Quasiparticle energy dispersion in doped two-dimensional quantum antiferromagnets

T. Xiang and J. M. Wheatley
Research Center in Superconductivity, University of Cambridge, Madingley Road, Cambridge CB3 0HE, United Kingdom
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The quasiparticle dispersion in the one-hole t-t'-t''-J model is studied. Both finite-size diagonalization and the self-consistent Born-approximation calculations have been performed and compared. The quasiparticle band structures in the hole- and electron-doped high-T_c cuprates are qualitatively different. In the hole-doped compounds, the band maxima are located at $(\pm\pi/2,\pm\pi/2)$, while in the electron-doped compounds the band maxima are located at $(\pi,0)$ and its equivalent points. The angle-resolved photoemission data for the quasiparticle dispersion of $Sr_2CuO_2Cl_2$ can be quantitatively reproduced using the one-band t-t'-t''-J model with the three-site hopping term. [S0163-1829(96)50842-8]

The energy dispersion of hole quasiparticles in the normal states of two-dimensional CuO planes is of fundamental interest for understanding the microscropic mechanism of high-temperature superconductivity. Due to the strong Coulomb repulsion between electrons, quasiparticles in high-T_c cuprates behave very differently from what was predicted by one-electron band calculations. Recently Wells *et al.*[1] reported an ARPES measurement on an insulating layered copper oxide $Sr_2CuO_2Cl_2$. This is by far the most direct measurement of the dispersion of a *single hole* in an antiferromagnetic background since $Sr_2CuO_2Cl_2$ is difficult to dope. It provides a direct test for the model Hamiltonians which are proposed for high-temperature superconductors. Wells *et al.* found that the hole bandwidth and the dispersion along the diagonal direction from (0,0) to (π,π) in the Brillouin zone agree well with the calculations based on the t-J model. However, near $(\pi,0)$ the data differ significantly from the prediction of the t-J model and the dispersion from $(\pi,0)$ to $(0,\pi)$ is much greater than that in the t-J model.

Recently Nazarenko *et al.*[2] calculated the hole dispersion in the one-band t-t'-J model under the self-consistent Born approximation (SCBA). They found that the presence of the t' term can enlarge the energy dispersion around $(0,\pi)$, but the overall band structure is inconsistent with the experimental one. Several groups have also calculated the energy dispersions of the hole in the three-band model based on either variational wave functions[2,3] or SCBA[4] and found that the results reproduce very well the experimental data. These studies seem to imply that the one-band model is inferior to the multiband model even for studying low-energy properties of high-T_c cuprates.[3] This is actually not true. To understand qualitatively the physics of a hole propagating in an antiferromagnetic background, the t-J or t-t'-J model might be sufficient. However, to fit quantitatively the result of a one-band model with the experimental data, the one-band model used should include all the terms which are deduced from the multiband Hubbard model by eliminating high-lying orbitals. At least two of those terms which are ignored in the previous study should be considered, one is the t'' term (i.e., the next-next neighbor hopping term) and the other is the three-site hopping term. Both the t' term and t'' term originated from the effective hopping (or wave function overlap) between two O $2p$ orbitals besides a Cu via the Cu $3d$ and $4s$ orbitals;[5] the t' term is the hopping between two nearest neighboring oxygens, and the t'' term is the hopping between two oxygens on the two sides of Cu. $|t''|$ is generally smaller than, but certainly of the same order of magnitude as $|t'|$.[6] The three-site hopping term is always present if the effective one-band model is derived from the one-band Hubbard model[7] or the multiband Hubbard model.[8] Both the t'' and three-site hopping terms involve hoppings on the same sublattices and are affected very weakly by antiferromagnetic correlations. They may therefore have substantial contributions to the quasiparticle dispersion. Other long-range hopping terms involve the wave function overlap of O orbitals not within the same unit cell and are generally small and negligible.

In this paper we report our theoretical results for the energy dispersion in the one-band model with one hole in two dimensions. Both the Lanczos diagonalization and the SCBA calculations are performed and compared. We find that the experimental data for $Sr_2CuO_2Cl_2$ can be quantitatively fitted by the t-t'-t''-J model with the three-site hopping term within the experimental error.

Let us first consider the t-t'-t''-J model without the three-site hopping term. The model Hamiltonian is defined in the Hilbert subspace without double occupied sites by

$$H=-\sum_{i\delta\sigma}(t_\delta c^\dagger_{i\sigma}c_{i+\delta\sigma}+\text{H.c.})+J\sum_{\langle ij\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j-\tfrac{1}{4}n_in_j), \tag{1}$$

where $\langle\ \rangle$ refers to the nearest neighbors, and $t_\delta=t$ for the nearest neighbor hopping ($\delta=\hat{x},\hat{y}$), t' for the next nearest neighbor hopping ($\delta=\hat{x}\pm\hat{y}$), and t'' for the next-next nearest neighbor hopping ($\delta=2\hat{x},2\hat{y}$). The rest of the notation is standard. For high-T_c materials, both t and J vary in a certain energy scale, $t\approx 0.3-0.4$ eV and $J\approx 0.1-0.2$ eV, depending on compounds. So far, accurate determinations for t and J from experiment are still not available. For concreteness in discussion, we take $t=0.35$ eV and $J=0.15$ eV. The quasiparticle bandwidth evaluated from this set of values of t and J is roughly the same as that for $Sr_2CuO_2Cl_2$ when $t'=t''=0$. In our calculation, we take t' and t'' as free parameters, but restrict $|t''|<|t'|<J$. If the Hamiltonian (1) is derived from the multiband Hubbard model including the Cu

$3d_{x^2-y^2}$ and $4s$ and O p_x and p_y orbitals, then t' is negative (positive) for hole- (electron-) doped materials and t'' has an opposite sign to t'.[5]

For a one-hole system, we can do a Galilean transformation to shift the origin of the frame of coordinates to the position of hole.[9] If the hole momentum is k, following the derivation of Ref. 9 it can then be shown that the Hamiltonian (1) is equivalent to an effective Hamiltonian

$$H_h(k) = -\sum_{\delta\sigma} (t_\delta e^{-i(P-k)\delta} c^\dagger_{\mathbf{0}\sigma} c_{\delta\sigma} + \text{H.c.}) + J\sum_{\langle ij\rangle} (\mathbf{S}_i\cdot\mathbf{S}_j - \tfrac{1}{4} n_i n_j), \quad (2)$$

where $\mathbf{0}=(0,0)$ and $P=\Sigma_{k\sigma} k c^\dagger_{k\sigma} c_{k\sigma}$ is the total momentum operator. In our exact diagonalization study, we solve this effective Hamiltonian on finite-size lattices with periodic boundary condition (PBC), but allow k to change continuously (i.e., k can take all values allowed in an infinite square lattice).

For each given k, we define the difference between the lowest energy of the one-hole Hamiltonian (2) with total spin 1/2, $E_{N-1}(k)$, and the ground state energy of the system without holes, E_N, as the coherent hole quasiparticle energy $E(k)=E_N-E_{N-1}(k)$. The quasiparticle energy $E(k)$ such defined corresponds directly to what was measured in experiments, since the ground state of $Sr_2CuO_2Cl_2$ is a spin singlet and the state with one electron removed from the ground state by high-energy photons has spin 1/2. On finite-size lattices, some higher spin states may have lower energies than $E_{N-1}(k)$ for certain values of k, so $E_{N-1}(k)$ may not always be the minimum energy of $H_h(k)$. However, in thermodynamic limit we believe that $E_{N-1}(k)$ will either be the minimum of $H_h(k)$ or differ infinitesimally small from the minimum energy of $H_h(k)$ for all k. Thus alternatively $E(k)$ can also be defined as the difference between the lowest eigeneigen of $H_h(k)$ and the ground state energy without holes. In thermodynamic limit the above two definitions should give the same result for $E(k)$.

Under the SCBA,[10,11] the quasiparticle energy is given by the position of coherence peak at the bottom of the spectral function $A(k,\omega)=-\text{Im}\, G(k,\omega)/\pi$, and the single particle Green's function $G(k,\omega)$ is determined by the self-consistent equation:

$$G(k,\omega)=\frac{1}{\omega-\varepsilon_k-(1/N)\sum_q \Gamma^2(k,q) G(k-q,\omega-\Omega_q)}, \quad (3)$$

where $\varepsilon_k=4t'\cos k_x\cos k_y+2t''(\cos 2k_x+\cos 2k_y)$ and $\Gamma(k,q)=4t(\gamma_{k-q}u_q+\gamma_k v_q)$ with $\Omega_q=4J\sqrt{1-\gamma_q}$, $u_k=[(1-\gamma_k^2)^{-1/2}+1]^{1/2}/\sqrt{2}$, $v_k=-\text{sgn}(\gamma_k)[(1-\gamma_k^2)^{-1/2}-1]^{1/2}/\sqrt{2}$, and $\gamma_k=(\cos k_x+\cos k_y)/2$. From Eq. (3), it is straightforward to show that $G(k,\omega)$ (and therefore the quasiparticle dispersion) is symmetric under the reflection about the magnetic Brillouin zone boundary (i.e., $k_x+k_y=\pi$) since ε_k is symmetric under this transformation. This symmetry is purely due to the approximations made in this approach; the original Hamiltonian (1) does not have this symmetry.

There are several approximations involved in the SCBA calculation: the linear spin-wave expansion and the neglect of crossing diagrams. These approximations ignore vertex corrections and the hole distortion to the spin background and do not guarantee the hard-core nature of the slave fermions and the Schwinger bosons. In the absence of the t' and t'' terms, the contribution from the two-loop crossing diagram to vertices is exactly zero.[12] Thus the vertex correction in the SCBA calculation for the t-J model is small. However, in the presence of these terms, the two-loop crossing diagrams are generally nonzero.

For the t-J model, the band structure of hole quasiparticles has been extensively studied by many groups,[11–14] and the agreement between the finite-size calculation[13,14] and the SCBA calculation[12] is remarkably good. The quasiparticle dispersion in this model shows many interesting features which are completely different from that in the ordinary metal. Firstly, the band maximum locates at $(\pm\pi/2,\pm\pi/2)$; secondly, the effective mass is very anisotropic, it has a larger value along the zone diagonal and a smaller value along the direction perpendicular; and thirdly, the bandwidth scales with a certain power of the exchange energy J ($\sim J^{2/3}$ when $t\ll J$) rather than the hopping constant t.

In the previous finite-size calculations, the Hamiltonian (1) with PBC were generally used. As the number of k points allowed in a finite lattice with PBC is limited, calculations on large lattices are generally required in order to obtain a complete picture of the quasiparticle band structure. However, if the Hamiltonian (2) with PBC is diagonalized and the hole momentum k in Eq. (2) is taken as a free parameter [this is equivalent to diagonalizing the Hamiltonian (1) with twisted boundary conditions as shown in Ref. 9], we find that even on a relatively small lattice, such as $N=20$, a comprehensive picture of the quasiparticle band structure can be obtained.

In Fig. 1(a), our finite-size diagonalization results for $E(k)$ on $N=16$ and 20 are shown and compared with the SCBA ones for the t-J model. The agreement between the finite lattice calculation and the SCBA calculation in the whole Brillouin zone is good, in agreement with the previous calculations.[13,14] The finite-size effect, as revealed by the difference between the $N=16$ and $N=20$ results and the difference between the finite lattice result and that of SCBA is small. On finite lattices, the band maxima locate not exactly at $(\pm\pi/2,\pm\pi/2)$, but they tend to move towards these points as N increases.[9]

The presence of the next nearest neighbor and the next-next neighbor hopping terms changes largely the energy dispersion of quasiholes. Let us consider the contribution of the t' term first. When $t'<0$, as shown in 1(b), the energy dispersion along the line $(\pi,0)-(0,\pi)$ is enlarged. Around $(\pi,0)$, the dispersion is relatively small, but $E(k)$ falls much below the band maximum. These features are qualitatively consistent with the experimental results for $Sr_2CuO_2Cl_2$.[1] However, the overall dispersion of $E(k)$ [except at the vicinity of (π,π)] is largely reduced by the t' term. If fitting the experimental data of $Sr_2CuO_2Cl_2$ using the t-t'-J model, we find that a rather large J value, about twice as large as what has been found in experiments, is needed.

When $t'>0$, as shown in Fig. 1(c), $E(k)$ behaves quite differently from the case $t'<0$: (1) In this case the band

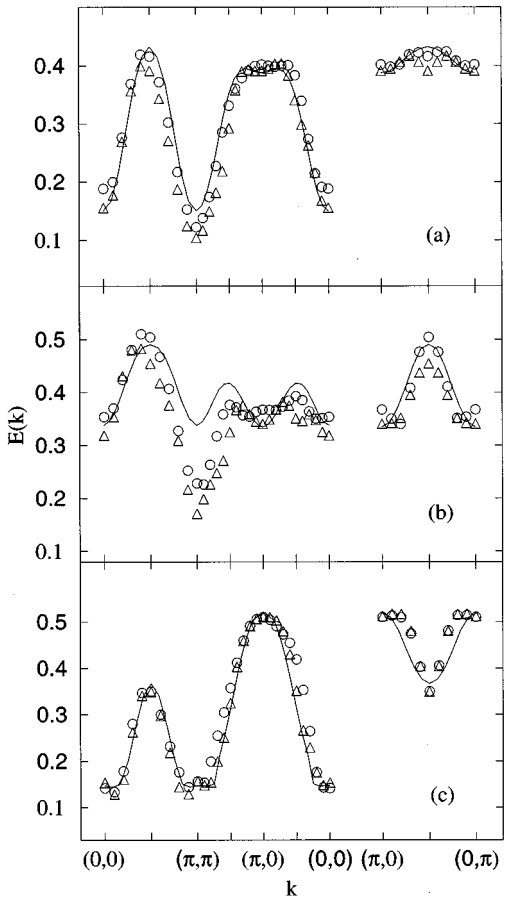

FIG. 1. Comparison of the quasiparticle dispersion relation $E(k)$ (unit: eV) obtained from the SCBA method on 24×24 lattice (solid line) with that obtained from the finite-size diagonalization method on $N=16$ (triangle) and $N=20$ (circle) lattices for the t-t'-J model with $t=0.35$ eV, $J=0.15$ eV and (a) $t'=0$, (b) $t'=-0.08$ eV, and (c) $t'=0.08$ eV.

maxima locate at $(\pi,0)$ and its equivalent points, consistent with other theoretical results;[15] (2) the bandwidth is enlarged compared with the t-J model ; (3) $E(k)$ becomes more symmetric about the magnetic Brillouin zone boundary and shows a large dispersion along the line $(\pi,\pi)-(\pi,0)-(0,0)$; (4) The agreement between the SCBA and the finite-size calculations is fairly good and the finite-size effect is even smaller than that for the t-J model. However, as t' gets larger, there is no well-defined coherent peak at the bottom of a quasiparticle spectrum when k is in the vicinity of (0,0) in the SCBA. So far no ARPES data are available for electron-doped cuprates for comparison. If we believe that the asymmetry between the electron and hole-doped high-T_c materials is mainly due to the next nearest neighbor hopping term, then the above features of $E(k)$ should in principle be observable in the ARPES spectrum in electron-doped materials.

For the t-t'-J model with a negative t' term, the overall agreement between the finite-size calculation and the SCBA calculation is not as good as for the $t'\geqslant0$ cases. This disagreement is probably due to the linear spin-wave approximation in the SCBA approach which ignores the influence of holes to the quantum antiferromagnetic Néel state. A positive (negative) t' term can enhance (reduce) the antiferromagnetic correlations in the one band-model.[16] So in the presence of a negative t' term, the distortion of a hole to the quantum antiferromagnetic Néel state is enlarged. In this case to obtain a more quantitative description for the quasiparticle dispersion, exact diagonalizations on larger lattices are needed.

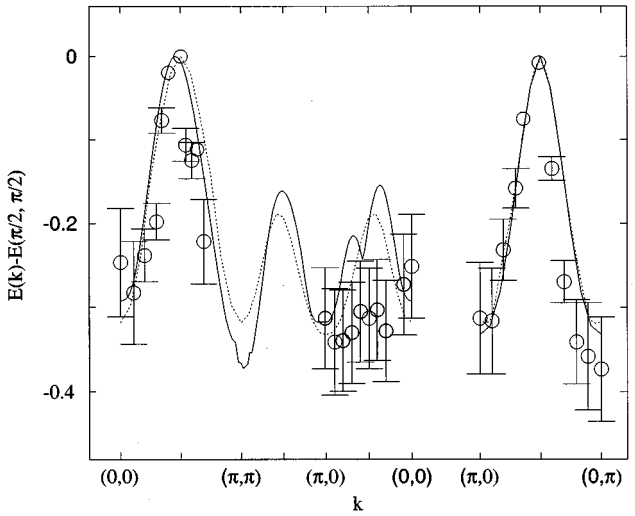

FIG. 2. Comparison of the quasiparticle energy $E(k)-E(\pi/2,\pi/2)$ (unit: eV) in $Sr_2CuO_2Cl_2$ (circle) with the corresponding results for the t-t'-t''-J model obtained from the exact diagonalization with $N=20$ (solid line) and the SCBA approach (dashed line). $t=0.35$ eV, $t'=-0.12$ eV, $t''=0.08$ eV, and $J=0.15$ eV.

The above discussion indicates that the bandwidth of the t-t'-J model is too small compared with the experimental one for $Sr_2CuO_2Cl_2$ within the physically reasonable region of parameters, consistent with the previous study.[2] A finite t'' term, however, can change this situation significantly. The contribution of the t'' term to $E(k)$ is similar to a $-t'$ term, for example for the t-t''-J model ($t'=0$) the band maximum locates at $(\pi/2,\pi/2)$ if $t''>0$ or $(\pi,0)$ if $t''<0$, but the overall energy dispersion is always enlarged by the t'' term.

In Fig. 2 the quasiparticle dispersions for the t-t'-t''-J model are shown and compared with the experimental data for $Sr_2CuO_2Cl_2$. Along two diagonal lines, $(0,0)-(\pi,\pi)$ and $(\pi,0)-(0,\pi)$, the finite-size effect is small and the agreement between the experimental data and our calculation is very good. Compared with Fig. 1(b), we find that the bandwidth is largely enhanced by even a small t'' term. Along the line $(\pi\pi)-(\pi,0)-(0,0)$, the energy dispersion obtained from both the exact diagonalization and SCBA calculations is larger than the experimental one, and the agreement between the exact diagonalization and the SCBA results along this line is also not as good as along two diagonal lines. A subpeak appears in the curve of the exact diagonalization result on the line $(\pi,0)-(0,0)$. This is purely due to the finite-size effect.

Now let us consider the three-site hopping term. The Hamiltonian for the three-site hopping term is given by[7,8,17]

$$H_{3\text{-site}}=\frac{J}{4}\sum_{\langle ij\rangle\neq\langle ik\rangle\sigma}(c^{\dagger}_{i\bar{\sigma}}c_{i\sigma}c^{\dagger}_{j\sigma}c_{k\bar{\sigma}}-n_{i\bar{\sigma}}c^{\dagger}_{j\sigma}c_{k\sigma}). \qquad (4)$$

This term describes an effective hopping of a hole to one of its next or next-next neighbor sites by exchanging spins with another hole on its nearest neighbor site. From the calculation we find that this term has a very weak effect on the quasiparticle dispersion along two diagonal lines. However, it has a relatively larger effect on $E(k)$ when k varies along $(\pi,\pi)-(\pi,0)-(0,0)$. It suppresses the dispersion of $E(k)$ on $(\pi,\pi)-(\pi,0)-(0,0)$ and therefore improves the agreement between the theoretical result and the experimental data. Figure 3 compares the energy dispersion of the t-t'-t''-J model with the three-site term on a $N=20$ lattice with that of $Sr_2CuO_2Cl_2$. It is easy to see that the one-band t-t'-t''-J model with the three-site hopping term gives a good account for the quasiparticle dispersion in $Sr_2CuO_2Cl_2$. This result is consistent with the previous studies for the quasiparticle dispersion based upon the multiband Hubbard model.[2–4] It implies that the multiband Hubbard model is indeed equivalent to a one-band model in describing low-energy excitations of high-T_c cuprates.

In conclusion, we have studied the energy dispersion of hole quasiparticles in an antiferromagnetically correlated background using the exact diagonalization and the SCBA methods. In the exact diagonalization study, we first derive an effective Hamiltonian for the one-hole t-J model using the Galilean transformation for each given hole momentum k (which can take all allowed values in an infinite lattice), and then diagonalize this effective Hamiltonian on finite lattices with PBC. As there is no limitation for k values, this allows us to have a comprehensive study for the band structure of quasiparticles with the finite-size diagonalization even on a $N=20$ lattice. We find that the finite-size diagonalization results agree well with the SCBA ones, especially when $t'\geqslant 0$. For hole-doped high-T_c compounds, the band maxima locate at $(\pm\pi/2,\pm\pi/2)$ in thermodynamic limit. However, for electron-doped compounds, the band maxima locate at $(\pi,0)$ and its equivalent points. The experimental data for $Sr_2CuO_2Cl_2$ can be quantitatively understood from the one band t-t'-t''-J model with the three-site hopping term.

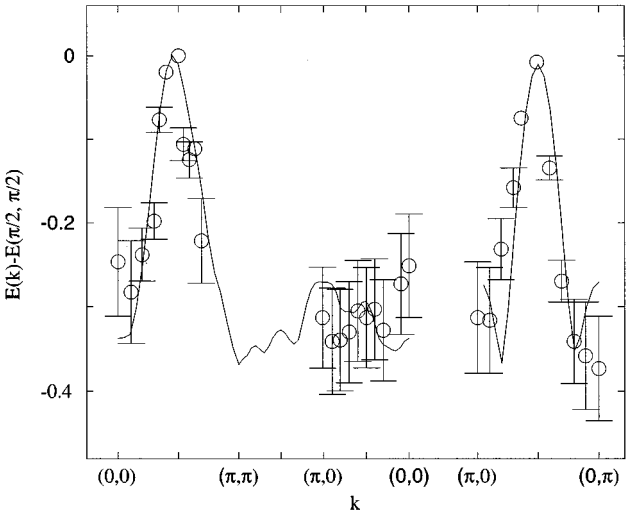

FIG. 3. Comparison between the quasiparticle energy $E(k)-E(\pi/2,\pi/2)$ (unit: eV) of the t-t'-t''-J model with the three-site hopping term on a $N=20$ lattice (curve) and that of $Sr_2CuO_2Cl_2$. $t=0.35$ eV, $t'=-0.12$ eV, $t''=0.08$ eV, and $J=0.15$ eV.

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