flat band along the $(0,0) \rightarrow (\pi,0)$ line presents a problem for this model. This flat region is absent in the t - J model quasiparticle band. A simple t' term adds the “bare” hole dispersion in the form $\epsilon_{\mathbf{k}}^0 = 4t' \cos k_x \cos k_y$. Considering this term as the correction to the pure t - J model dispersion one can see that it *does not* lift the $(\pi/2,0)$ point from its t - J model position, and so it cannot provide the flat dispersion in principle. Increasing of the t' parameter leads to the narrowing of the theoretical spectrum and to a worse agreement with experiment. These failures were the reason⁴ to consider the more general model for the interpretation of the experiment. Moreover, they have made questionable the further use of the t - J -like models, which were considered as the candidates for description of the low-energy physics and superconductivity in cuprates.

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.^{4–6} These calculations reproduce the experimental band structure 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 data³ and electronic structure works.⁷

From our point of view the experimental and *pure* t - t' - J model discrepancy is the reason to revise approximations made in obtaining this model for the CuO_2 plane, not to deny it.

In our previous works⁸ we developed ideas of the three-band model low-energy reduction, proposed by Zhang and Rice.⁹ We performed the consistent quantitative mapping of the initial model to the single-band one using Wannier-orthogonalized 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 statement¹¹ is that there are physical reasons for including some other terms except the t' one, namely, hopping terms to the next-next-nearest neighbors and the so-called “three-site” terms, into the 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 \mathbf{k} points quite well.

The Hamiltonian of the generalized t - t' - J model has the form¹¹

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

$$H_{t-J} = t \sum_{\langle ij \rangle, \alpha} \tilde{c}_{i, \alpha}^\dagger \tilde{c}_{j, \alpha} + J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (1)$$

$$H_{t'} = t' \sum_{\langle ij \rangle_2, \alpha} \tilde{c}_{i, \alpha}^\dagger \tilde{c}_{j, \alpha} + t'' \sum_{\langle ij \rangle_3, \alpha} \tilde{c}_{i, \alpha}^\dagger \tilde{c}_{j, \alpha} \\ + t^N \sum_{\langle ilj \rangle, \alpha} \tilde{c}_{i, \alpha}^\dagger \tilde{c}_{j, \alpha} \hat{N}_l + t^S \sum_{\langle ilj \rangle, \alpha \beta} \tilde{c}_{i, \alpha}^\dagger \boldsymbol{\sigma}_{\beta \alpha} \tilde{c}_{j, \beta} \cdot \mathbf{S}_l,$$

in standard notation of the constrained Fermi operators, brackets denoting first ($\langle \rangle$), second, and third ($\langle \rangle_{2,3}$) neighbor sites, respectively. Three-site terms are written in the rotationally invariant form, and N_l and \mathbf{S}_l 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 the triplet state.

Ranges for the parameters of the model (1) are¹¹ $t/J = 2.4$ – 2.7 , $t' = 0.01$ to -0.25 , $t'' = 0.12$ – 0.16 , $t_N = 0.01$ – 0.07 , and $t_S = -0.07$ to -0.16 . It is worth noting that the t' amplitude is smaller than follows from the cluster calculation³ and t'' is not small compared to t' . As discussed in Ref. 11 and in the work by Jefferson *et al.*,¹² the main reason for the difference between Cu_2O_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 a not small and weakly varied t'' , whereas $t''_{\text{Cu-O}} (t''_{\text{O-O}}) \ll t'_{\text{Cu-O}} (t'_{\text{O-O}})$.

Previously¹¹ 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, as is clear by now, not enough for the correct treatment 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 the constraint on the fermion degrees of freedom fulfilled exactly,¹⁵ and the only approximation is the spin-wave one. Hamiltonian of the model (1) becomes

$$H \approx \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} h_{\mathbf{k}}^\dagger h_{\mathbf{k}} + \sum_{\mathbf{q}} \omega_{\mathbf{q}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \\ + \sum_{\mathbf{k}, \mathbf{q}} (M_{\mathbf{k}, \mathbf{q}} h_{\mathbf{k}-\mathbf{q}}^\dagger h_{\mathbf{k}} a_{\mathbf{q}}^\dagger + \text{H.c.}) + H^{(2)}, \quad (2)$$

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

$$\epsilon_{\mathbf{k}} = \epsilon_{\mathbf{k}}^0 + \delta \epsilon_{\mathbf{k}}, \quad (3)$$

$$\epsilon_{\mathbf{k}}^0 = 4(t' + 2t_N - t_S)[\gamma_{\mathbf{k}}^2 - (\gamma_{\mathbf{k}}^-)^2] \\ + 8(t'' + t_N - t_S/2)[\gamma_{\mathbf{k}}^2 + (\gamma_{\mathbf{k}}^-)^2 - 0.5],$$

where we used shorthand notation $\gamma_{\mathbf{k}} = \frac{1}{2}[\cos(k_x) + \cos(k_y)]$, $\gamma_{\mathbf{k}}^- = \frac{1}{2}[\cos(k_x) - \cos(k_y)]$. $\delta \epsilon_{\mathbf{k}}$ is the addition from zero-point fluctuations:

$$\delta \epsilon_{\mathbf{k}} = 4\alpha_1(t' + 2t_N + t_S)[\gamma_{\mathbf{k}}^2 - (\gamma_{\mathbf{k}}^-)^2] + 8\alpha_2(t'' + t_N + t_S/2) \\ \times [\gamma_{\mathbf{k}}^2 + (\gamma_{\mathbf{k}}^-)^2 - 0.5] + 4\beta t_S(4\gamma_{\mathbf{k}}^2 - 1), \quad (4)$$

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

Using the SCBA we find the Green function of the hole as $G(\mathbf{k}, \omega) = [\omega - \epsilon_{\mathbf{k}} - \Sigma(\mathbf{k}, \omega - \omega_{\mathbf{q}})]^{-1}$ with the self-energy

$$\Sigma(\mathbf{k}, \omega - \omega_{\mathbf{q}}) = \frac{1}{N} \sum_{\mathbf{q}} M_{\mathbf{k}, \mathbf{q}}^2 G(\mathbf{k} - \mathbf{q}, \omega - \omega_{\mathbf{q}}). \quad (5)$$

It was proved earlier¹⁶ that the first-order correction to the hole-magnon vertex is absent and the highest are very small.

Recently Bala, Oles, and Zaanen¹⁷ showed that the higher-order vertices ($H^{(2)}$) do not change the SCBA results and confirmed that one-magnon couplings are accurate enough to reproduce the realistic properties of the t - J -like models.

Equation (5) was solved numerically by the simple iteration procedure. We found no significant changes of the results for 16×16 \mathbf{k} points (in MBZ) and 1000 ω 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 in 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 $\epsilon_{\mathbf{k}}^0$, Eq. (3), t_N and t_S terms enter in a combination $(2t_N - t_S)$, which realistic range is $[\frac{1}{4}J - \frac{3}{4}J]$, and so we simply take its Hubbard value $(2t_N - t_S) = J/2 = 0.2t$. We used $t/J = 2.5$, $t_N = J/8$, $t_S = -J/4$, and $J = 0.14$ eV (from Ref. 19). For t' and t'' we used $t' = -0.2t$, $t'' = 0.15t$. Note that the bare dispersion (3) consists of two terms, which can be considered as the $t'_{\text{eff}} (= t' + 2t_N - t_S)$ and t''_{eff}

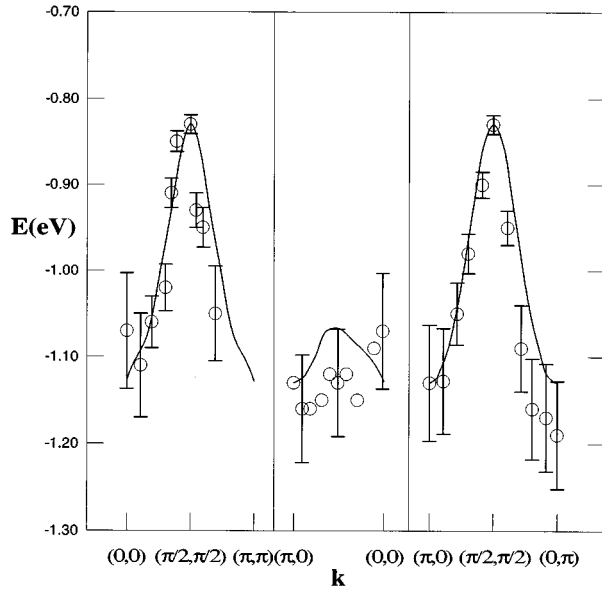


FIG. 1. Dispersion curve of a hole in the generalized t - t' - J model (1), (2) along the main directions $(0,0) \rightarrow (\pi, \pi)$, $(\pi, 0) \rightarrow (0,0)$, and $(\pi, 0) \rightarrow (0, \pi)$ (solid curve). Model parameters that provide this $E_{\mathbf{k}}$ are $t/J=2.5$, $t'=-0.2t$, $t''=0.15t$,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

($=t''+t_N-t_S/2$), 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 a good agreement with experiment along $(\pi, 0)$ - $(0, \pi)$ as well as along $(0, 0)$ - $(\pi, 0)$ lines. Notice that the experimental error bars are much broader for the top of the hole band than for the bottom. It is due to the fact that the energy distribution curves (EDC's) have a broad maximum for these \mathbf{k} points and it is hard to identify the quasiparticle peak in the EDC spectra.¹ This feature of the ARPES can be explained in the spin polaron approach. A lower intensity of the photoemission peaks at the top of the hole band easily connected to the lower quasiparticle residue at $(0, 0) \rightarrow (\pi, 0)$ points which can be lower than the experimental resolution. It is interesting that the spectral function at these \mathbf{k} points shows not only small intense of the lower quasiparticle peak but the wide group of peaks (see also Ref. 17). It can be directly related to the broad peak in the energy distribution curves. The origin of these peaks is due to importance of the multimagnon 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 , and t_N are not small (average and larger), the shape of the band 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. 2. 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)

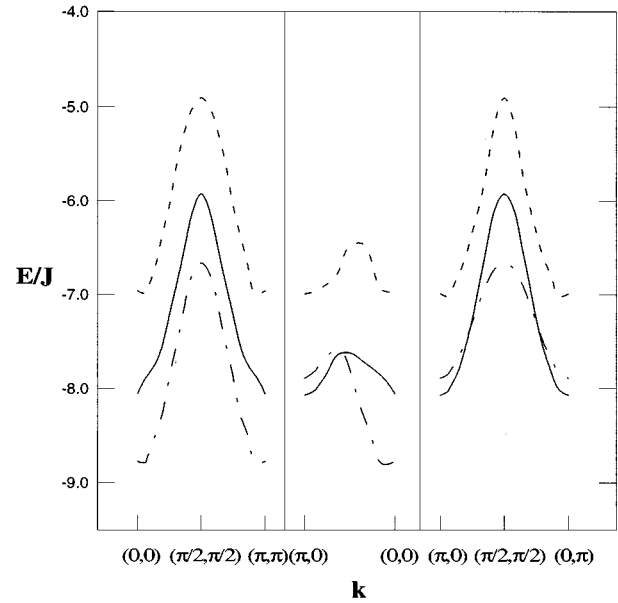


FIG. 2. Dispersion relation of a hole in the generalized t - t' - J model for the different sets of parameters: $t'=-0.2t$, $t''=0.15t$ (solid curve), $t'=-0.5t$, $t''=0.15t$ (dashed curve), and $t'=-0.2t$, $t''=0$ (dotted-dashed curve). Other parameters are $t/J=2.5$ and $t_S=-2t_N=-J/4$.

touch only the higher states, which are unstable. It is interesting that the further increasing of t'' ($>0.15t$) also does 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 describes very well the experimental results of ARPES on $\text{Sr}_2\text{CuO}_2\text{Cl}_2$ system.¹ Parameters of the model, for which good agreement is achieved, are from realistic regions¹¹ and so they are strongly justified. The hopping integral to the next-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 arises at any (not very small) t' , t'' , t_S , and 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. The smaller intensity of the photoemission peaks at the top of the band can be directly related to the small quasiparticle residues at these points.

Xiang and Wheatly²⁰ and Hayn, Barabanov, and Schulenburg²¹ have recently proposed the same models for description of an experimental spectrum. Good coincidence with ARPES results is reported.

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