PHYSICAL REVIEW B VOLUME 46, NUMBER 21 1 DECEMBER 1992-I

Band structure, magnetic fluctuations, and quasiparticle nature of the two-dimensional three-band Hubbard model

Hong-Qiang Ding, Gladys H. Lang, and William A. Goddard III
Materials Simulation Center, Beckman Institute, California Institute of Technology, Pasadena, California 91125
(Received 27 August 1992; revised manuscript received 30 September 1992)

A single hole doped into the CuO_2 plane of a high-T_c superconductor is studied via exact calculations of the three-band Hubbard model (large-U limit) on a 4×4 periodic cluster. The quasiparticle band has its bottom at $\mathbf{k}=(\pi/2,\pi/2)$ and disperses strongly towards Γ and X with a dispersion $1.7J_{dd}=0.22$ eV. The quasiparticle has a nearly isotropic effective mass ($\sim4m_e$) and the dressing effects are well localized (~8 Å) with characteristic features of both the three-spin polaron and the Zhang-Rice singlet (although solutions of the t-J model are substantially different).

INTRODUCTION

Strongly correlated electron systems such as Hubbard models have been reexamined with great interest since the discovery of high-T_c superconductivity. The one-band Hubbard model, especially the strong-coupling limit (the t-J model), has been extensively studied. The more realistic three-band model has been also analyzed with a variety of methods by many groups.[1-8] The low-lying excitations are sometimes described using a one-band model, however, there are indications that the one-band picture breaks down in the charge-transfer regime.[2] Equally important is the role of direct oxygen-oxygen hopping. Local-density-functional (LDF) calculations[9,10] and generalized valence bond calculations[11] now agree, indicating that doped holes are primarily on the oxygen sites with a large oxygen hopping integral, $t_{pp}\simeq0.65$ eV.

In this paper, we report an exact calculation of the three-band model using a 4×4 periodic finite cluster. The emphasis is on characterizing the nature of the quasiparticle and we find that O-O hopping has a dramatic effect. We study the large-U limit where the spins at the Cu sites are localized and a single hole hops in the oxygen network which interacts with the localized Cu holes.[1,6,7] In the parameter regime relevant to high-T_c materials, we find that the quasiparticle disperses strongly from the band bottom at $S=(\pi/2,\pi/2)$ toward $\Gamma=(0,0)$ or $X=(\pi,\pi)$ with a dispersion of $1.7J=0.22$ eV. The dispersion from S toward $M=(\pi,0)$ or $(0,\pi)$ is also large, $0.86J_{dd}=0.11$ eV. The nearly isotropic effective mass at S is $m^*\sim4m_e$. The hole spin has strong antiferromagnetic (AF) correlations with the two neighboring Cu spins $\langle S_O\cdot S_{Cu}\rangle=-0.464$, but the correlations decrease quickly with distance (the next-near-neighbor correlation drops by a factor of 10), indicating a linear size of $\sim2a=7.6$ Å for the quasiparticle magnetic dressing effects. The hole carries a small but nonzero spin projection, $\langle S_O^z\rangle\simeq-0.014$, and appears to be constantly scattered between spin-up and spin-down three-spin polarons (Emery) states. The AF magnetic long-range order is destroyed.

We also examined the Zhang-Rice (ZR) singlet[12] (originally constructed in the $t^{pp}=0$ limit) within the three-band model. We find that the coherence of the four O-Cu bond states sharing the same Cu is quite large, leading to a projection probability of 68% of the ZR singlet onto the ground state. However, the solutions of the t-J model show substantial differences from that of the three-band model, both in band structure and in magnetic fluctuations.

The model for the CuO_2 plane in the present study is the standard three-band extended Hubbard model[1,2]

$$\begin{aligned}H=&\epsilon_d\sum_i n_i+\epsilon_p\sum_k n_k+U_d\sum_i n_i n_i+U_p\sum_k n_k n_k\\&+U_{pd}\sum_{\langle ik\rangle} n_i n_k+t_{pd}\sum_{ik\sigma}(d_{i\sigma}^\dagger p_{k\sigma}+\text{H.c.})\\&+K_{pd}\sum_{ik\sigma\sigma'} d_{i\sigma'}^\dagger p_{k\sigma}^\dagger d_{k\sigma}p_{i\sigma'}+t_{pp}\sum_{kl,\sigma}(p_{k\sigma}^\dagger p_{l\sigma}+\text{H.c.}),\end{aligned}\tag{1}$$

where i,j label the Cu sites, k,l the O sites, and σ the spin. Here $p_k^\dagger$, p_k are the creation and destruction operators for oxygen $2p\sigma$ states and $d_i^\dagger$, d_i for Cu $3d_{x^2-y^2}$ states. U_p, U_d are on-site Coulomb repulsions and ϵ_p, ϵ_d are site energies. U_{pd} and K_{pd} are the Coulomb repulsion and the direct spin exchange between Cu and O sites. t_{pp} is the matrix element for oxygen-oxygen hopping while t_{pd} is for O-Cu hopping. $n_i=\sum_\sigma d_{i\sigma}^\dagger d_{i\sigma}$ and $n_k=\sum_\sigma p_{k\sigma}p_{k\sigma}$. This model has been studied by a number of authors[1-8] in various limits.

In undoped cases such as La_2CuO_4 or $YBa_2Cu_3O_6$, each Cu has a $3d^9$ configuration with no holes on oxygen sites. This half-filled system is a charge-transfer insulator with an antiferromagnetic spin coupling J_{dd} between the localized Cu spins (due to the large on-site repulsion U_d). This leads to a Heisenberg spectrum of states. With small doping, the additional holes go largely to oxygen sites and we can simplify the three-band model into an effective large-U Hamiltonian through second-order perturbation theory[1,6,7]

$$H_{\text{eff}}=J_{dd}\sum_{\langle ij\rangle}{}' S_i\cdot S_j+J_{pd}\sum_{\langle ik\rangle} S_i\cdot S_k n_k$$
$$+t_{pp}\sum_{\langle kl\rangle}(p^{\dagger}_{k\sigma}p_{l\sigma}+\text{H.c.})$$
$$+\sum_{\langle kil\rangle\sigma}(t_a p^{\dagger}_{k\sigma}n_{i,-\sigma}p_{l\sigma}-t_b P^{\dagger}_{k\sigma}n_{i,\sigma}p_{l\sigma}$$
$$-t_c p^{\dagger}_{k,\sigma}d^{\dagger}_{i,-\sigma}d_{i,\sigma}p_{l,-\sigma}+\text{H.c.})\,. \quad (2)$$

Here the J_{dd} term is the Cu-Cu Heisenberg term and the J_{pd} term describes bond pairing (a Kondo-like spin coupling) between the oxygen hole and the two nearest Cu spins. These terms both arise from the strong d-p hopping t_{pd}. The d-p hopping also induces effective spin-preserving hopping t_a, t_b terms and spin-exchange hopping t_c terms, implicitly taking into account the charge-transfer processes. This effective Hamiltonian has been studied previously[1,6,7] (the model without the second-order charge-transfer t_a,t_b,t_c terms has also been considered[8]).

The parameter of H_{eff} were obtained by exactly diagonalizing an O-Cu-O cluster using the original three-band Hamiltonian and extracting the effective hopping parameters $t_a,t_b(t_c=t_a+t_b)$ as the energy splitting between the symmetric and/or antisymmetric states. The Kondo coupling J_{pd} together with a modified Heisenberg term J'_{dd} (the Cu-Cu spin coupling when a doped hole resides at the middle oxygen site) was obtained as the energy splitting between the three lowest states of a Cu-O-Cu cluster. Using the Hubbard parameters of McMahan, Annett, and Martin[9] (the results of Hybertsen and co-workers[10] and of Goddard and co-workers[11] lead to slightly different effective parameters, but all physical properties remain very much the same), we obtain (all in eV) $J_{dd}\simeq 0.132$, $J'_{dd}\simeq 0.054$, $J_{pd}\simeq 0.92$, $t_a\simeq 0.33$, $t_b\simeq 0.39$, and $t_{pp}\simeq 0.6$. This J_{dd} is very close to the values determined[13] by fitting correlation lengths in neutron scattering (0.125 eV), from Raman scattering (0.128 eV), and from the spin-wave velocity (0.126 eV). In the following, we express all energies in units of J_{dd}. For the t-J model, we used $t_{t\text{-}J}\simeq 0.46$ eV$=3.5J_{dd}$.[10] H_{eff} is solved exactly for a periodic lattice with 4×4 unit cells (16 Cu sites and 32 O sites). We work in $M_s=\sum S^z_{\text{Cu}}+S^z_{\text{O}}=\frac{1}{2}$ subspace, which contains all S states $S=\frac{15}{2},-\frac{13}{2},\ldots,\frac{13}{2},\frac{15}{2}$.

BAND STRUCTURE AND MAGNETIC FLUCTATIONS

Figure 1(a) shows the lowest energy[14] of the hole at all nonequivalent $\mathbf{k}$ with $S=\frac{1}{2}$. There is a large dip at S. Such a strong dispersion implies a sharp Fermi surface midway between Γ and X, as in LDF band-structure calculations.[15] The crossing of the sharp Fermi surface along this line has been clearly seen in the angle-resolved photoemission experiments.[16] The dispersions from M to Q and to P are both rather flat, which also agree qualitatively with LDF results. That X is close to Γ in energy and P is close to Q is reminiscent of the antiferromagnetic spin-wave spectrum in the undoped case where the spectrum is symmetric about the S-M line. This differs from the LDF results. Overall, the quasiparticle band can be approximated by $E(k)/J_{dd}=0.86\cos(k_xa+k_ya)-0.47\cos(k_xa-k_ya)$, leading to a nearly isotropic quasiparticle effective mass at S: $m^*_{[1,-1]}/m^*_{[1,1]}=1.8$, and $m^*_{[1,1]}\simeq\hbar^2/J_{dd}a^2=4.0m_e$ (in terms of the effective mass for the O-O hopping, $m^*_{[1,1]}/m^*_{pp}\simeq 4.6$).

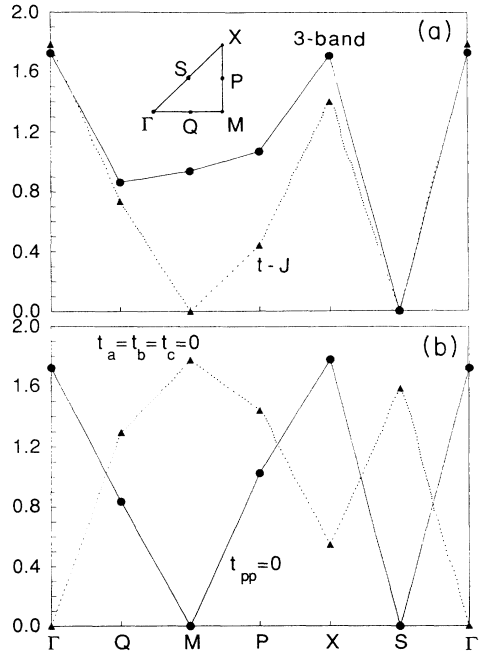

FIG. 1. (a) The quasiparticle band for a doped hole in the half-filled CuO_2 plane for the three-band model. Also shown is the band for the t-J model. (b) The effect on the quasiparticle band of deleting charge-transfer hopping $t_a=t_b=t_c=0$ or O-O hopping $ta_{pp}=0$.

The band for the t-J model [also shown in Fig. 1(a)] is similar along the Γ-X line, but differs substantially along the X-M-Γ line: the bottom of the band is degenerate in M and S. Although on larger lattices this degeneracy is lifted, the dispersion along M-S-M' [$M'=(0,\pi)$] remains small, leading to[17] $m^*_{[1,-1]}/m^*_{[1,1]}\simeq 27$, in sharp contrast to the three-band results.

How important are the second-order (charge-transfer) hoppings, t_a,t_b,t_c? Ignoring them completely (the case considered in Ref. 8) changes the band dramatically [Fig. 1(b)]. In this case, the bottom of the band is (0,0), involving primarily the O-O hopping. Alternatively, neglecting O-O hopping (setting $t_{pp}=0$) leads to a band similar to the t-J band, with degenerate ground states at S and M. This band is in qualitative agreement with quantum Monte Carlo simulations[4] near the Fermi energy ($E_F=0$ in Fig. 1).

As the oxygen hole hops around, the Cu-Cu AF spin correlations are reduced significantly, as shown in Fig. 2 for a Cu spin next to the oxygen hole. The spin correlations are reduced rapidly from that of the Heisenberg ground state. The staggered magnetization is $m^2=0.187$ for the three-band model ($m^2=0.277$ for the undoped case and $m^2=0.206$ for the t-J model). Thus the long-range AF order disappears even for moderate doping

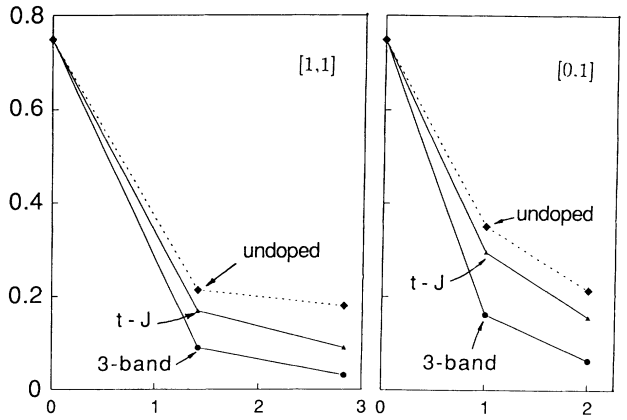

FIG. 2. Cu-Cu spin correlation $|\langle S_1 \cdot S_r \rangle|$ along the [1,1] and [0,1] directions. Here S_1 is adjacent to the hole, and the normalization is $\langle S_1 \cdot S_1 \rangle = 0.75$.

(6%). In the three-band model, the AF Cu-Cu spin-wave excitations are suppressed more strongly than in the *t-J* model. Another measure is the magnetic energy for Cu-Cu spin coupling, $E_{\text{mag}} = \sum_{\langle ij \rangle} J_{dd} \langle S_i \cdot S_j \rangle$. On the 4×4 cluster, the Heisenberg model has $E_{\text{mag}} = -11.23 J_{dd}$ and the three-band model has $E_{\text{mag}} = -8.25 J_{dd}$, implying $(11.23-8.25)/0.351 = 8.5$ broken bonds in the three-band model. In the static limit (all hoppings are ignored), $E_{\text{mag}} = -9.24 J_{dd}$. Thus out of the 8.5 broken bonds, $(9.24-8.33)/0.351 = 2.6$ are due to dynamical effects. In the *t-J* model $E_{\text{mag}} = -8.33 J_{dd}$ ($E_{\text{mag}} = -9.88 J_{dd}$ in the static limit). Hence out of the $(11.23-8.33)/0.351 = 8.3$ broken bonds, 4.4 bonds are due to dynamic effects in the *t-J* model.

QUASIPARTICLE

The first question about the nature of the quasiparticle is its spin state. A free hole moving on the oxygen network would have $\langle S^z_{\text{O}} \rangle = \frac{1}{2}$. For the ground state of the three-band model, we find $\langle S^z_{\text{O}} \rangle = -0.014$, indicating the presence of strong interactions. (Setting $t_{pp} = 0$ leads to $\langle S^z_{\text{O}} \rangle \sim -0.005$.) The net spin of the Cu spin is $\langle (\sum S_{\text{Cu}})^2 \rangle = 1.54$. This would be 2 for a pure triplet state, indicating $S \simeq 1$ for the Cu spins. Given net spins of $S = 1$ for the Cu and $S = \frac{1}{2}$ for the oxygen hole, we can construct two states with $S_{\text{total}} = S^z_{\text{total}} = \frac{1}{2}$: (a) one with $S^z_{\text{Cu}} = 0$ and $S^z_{\text{O}} = \frac{1}{2}$, (b) another with $S^z_{\text{Cu}} = 1$ and $S^z_{\text{O}} = -\frac{1}{2}$. The measured $\langle S^z_{\text{O}} \rangle$ indicates that the two occur with approximately equal probability.

Because of the large J_{pd} between the oxygen hole spin and Cu spins, Emery[1] proposed the spin polaron $\chi_\uparrow = (1/\sqrt{6})\{2|\text{Cu}_\uparrow \text{O}_\downarrow \text{Cu}^\uparrow\rangle - \text{Cu}_\uparrow \text{O}_\uparrow \text{Cu}_\downarrow\rangle - |\text{Cu}_\downarrow \text{O}_\uparrow \text{Cu}_\uparrow\rangle\}$ as the quasiparticle. *Ab initio* calculations[11] indicate a strong resonance between the Cu-O bond and the O-Cu bond, supporting this three-spin polaron picture. The present study finds strong evidence for this polaron character in the large (93%) projection probability[7(b)] onto the ground state, $|\langle \chi_\uparrow g \rangle|^2 = 0.52$ and $|\langle X_\downarrow | g \rangle|^2 = 0.41$. A check on this is to estimate $\langle S^z_{\text{O}} \rangle$ for the polaron. Since $\langle \chi_\uparrow | S^z_{\text{O}} | \chi_\uparrow \rangle = -\frac{1}{6}$, the polaron contribution should be $\langle S^z_{\text{O}} \rangle = 0.52(-1/6) + 0.41(1/6) = -0.018$, quite close to the actual value of -0.014.

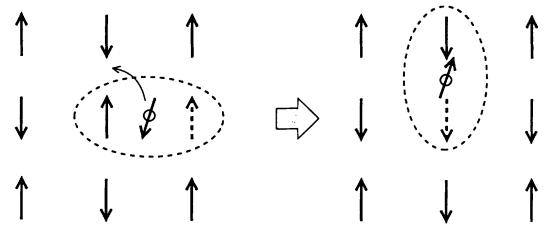

FIG. 3. Scattering of the three-spin polaron from the spin-up state to the spin-down state in the Néel background. The dashed spin indicates an overturned spin with respect to the Néel state.

Correlation functions characteristic of the polaron can be measured. For an isolated polaron, the correlation between the two Cu spins is $\langle \chi_\uparrow | S_{\text{Cu}(1)} \cdot S_{\text{Cu}(2)} | \chi_\uparrow \rangle = \frac{1}{4}$ and the correlation between the O hole spin and the Cu spin is $\langle \chi_\uparrow | S_{\text{O}} \cdot S_{\text{Cu}(1)} | \chi_\uparrow \rangle = -\frac{1}{2}$. In the ground state of the many-body system, we obtained $\langle S_{\text{Cu}(1)} \cdot S_{\text{Cu}(2)} \rangle = 0.181$ and $\langle S_{\text{O}} \cdot S_{\text{Cu}(1)} \rangle = -0.464$. These values are 72% and 93% of the saturation, respectively, giving strong evidence for the Emery polaron character. It is important to note[7(b)] that this three-spin polaron character in the exact state is dominated by the large spin-exchange hopping (t_c), rather than the large J_{pd} spin coupling. Setting $J_{pd} = 0$ still leads to a polaron: $\langle S_{\text{Cu}(1)} \cdot S_{\text{Cu}(2)} \rangle = 0.166$ and $\sum_\sigma |\langle \chi_\sigma | g \rangle|^2 = 91\%$. On the other hand, ignoring the t_c hopping, leads to $\langle S_{\text{Cu}(1)} \cdot S_{\text{Cu}(2)} \rangle = -0.192$ and $\sum_\sigma |\langle \chi_\sigma | g \rangle|^2 = 0.39$, and further setting $t_{pp} = 0$ leads to $\langle S_{\text{Cu}(1)} \cdot S_{\text{Cu}(2)} \rangle = -0.047$ and $\sum_\sigma |\langle \chi_\sigma | g \rangle|^2 = 0.61$. In both latter cases, the characteristic ferromagnetic correlation between the Cu(1)-Cu(2) spins is absent. These latter results also indicate that a mere 61% projection to a trial function does not necessarily imply the validity of the trial function—some essential characteristics could be missing.

The above results that the quasiparticle has $\langle S^z_{\text{O}} \rangle \sim 0$ with $|\langle \chi_\uparrow | g \rangle|^2 \sim |\langle \chi_\downarrow | g \rangle|^2$ indicate that the spin polaron is scattered constantly between up and down states as it propagates (Fig. 3). This is primarily due to the t_c spin-exchange hopping term. This spin-flip process is strongest when the hole has pure singlet coupling to the Cu, which leads to hopping amplitude ($t^s_c = t_a + 2t_b$) instead of ($t_c = t_a + t_b$) in Eq. (2). This raises an important point regarding the quasiparticle: the singlet character of the O hole with a neighboring Cu spin is $(p^\dagger_\uparrow d^\dagger_\downarrow - p^\dagger_\downarrow d^\dagger_\uparrow)/\sqrt{2} \equiv (\text{O},\text{Cu})_s$. The projection probability of $(\text{O}, \text{Cu})_s$ onto the ground state is quite high (71.4%). This singlet pairing underlies the three-spin polaron, which can be regarded as the symmetrized combination of two such singlet pairs for Cu-O-Cu:

$$\chi_\uparrow = [\text{Cu}(1)_\uparrow (\text{O},\text{Cu}(2))_s - (\text{Cu}(1),\text{O})_s \text{Cu}(2)_\uparrow]/\sqrt{3} \ .$$

The singlet Cu-O pairing also underlies the Zhang-Rice singlet.[12] Instead of the Cu-O-Cu cluster of the three-spin polaron, the ZR singlet consists of four O's surrounding a center Cu. We find that a combination of two states, $\psi = (\text{Cu},\text{O}_1)_s - (\text{Cu},\text{O}_2)_s$, gets a large enhancement due to the cross term: $\langle g | \text{Cu},\text{O}_1)_s | (\text{Cu},\text{O}_2)_s | g \rangle \simeq -0.33$.

The ZR singlet in the Hubbard approximation can be written as

$$\psi_{ZR}^{H}=\tfrac{1}{2}[(Cu,O_1)_s+(Cu,O_2)_s-(Cu,O_3)_s-(Cu,O_4)_s] .$$

In the projection, we find that the sign of the cross terms always goes according to the sign of the t_{pd} hopping matrix element and thus each cross term always contributes positively, leading to

$$|\langle\psi|g\rangle|^2=\tfrac{1}{4}[4 \text{ diagonal terms}+12 \text{ cross terms}]$$
$$=0.357+(0.331+0.338+0.334)=1.36 .$$

Thus the enhancement factor due to the coherence is 1.36/0.357 = 3.8 (compared with the factor 4 from second-order energy considerations). The net projection probability is $\frac{1}{2}|\langle\psi|g\rangle|^2=0.677$ for this local ZR singlet state.

EXPERIMENT

These results are consistent with several experiments on high-T_c materials. The sharp Fermi surface midway between Γ and X has been demonstrated in photoemission experiments.[16] NMR relaxation rates on the O sites and on the Cu sites are reported[18] to have the same temperature dependence, indicating that the O spin couples strongly with the Cu spins. Our results suggest that O-Cu spin correlation is much stronger than the Cu-Cu correlation [$\langle S_O\cdot S_{Cu}\rangle=-0.46$ versus $\langle S_{Cu}\cdot S_{Cu}\rangle=-0.35$], which is quite consistent with the NMR data. The optical and dc conductivity measurements[19] indicate that the charge carriers are strongly scattered, even for low doping. This is consistent with our result that the three-spin polaron is constantly scattered between up and down states.

ACKNOWLEDGMENTS

This research was initiated with support by NSF-DMR-MRG and completed with support from NSF-CHE. The facilities of the MSC are also supported by grants from DOE-AICD, Allied-Signal, Asahi Chemical, Asahi Glass, BP America, Chevron, and Xerox.

[1]V. J. Emery, Phys. Rev. Lett. **58**, 2794 (1987); V. J. Emery and G. Reiter, Phys. Rev. B **38**, 4547 (1988).

[2]P. B. Littlewood, C. M. Varma, and E. Abrahams, Phys. Rev. Lett. **60**, 379 (1987); C. M. Varma, S. Schmitt-Rink, and E. Abrahams, Solid State Commun. **62**, 681 (1987).

[3]J. E. Hirsch, Phys. Rev. Lett. **59**, 228 (1987); J. E. Hirsch, S. Tang, E. Loh, and D. J. Scalapino, Phys. Rev. B **69**, 1668 (1988).

[4]G. Dopf *et al.*, Phys. Rev. Lett. **68**, 2082 (1992); R. T. Scalettar *et al.*, Phys. Rev. B **44**, 770 (1991); J. Wagner, W. Hanke, and D. J. Scalapino, *ibid.* **43**, 10 517 (1991).

[5]G. Kotliar, P. A. Lee, and N. Read, Physica C **153-155**, 538 (1988); J. H. Kim, K. Levin, and A. Auerbach, Phys. Rev. B **39**, 11 633 (1989); M. Grilli *et al.*, *ibid.* **42**, 329 (1990); C. A. Balseiro *et al.*, Phys. Rev. Lett. **62**, 2624 (1989).

[6]J. Zaannen and A. M. Olés, Phys. Rev. B **37**, 9423 (1988).

[7](a) M. Ogata and H. Shiba, J. Phys. Soc. Jpn. **57**, 3074 (1988); (b) D. M. Frenkel, R. J. Gooding, B. I. Shraiman, and E. D. Siggia, Phys. Rev. B **41**, 350 (1990).

[8]G. Chen and W. A. Goddard, Science **239**, 899 (1988); A. Aharony *et al.*, Phys. Rev. Lett. **60**, 1330 (1988); R. J. Birgeneau, M. K. Kastner, and A. Aharony, Z. Phys. B **71**, 57 (1988); J. P. Lu, Q. Si, and K. Levin, Physica C **162-164**, 1465 (1989); C. X. Chen, H. B. Schuttler, and A. J. Fedro, Phys. Rev. B **41**, 2581 (1990).

[9]A. K. McMahon, J. F. Annett, and R. M. Martin, Phys. Rev. B **42**, 6268 (1990).

[10]M. S. Hybertsen, M. Schluter, and N. E. Christensen, Phys. Rev. B **39**, 9028 (1989); M. S. Hybertsen, E. B. Stechel, M. Schluter, and D. R. Jennison, Phys. Rev. B **41**, 11 068 (1990).

[11]Y. Guo, J-M. Langlois, and W. A. Goddard, Science **239**, 896 (1988); W. A. Goddard, Y. Guo, G. Chen, H. Q. Ding, J.-M. Langlois, and G. H. Lang, in *Proceedings from High Temperature Superconductivity, Materials, Mechanisms and Devices, St. Andrews, Scotland,* edited by D. P. Tunstall and W. Barford (Adam Hilger, Bristol, 1991).

[12]F. C. Zhang and T. M. Rice, Phys. Rev. B **37**, 3759 (1988). For a review on finite cluster study on the *t-J* model, see E. Dagotto, Int. J. Mod. Phys. B **5**, 907 (1991).

[13]H.-Q. Ding and M. S. Makivic, Phys. Rev. Lett. **64**, 1449 (1990); R. R. P. Singh *et al.*, *ibid.* **62**, 2736 (1989); G. Aeppli *et al.*, *ibid.* **62**, 2052 (1989).

[14]At Γ, the lowest state has $S=\frac{3}{2}$. Thus we use the second lowest state, which has $S=\frac{1}{2}$. At X, the first two lowest states both have $S=\frac{3}{2}$ and we use the third lowest state, which has $S=\frac{1}{2}$. This also occurs at Γ for the *t-J* model. The lowest state at all other points has $S=\frac{1}{2}$. The energy increases at Γ,X by restricting the band to only the $S=\frac{1}{2}$ state are $\sim 0.5J_{dd}$.

[15]M. S. Hybertsen and L. F. Mattheiss, Phys. Rev. Lett. **60**, 1661 (1988); H. Krakauer and W. E. Pickett, *ibid.* **60**, 1665 (1988).

[16]C. G. Olson *et al.*, Phys. Rev. B **42**, 381 (1990).

[17]S. A. Trugman, Phys. Rev. B **41**, 892 (1990).

[18]P. C. Hammel *et al.*, Phys. Rev. Lett. **63**, 1991 (1989); M. Takigawa *et al.*, *ibid.* **63**, 1865 (1989).

[19]B. Batlogg, in *High Temperature Superconductivity Proceedings: Los Alamos Symposium 1989,* edited by K. S. Bedell *et al.* (Addison-Wesley, Reading, MA, 1990).

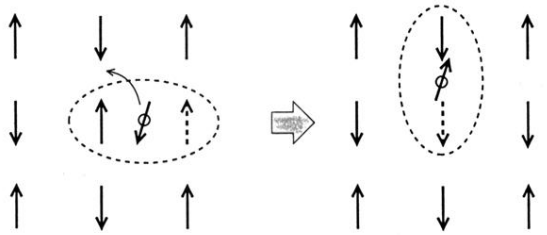

FIG. 3. Scattering of the three-spin polaron from the spin-up state to the spin-down state in the Néel background. The dashed spin indicates an overturned spin with respect to the Néel state.