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

The quasiparticle dispersion in the one-hole \( t - t' - t'' - J \) model is studied. Both the 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 located at \((\pm \pi/2, \pm \pi/2)\), while in the electron doped compounds the band maxima locate at \((\pi, 0)\) and its equivalent points. The angle-resolved photoemission data for the quasiparticle dispersion of \( \text{Sr}_2\text{CuO}_2\text{Cl}_2 \) can be quantitatively reproduced using the one band \( t - t' - t'' - J \) model with the three-site hopping term.

The energy dispersion of hole quasiparticles in the normal states of two-dimensional CuO planes is of fundamental interest for understanding the microscopic mechanism of high temperature superconductivity. Due to the strong Coulomb repulsion between electrons, quasiparticles in high-\( T_c \) cuprates behave very differently from what predicted by one-electron band calculations. Recently Wells et al. \cite{1} has reported an ARPES measurement on an insulating layered copper oxide \( \text{Sr}_2\text{CuO}_2\text{Cl}_2 \). This is by far the most direct measurement of the dispersion of a single hole in an antiferromagnetic background since \( \text{Sr}_2\text{CuO}_2\text{Cl}_2 \) is difficult to dope. It provides a direct test for the model Hamiltonians which are proposed for high temperature superconductors. Wells et al. has found that the the hole bandwidth and the dispersion along the diagonal direction from \((0, 0)\) to \((\pi, \pi)\) in 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. \cite{2} has 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 bandstructure is inconsistent with the experimental one. Several groups have also calculated the energy dispersions of hole in the three bands model based on either variational wavefunctions \cite{3,4} or SCBA \cite{5} 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 \cite{1}. 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 highlying 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 are originated from the effective hopping (or wavefunction overlap) between two O 2p orbitals besides a Cu via the Cu 3d and 4s orbitals \cite{6}; 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 \( |t'| \). \cite{7} The three site hopping term is always present if the effective one band model is derived from the one band Hubbard model \cite{8} or the multiband Hubbard model \cite{9}. Both the \( t'' \) and three-site hopping terms involve hoppings on 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 wavefunction 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 \( \text{Sr}_2\text{CuO}_2\text{Cl}_2 \) 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

\[
H = -\sum_{\delta \sigma}(t_{\delta} \hat{c}_{i, \sigma}^{\dagger} c_{i+\delta \sigma} + H.c.) + J \sum_{\langle ij \rangle} \langle \mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4}n_i n_j \rangle,
\]

where \( \langle \cdot \rangle \) refers 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 notation is standard. For high-\( T_c \) materials, both \( t \) and \( J \) vary in a certain energy scale, \( t \approx 0.3 \sim 0.4\text{eV} \) and \( J \approx 0.1 \sim 0.2\text{eV} \), depending on compounds. So far accurate determinations for \( t \) and \( J \) from experiment are
the spectral function without holes. In thermodynamic limit the above two minimum energy of the Hamiltonian \( \mathcal{H} \) 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. However, in thermodynamic limit we believe that the quasiparticle energy is restricted to shift the origin of the frame of coordinates to \( k \) when \( t' \) and \( t'' \) change continuously \( \left( i.e. \ t' \right. \) or \( \left. t'' \right| < J \). If the Hamiltonian \( \mathcal{H} \) is taken as a free parameter (this is equivalent to different from that in the ordinary metal. Firstly, the band structure of Sr\( _2 \)CuO\( _2 \)Cl\( _2 \) 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 \( E_{N-1} \) for certain values of \( k \), so \( E_{N-1} \) may not always be the minimum energy of \( H_h(k) \). However, in thermodynamic limit we believe that \( E_{N-1} \) 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, 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:

\[
G(k, \omega) = \frac{1}{\omega - \varepsilon_k - \frac{1}{\pi} \sum_q \Gamma^2(k, q)G(k - q, \omega - \Omega_q)}, \tag{3}
\]

where \( \varepsilon_k = 4t' \cos k_x \cos k_y + 2t'' \cos 2k_x + \cos 2k_y \) and \( \Gamma(k, q) = 4t(\gamma_1 \cos q_y + \gamma_2 \cos q_y) \) with \( \Omega_q = 4J \sqrt{1 - \gamma^2} \), \( u_k = [(1 - \gamma^2)^{-1/2} + 1]^{1/2}/\sqrt{2} \), \( v_k = -\text{sgn}(\gamma_k) [(1 - \gamma^2)^{-1/2} - 1]^{1/2}/\sqrt{2} \), 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 \( \varepsilon_k \) is symmetric under this transformation. This symmetry is purely due to the approximations made in this approach; the original Hamiltonian \( \mathcal{H} \) 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 vertexs is exactly zero \( \mathcal{H} \). Thus the the vertex correction in the SCBA calculation for the \( t-J \) model is small. However, in the presence of these terms, the two-crossing diagrams are generally nonzero.

For the \( t-J \) model, the band structure of hole quasiparticles has been extensively studied by many groups \( \mathcal{H} \) and \( \mathcal{H} \), and the agreement between the finite size calculation \( \mathcal{H} \) and the SCBA calculation \( \mathcal{H} \) 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 band width scales with \( N \) and that of SCBA is small. On finite lattices, the finite size calculation and the SCBA calculation in \( \mathcal{H} \) is taken as a free parameter (this is equivalent to diagonalizing the Hamiltonian \( \mathcal{H} \) with twisted boundary conditions as shown in Ref. \( \mathcal{H} \)), 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. 1a, 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. 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.
been found in experiments, is needed.

differently from the case of SrCl₂,

tpersion of the line (π, π, π)

the energy dispersion along the line (π, π, π)

The presence of the next nearest neighbor and the

The above discussion indicates that the bandwidth of the
t→J model is too small compared with the experimental one for Sr₂CuO₂Cl₂ within the physically reasonable region of parameters, consistent with the previous study [9]. 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 (π/2, π/2) if t'' > 0 or (π, 0) if t'' < 0, but the overall energy dispersion is always enlarged by the t'' term.

In Fig. 3 the quasiparticle dispersions for the t − t' − t'' − J model are shown and compared with the experi-

![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 = 0.35ev, J = 0.15ev and (a) t' = 0, (b) t' = -0.08ev , and (c) t' = 0.08ev.](image1)

![FIG. 2. Comparison of the quasiparticle energy E(k) = E(π/2, π/2) (unit: ev) in Sr₂CuO₂Cl₂ (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 = 0.35ev, t' = -0.12ev, t'' = 0.08ev, and J = 0.15ev.](image2)
mental data for Sr$_2$CuO$_2$Cl$_2$. Along two diagonal lines, $(0,0) - (\pi, \pi)$ and $(\pi, 0) - (0,0)$, the finite size effect is small and the agreement between the experimental data and our calculation is very good. Compared with Fig. 1b, 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 sub-peak 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.

![Graph](image)

**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$_2$CuO$_2$Cl$_2$. $t = 0.35$eV, $t' = -0.12$eV, $t'' = 0.08$eV, and $J = 0.15$eV.

Now let us consider the three-site hopping term. The Hamiltonian for the three-site hopping term is given by

$$H_{3-site} = \frac{J}{4} \sum_{(ij)\neq (ik)\sigma} \left( c_{i\sigma}^\dagger c_{i\sigma} c_{j\sigma}^\dagger c_{k\sigma} - n_{i\sigma} c_{j\sigma}^\dagger c_{k\sigma} \right). \quad (4)$$

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 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. Fig. 4 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$_2$CuO$_2$Cl$_2$. 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$_2$CuO$_2$Cl$_2$. This result is consistent with the previous studies for the quasiparticle dispersion based upon the multiband Hubbard model.

It implies that the 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 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 $t' > 0$. 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$_2$CuO$_2$Cl$_2$ can be qualitatively understood from the one band $t - t' - t'' - J$ model with the three-site hopping term.

---

1. B. O. Wells, Z.-X. Shen, A. Matsuura, D. M. King, M. A. Kastner, M. Greven, and R. J. Birgeneau, Phys. Rev. Lett. 74, 964 (1995).
2. A. Nazarenko, K. J. E. Vos, S. Haas, E. Dagotta, and R. J. Gooding, Phys. Rev. B 51, 8676 (1995).
3. K. J. E. Vos and R. J. Gooding, cond-mat/9511030, to be published in Z. Phys. B.
4. O. A. Starykh, O. F. de A. Bonfim, and G. F. Reiter, Phys. Rev. B 52, 15254 (1995).
5. D. C. Mattis and J. M. Wheatley, Mod. Phys. Lett. 9, 1107 (1995).
6. More precious calculation for the values of $t'$ and $t''$ needs consider the orthogonality of the Wannier representation of O 2p bonding and nonbonding orbitals. Direct O-O wavefunction overlap may have also a small contribution to $t'$.
7. J. E. Hirsch, Phys. Rev. Lett. 54, 1317 (1985).
8. M. Ogata and H. Shiba, J. Phys. Soc. Jpn. 57, 3074 (1988).
9. T. Xiang, Phys. Rev. B 44, 2276 (1991).
10. S. Schmitt-Rink, C. M. Varma, and A. E. Ruckenstein, Phys. Rev. Lett. 60, 2793 (1988).
11. C. Kane, P. A. Lee, and N. Read, Phys. Rev. B 39, 6880 (1989).
12. Z. Liu and E. Manoussakis, Phys. Rev. B 45, 2425 (1992).
13. E. Dagotta, A. Nazarenko, and M. Boninsegni, Phys. Rev. Lett. 73, 728 (1994).
14. P. W. Leung and R. J. Gooding, Phys. Rev. B (1996).
[15] T. Tohyama and S. Maekawa, Phys. Rev. B 49, 3596 (1994).