

## Quasiparticle photoemission intensity in doped two-dimensional quantum antiferromagnets

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Using the self-consistent Born approximation, and the corresponding wave function of the magnetic polaron, we calculate the quasiparticle weight corresponding to destruction of a real electron (in contrast to creation of a spinless holon), as a function of wave vector for one hole in a generalized  $t$ - $J$  model and the strong-coupling limit of a generalized Hubbard model. The results are in excellent agreement with those obtained by exact diagonalization of a sufficiently large cluster. Only the Hubbard weight compares very well with photoemission measurements in  $\text{Sr}_2\text{CuO}_2\text{Cl}_2$ . [S0163-1829(97)05821-9]

The problem of a single hole in an antiferromagnetic background has been a subject of considerable interest since the discovery of high- $T_c$  systems. One of the most powerful tools for this study is the self-consistent Born approximation (SCBA).<sup>1-4</sup> Excellent agreement has been obtained between the position of the lowest pole of the holon Green function of the SCBA and the quasiparticle dispersion obtained by exact diagonalization of small systems.<sup>3-5</sup> An important advance in the understanding of the SCBA has been the explicit construction of the corresponding wave function by Reiter.<sup>6</sup>

The interest in the problem has been revived by recent angle-resolved photoemission experiments on insulating  $\text{Sr}_2\text{CuO}_2\text{Cl}_2$ , in which the hole dispersion and quasiparticle weight have been measured.<sup>7</sup> While it was clear that the ‘‘bare’’  $t$ - $J$  model was unable to explain the observed dispersion, several works have appeared fitting the experimental dispersion using generalized  $t$ - $J$  models,<sup>5,8,9</sup> a generalized Hubbard model<sup>10</sup> and the spin-fermion (or Kondo-Heisenberg) model for the cuprates.<sup>11</sup> Except for the fact that the bandwidth is  $\sim 10\%$  narrower than the experimental result if the experimental value of  $J$  is taken,<sup>12</sup> the generalized  $t$ - $J$  model including hopping to second and third nearest neighbors (NN) and the three-site term  $t''$ , reproduces well the experimental dispersion<sup>5,9</sup> and also other properties of the spin-fermion and three-band Hubbard models.<sup>12</sup> A consistent picture of the observed spin and charge excitations has been obtained using a generalized one-band Hubbard model.<sup>10</sup>

However, very little attention has been devoted to the explanation of the intensity of the observed quasiparticle peaks. This task is difficult for the following reasons: (i) exact results for quasiparticle intensities in sufficiently large clusters (containing more than 16 unit cells, as discussed below) exist only for the ‘‘bare’’  $t$ - $J$  model and only at a few wave vectors. (ii) The SCBA provides the Green function of the spinless holon, while the Green function of the real particles contain spin-wave excitations and simple decoupling approximations do not provide reasonable results. The holon weights are the same for wave vectors differing in  $(\pi, \pi)$  contrary to experiment. (iii) While a lot of work has been devoted to the mapping of the three-band Hubbard model for the cuprates to low-energy effective models, less attention has been devoted to the mapping of the corresponding operators.<sup>12,14,15</sup> This information as well as the photoionization cross sections for Cu and O are necessary if accurate weights are wished.

In this paper we calculate the photoemission quasiparticle weight for removing an electron, as a function of wave vector in generalized  $t$ - $J$  and strong-coupling Hubbard models, using the SCBA and the wave function of the polaron.<sup>6</sup> The Hamiltonian has the form

$$\begin{aligned}
 H = & - \sum_{i\delta\sigma} t_{\delta} c_{i+\delta\sigma}^{\dagger} c_{i\sigma} - t'' \\
 & \times \sum_{i\eta\neq\eta'\sigma} c_{i+\eta'\sigma}^{\dagger} c_{i+\eta\sigma} \left( \frac{1}{2} - 2\mathbf{S}_i \cdot \mathbf{S}_{i+\eta} \right) \\
 & + \frac{J}{2} \sum_{i\eta} \left( \mathbf{S}_i \cdot \mathbf{S}_{i+\eta} - \frac{1}{4} n_i n_{i+\eta} \right). \quad (1)
 \end{aligned}$$

The first term contains hopping to first-, second-, and third- nearest neighbors (NN) with parameters  $t_1, t_2, t_3$ , respectively. The first NN of site  $i$  are labeled as  $i + \eta$ . Equation (1) is obtained from a standard canonical transformation of a Hubbard model with hoppings  $t_1, t_2, t_3$ , if (complicated) terms smaller than  $t'' = t^2/U$  are neglected.<sup>16</sup> The difference between generalized  $t$ - $J$  and strong-coupling Hubbard models is the meaning of the operator  $c_{i\sigma}$ , as explained below. The Hamiltonian can be written in terms of spinless fermions and spin-wave operators.<sup>1-4,16</sup> We adopt the procedure and notation used by Martínez and Horsch,<sup>3</sup> slightly generalized to include second- and third- NN hoppings and the three-site term:<sup>16</sup> The sublattice  $A$  is defined as that of positive magnetization. The spins of sublattice  $B$  are rotated  $180^\circ$  around the  $x$  axis. In this way the Néel state is converted into a fully polarized ferromagnetic state, restoring the translational symmetry of the nonmagnetic state at the price of losing the conservation of spin. Then, the  $c_{i\uparrow}$  operator is defined as a spinless holon creation operator  $h_i^{\dagger}$ , while  $c_{i\downarrow}$  becomes a composite operator involving a local spin deviation  $a_i$ . The result of both operations is the following representation:

$$\begin{aligned}
 c_{i\uparrow} &= h_i^{\dagger}, \quad c_{i\downarrow} = h_i^{\dagger} a_i, \quad \text{if } i \in A, \\
 c_{i\uparrow} &= h_i^{\dagger} a_i, \quad c_{i\downarrow} = h_i^{\dagger}, \quad \text{if } i \in B. \quad (2)
 \end{aligned}$$

In the exchange part [last term of Eq. (1)] the fermion occupation numbers are averaged and the bosonic quadratic part is diagonalized by a standard canonical transformation:

$$\alpha_q = u_q a_q - v_q a_{-q}^\dagger, \quad (3)$$

where  $u_q^2 = v_q^2 + 1 = 1/2 + 1/(2\nu_q)$ ,  $\nu_q = (1 - \gamma_q^2)^{1/2}$ ,  $u_q > 0$ ,  $\text{sgn}(v_q) = \text{sgn}(\gamma_q)$ , and  $\gamma_q = (\cos q_x + \cos q_y)/2$ . Retaining only linear terms in spin deviations for the rest of Eq. (1), the Hamiltonian becomes

$$H = E_J^0 + \sum_q \omega_q \alpha_q^\dagger \alpha_q + \sum_k \epsilon_k h_k^\dagger h_k + \frac{4t_1}{\sqrt{N}} \sum_{kq} M(k, q) (h_k^\dagger h_{k-q} \alpha_q + \text{H.c.}), \quad (4)$$

where  $E_J^0$  is a constant,  $\omega_q = 2J\nu_q$ ,  $\epsilon_k = [t_2 + 2(1-x)t']\epsilon_2(k) + [t_3 + (1-x)t']\epsilon_1(2k)$ , and  $M(k, q) = (u_q \gamma_{k-q} + v_q \gamma_k)$ , with  $\epsilon_1(k) = 4\gamma_k$  and  $\epsilon_2(k) = 4\cos k_x \cos k_y$ . In the present case, the doping  $x=0$ . The constraint that at the same site there cannot be both a hole and a spin deviation is neglected since it does not affect the results for motion of a hole in a *quantum* antiferromagnet.<sup>3</sup> The holon Green function  $G_h(k, \omega)$  is obtained from the self-consistent solution of the following two equations:

$$\Sigma(k, \omega) = \frac{4t_1}{N} \sum_q M^2(k, q) G_h(k-q, \omega - \omega_q),$$

$$G^{-1}(k, \omega) = \omega - \epsilon_k - \Sigma(k, \omega) + i\epsilon. \quad (5)$$

We have solved Eqs. (5) in clusters of  $16 \times 16$  and  $20 \times 20$  sites. In order to obtain accurate values of the holon quasiparticle weight  $Z_h$ , we have discretized the frequencies in intervals of  $\Delta\omega = 10^{-4}t_1$  and have taken the small imaginary part  $\epsilon = 5\Delta\omega$ . As an alternative method to that used by Liu and Manousakis,<sup>4</sup> we have fitted the part of the spectral weight nearest to the quasiparticle peak by a sum of several Lorentzian functions. The resulting width of the quasiparticle peak was practically identical to  $2\epsilon$  and from its integrated weight we determined  $Z_h$ . We have verified that using this method there are practically no finite-size effects in our clusters.

In the sudden approximation, the angle-resolved photoemission spectrum is proportional to the spectral density of states for Cu and O at wave vector  $k$ . These in turn are related to the imaginary part of the Green function for the generalized  $t$ - $J$  operator  $c_{k\sigma}$  or the generalized Hubbard operator  $\tilde{c}_{k\sigma}$  through a low-energy reduction procedure.<sup>12,15</sup> In linear order in  $1/U$ , the well-known procedure of the canonical transformation<sup>14,17</sup> applied to the generalized Hubbard model, in the subspace of no double occupancy, leads to

$$\tilde{c}_{i\sigma} = c_{i\sigma} + \sum_{\delta} \frac{t_{\delta}}{U} (n_{i\bar{\sigma}} c_{i+\delta\bar{\sigma}} - c_{i\bar{\sigma}}^\dagger c_{i+\delta\bar{\sigma}}). \quad (6)$$

Calling  $|0\rangle$  ( $|\psi_k\rangle$ ) the ground state of Eq. (4) for the undoped (hole doped with wave vector  $k$ ) system, and using the Lehmann representation of the wave function, one realizes that while the holon quasiparticle weight is

$$Z_h(k) = |\langle \psi_k | h_k^\dagger | 0 \rangle|^2, \quad (7)$$

the weight for emitting a Hubbard electron is

$$Z_{c\sigma}^{GH}(k) = |\langle \psi_k | \tilde{c}_{k\sigma} | 0 \rangle|^2 + |\langle \psi_{k+Q} | \tilde{c}_{k\sigma} | 0 \rangle|^2, \quad (8)$$

where  $Q = (\pi, \pi)$ , and  $|\psi_k\rangle$  and  $|\psi_{k+Q}\rangle$  are the *degenerate* eigenstates of the lowest energy of Eq. (4) with a finite overlap with  $\tilde{c}_{k\sigma}|0\rangle$ . The corresponding result for the generalized  $t$ - $J$  model  $Z_{c\sigma}^{GIJ}(k)$  is obtained taking infinite  $U$ . Since  $Z_{c\uparrow}(k) = Z_{c\downarrow}(k)$  we restrict to spin up in the following. The states  $|\psi_k\rangle$  can be constructed following the procedure used by Reiter.<sup>6</sup> The only change in Eqs. (1)–(10) of Ref. 6, is that the quasiparticle energy  $\lambda_k = \lambda_{k+Q}$  is replaced by  $\lambda_k - \epsilon_k$  in Eqs. (3), (6), and (9), and by  $\lambda_k - \epsilon_{k-q}$  in Eq. (4). Thus, writing explicitly only the terms with less than two spin-wave excitations we have

$$|\psi_k\rangle = A_0(k) h_k^\dagger |0\rangle + \frac{1}{\sqrt{N}} \sum_q A_1(k, q) h_{k-q}^\dagger \alpha_q^\dagger |0\rangle + \dots, \quad (9)$$

where

$$A_1(k, q) = 4t_1 M(k, q) G_h(k-q, \lambda_k - \omega_q) A_0(k). \quad (10)$$

Using Eqs. (2) and (6) and retaining only term lines in spin deviations we obtain

$$\tilde{c}_{i\uparrow} = h_i^\dagger - \frac{t_1}{U} (1-x) \sum_{\eta} h_{i+\eta}^\dagger a_i^\dagger, \quad \text{if } i \in A,$$

$$\tilde{c}_{i\uparrow} = h_i^\dagger a_i + \frac{1-x}{U} \times \left[ t_1 \sum_{\eta} h_{i+\eta}^\dagger + \sum_{\delta \neq \eta} t_{\delta} h_{i+\delta}^\dagger (a_{i+\delta} - a_i) \right], \quad i \in B. \quad (11)$$

The most important correction of order  $1/U$  is the first term between brackets in the second Eq. (11) and reflects the fact that in the ground state of the undoped Hubbard model, there is a finite double occupancy at sites  $B$  and an electron with spin up can be destroyed there, leaving a hole in one of its NN [this leads to the second term between brackets in Eqs. (12) and (14)].

Expressing Eqs. (11) in Fourier components, and using  $\sum_{i \in A(B)} e^{ikR_i} = (\delta_{k,0} + e^{iQR_i} \delta_{k,Q}) N/2$ , we obtain

$$\tilde{c}_{k\uparrow} = \frac{1}{2} [1 + f(k)] (h_k^\dagger + s_A h_{k+Q}^\dagger) + \frac{1}{2\sqrt{N}} \sum_q (h_{k+q}^\dagger - s_A h_{k+q+Q}^\dagger) \times \{ [1 + g(k, q)] a_q - f(k) a_q^\dagger \}, \quad (12)$$

where the phase  $s_A = e^{iQR_i}$  with  $i \in A$ , and

$$f(k) = \frac{t_1}{U} (1-x) \epsilon_1(k),$$

$$g(k, q) = \frac{1-x}{U} \{ t_2 [\epsilon_2(k) - \epsilon_2(k+q)] + t_3 [\epsilon_1(2k) - \epsilon_1(2k+2q)] \}. \quad (13)$$

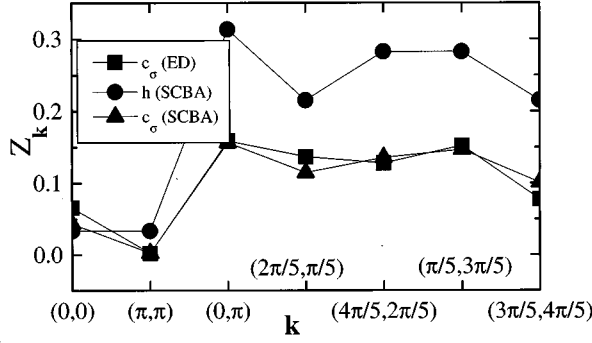


FIG. 1. Quasiparticle weight of the  $t$ - $J$  model  $Z_{c\sigma}^{tJ}(k)$  calculated with the SCBA in a  $20 \times 20$  lattice for several wave vectors (triangles), compared with exact diagonalization results in a square cluster of 20 sites  $Z_{ED}^{tJ}(k)$  (Refs. 13,18) (squares), and the spinless holon weight  $Z_h(k)$  of the SCBA (circles). Parameters are  $t_1=1$ ,  $J=0.3$ ,  $t_2=t_3=t''=0$ .

Using Eqs. (3), (7), (8), (9), (10), and (12) we obtain the desired result

$$\frac{Z_{c\sigma}^{GH}(k)}{Z_h(k)} = \frac{1}{2} \left| 1 + f(k) + \frac{8t_1}{N} \sum_q' M(k,q) G_h(k-q, \lambda_k - \omega_q) \right. \\ \left. \times \{v_q[1 + g(k,q)] - u_q f(k)\} \right|^2. \quad (14)$$

The sum is restricted to the magnetic Brillouin zone and the term with  $q=0$  is excluded (there are no magnons with  $q=0$  or  $q=Q$  in the  $|\psi_k\rangle$ ). The weight  $Z_{c\sigma}^{tJ}$  for the generalized  $t$ - $J$  model operator  $c_{i\sigma}$  is given by Eq. (14) with the Hubbard perturbative corrections  $f(k)$  (first NN) and  $g(k,q)$  (second and third NN) set to zero.

In Fig. 1 we compare the weight for the  $t$ - $J$  model obtained by exact diagonalization  $Z_{ED}^{tJ}(k)$  in a square lattice of 20 sites<sup>13</sup> with our results  $Z_{c\sigma}^{tJ}(k)$  for the  $20 \times 20$  cluster at equivalent wave vectors. The comparison between exact results for square clusters of 16, 18, 20, and 26 sites suggest that while the  $Z_{ED}^{tJ}(k)$  are nearly 20% larger for the  $4 \times 4$  cluster, the finite-size effects are of the order of 5% for larger clusters.<sup>13</sup> The agreement between the exact  $Z_{ED}^{tJ}(k)$  and SCBA  $Z_{c\sigma}^{tJ}(k)$  results is quite satisfactory. Note that the very small value of  $Z^{tJ}(Q)$  is a severe test to Eq. (14), since it requires a near cancellation of the different terms. Instead, the ‘bare’ SCBA result satisfies  $Z_h(k) = Z_h(k+Q)$  and cannot reproduce the shape of the exact results.

With the confidence gained by the above comparison, we have calculated the generalized  $t$ - $J$  and Hubbard weights for parameters which fit the observed quasiparticle dispersion  $\lambda_k$  in  $\text{Sr}_2\text{CuO}_2\text{Cl}_2$ .<sup>7</sup> There are several choices of  $t_2$ ,  $t_3$ , and  $t''$ , including different signs of  $t''$  which produce nearly identical results. We took the parameters of Ref. 5. The resulting dispersion and weights are represented in Fig. 2. Compared with the parameters of Fig. 1, the effects of  $t_2$ ,  $t_3$ , and  $t''$  are dramatic. They push the  $\lambda_k$  towards the incoherent part of the spectrum and reduce considerably the weights for the lowest  $\lambda_k$  (in the electron representation of Fig. 2). As a consequence, we could not detect quasiparticles near  $k=0$ ,  $Q$  or  $(\pi,0)$  ( $Z_h < 10^{-4}$  for these  $k$ ). Therefore, the corre-

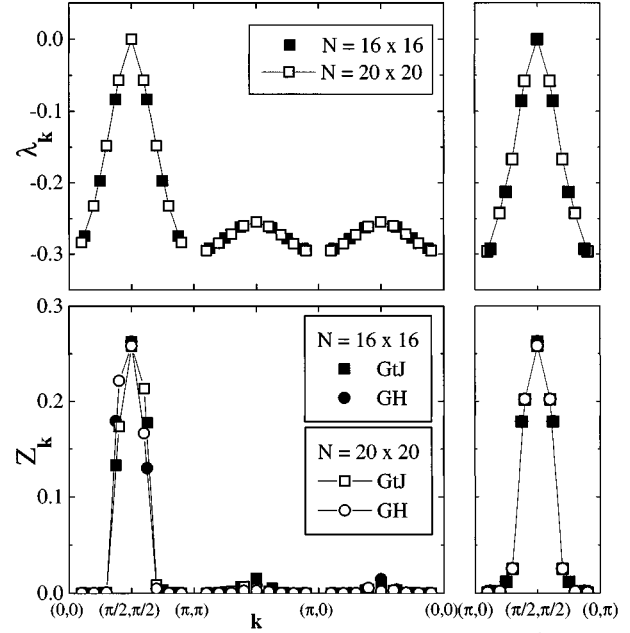


FIG. 2. Top: quasiparticle dispersion in clusters of  $16 \times 16$  (solid symbols) and  $20 \times 20$  sites (open symbols). Bottom: corresponding generalized  $t$ - $J$  (squares) and generalized Hubbard (circles) quasiparticle weights. Parameters are:  $t_1=0.35$ ,  $t_2=-0.12$ ,  $t_3=0.08$ ,  $J=0.15$ ,  $t''=J/4$ , and  $U=3.5$ .

sponding  $\lambda_k$  are not represented in Fig. 2. The weights for the generalized  $t$ - $J$  and Hubbard models have significant differences: in contrast to the results for  $t_2=t_3=t''=0$  (not shown),  $Z_{c\sigma}^{tJ}(k)$  is larger for  $k=(\pi/2+\varepsilon, \pi/2+\varepsilon)$  than for  $k=(\pi/2-\varepsilon, \pi/2-\varepsilon)$  with small  $\varepsilon$ . Instead,  $Z_{c\sigma}^{GH}(k)$ , in agreement with experiment, is larger inside the noninteracting Fermi surface. This effect is more noticeable for smaller values of  $U$  ( $t_1/U=0.1$  was taken in Fig. 2).<sup>19</sup>

In summary, using the SCBA and related wave function, we have calculated the dispersion and quasiparticle weight for removing a real electron in an undoped antiferromagnet described by a generalized  $t$ - $J$  or a generalized Hubbard model in the strong coupling limit. The weight for the  $t$ - $J$  model agrees very well with available exact results in sufficiently large clusters. While the generalized Hubbard can explain well both the measured dispersion *and* weight of the quasiparticle in  $\text{Sr}_2\text{CuO}_2\text{Cl}_2$ , the generalized  $t$ - $J$  model, without mapping the electron operators, cannot.

*Note added.* After submission of this manuscript we became aware of exact diagonalization results (EDR) of the  $t$ - $J$  model in a square cluster of 32 sites with periodic boundary conditions which has nine nonequivalent wave vectors (NEWV).<sup>20</sup> The dispersion relation  $\lambda_k$  agrees very well with the SCBA results except at the three NEWV nearest to  $k=(0,0)$  [ $k=(0,0)$ ,  $(\pi/4, \pi/4)$  and  $(\pi/2, 0)$ ], where finite-size effects in the EDR are obvious from the fact that  $\lambda_k \neq \lambda_{k+Q}$ . Except at the two NEWV nearest to  $k=(0,0)$  [ $k=(0,0)$  and  $(\pi/4, \pi/4)$ ], where the larger value of  $\lambda_k$  in the EDR leads to larger quasiparticle weights  $Z_k$ , these weights are in excellent agreement with our results using Eq. (14).

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- <sup>1</sup>S. Schmitt-Rink, C.M. Varma, and A.E. Ruckenstein, Phys. Rev. Lett. **60**, 2793 (1988).
- <sup>2</sup>C.L. Kane, P.A. Lee, and N. Read, Phys. Rev. B **39**, 6880 (1988).
- <sup>3</sup>G. Martínez and P. Horsch, Phys. Rev. B **44**, 317 (1991).
- <sup>4</sup>Z. Liu and E. Manousakis, Phys. Rev. B **45**, 2425 (1992).
- <sup>5</sup>T. Xiang and J.M. Wheatley, Phys. Rev. B **54**, R12653 (1996).
- <sup>6</sup>G.F. Reiter, Phys. Rev. B **49**, 1536 (1994).
- <sup>7</sup>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).
- <sup>8</sup>A. Nazarenko, K.J.E. Vos, S. Haas, E. Dagotto, and R. Gooding, Phys. Rev. B **51**, 8676 (1995).
- <sup>9</sup>V.I. Belinicher, A.L. Chernyshev, and V.A. Shubin, Phys. Rev. B **54**, 14 914 (1996).
- <sup>10</sup>F. Lema, J. Eroles, C.D. Batista, and E. Gagliano, Phys. Rev. B (unpublished).
- <sup>11</sup>O.A. Starykh, O.F. de Alcantara Bonfim, and G. Reiter, Phys. Rev. B **52**, 12 534 (1995).
- <sup>12</sup>J. Eroles, C.D. Batista, and A.A. Aligia, Physica C **261**, 237 (1996); references therein. For large O-O hopping the resulting three-site term  $t''$  favors a resonance-valence-bond superconducting state in the square lattice [C.D. Batista, and A.A. Aligia, Physica C **261**, 237 (1996); J. Low Temp. Phys. **105**, 591 (1996); Europhys. Lett. (to be published)] and shifts towards lower values of  $J$  the region of dominant superconducting correlations in one dimension [F. Lema, C.D. Batista, and A.A. Aligia, Physica C **259**, 287 (1996)].
- <sup>13</sup>D. Poilblanc, T. Ziman, H.J. Schulz, and E. Dagotto, Phys. Rev. B **47**, 14 267 (1993).
- <sup>14</sup>C.D. Batista and A.A. Aligia, Phys. Rev. B **47**, 8929 (1993).
- <sup>15</sup>L. Feiner, Phys. Rev. B **48**, 16 857 (1993).
- <sup>16</sup>J. Bala, A.M. Oleś, and J. Zaanen, Phys. Rev. B **52**, 4597 (1995).
- <sup>17</sup>H. Eskes, A.M. Oleś, M.B.J. Meinders, and W. Stephan, Phys. Rev. B **50**, 17 980 (1994); references therein.
- <sup>18</sup>When comparing our results with those of Poilblanc *et al.*, it should be taken into account that they took the opposite sign of  $t_1$  (positive for holes), what is equivalent to a shift in  $\mathbf{Q}=(\pi, \pi)$  of all wave vectors, and they summed over both spins, introducing a factor 2 with respect to our results. To compare with experiment the sign of  $t_1$  should be determined by the mapping procedure from the three-band Hubbard model  $H_{3b}$  with original phases (Ref. 12) (the usual change of phases of half of the orbitals of  $H_{3b}$  to have the same sign of the hoppings for all directions changes the sign of  $t_1$ ). After this mapping,  $c_{i1}^\dagger$  has the character of an effective electron creation operator (mainly of O character) over a vacuum state where all sites carry a Zhang-Rice singlet, and  $t_1 \sim 0.3-0.4$  eV  $>0$  results.
- <sup>19</sup>The effect of the correction term  $t_1/U$  has been studied recently using finite-size diagonalization by H. Eskes and R. Eder (unpublished), with results which agree with ours.
- <sup>20</sup>P.W. Leung and R.J. Gooding, Phys. Rev. B **52**, R15 711 (1995); **42**, 711(E) (1995).