Spatial distribution of mobile holes in the t - J model

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We have calculated the hole-hole correlation function for two holes doped into a $S=1/2$ antiferromagnetic insulator described by the t - J model on a 16-site $\sqrt{8} \times \sqrt{32}$ lattice and a 24-site $\sqrt{18} \times \sqrt{32}$ lattice using an exact diagonalization technique. We predict that the carriers described by this model, in the parameter range relevant to CuO_2 planes, tend to stay as far apart as possible. This result is in direct contradiction to previously published exact diagonalization data [e.g., D. Poilblanc, *Phys. Rev. B* **49**, 1477 (1994)]. We suggest that if the carriers do tend to stay as far apart from one another as possible, then the electron momentum distribution function shows evidence for hole pockets at $\vec{k}=(\pm\pi/2, \pm\pi/2)$, consistent with many recent studies of these models, including recent photoemission work.

A theoretical starting point for the study of the CuO_2 planes found in high-temperature superconductors is the strong-coupling limit of the single-band t - U Hubbard model.¹ It has been argued that the simpler t - J model^{2,3} adequately represents the important low-energy physics of these materials.⁴ Even though these two models are different, one expects some similarities in their physical properties in the strong-coupling limit. In this paper we will discuss the spatial distribution of a pair of carriers whose interactions in an antiferromagnetic insulator are described by the t - J model.

In a recent paper,⁵ the hole-hole correlation function for a pair of holes described by the t - J model was studied using an exact diagonalization technique on a large 26-site square lattice; this work augments earlier studies of square lattices of 16 sites^{6,7} and 18 and 20 sites,⁸ and a consistent picture emerges from these studies. Qualitatively, it was found that in the parameter region believed to be appropriate for the high- T_c materials a pair of carriers tended to want to be close together. For example, for the large 26-site square lattice studied, the findings of Ref. 5 are that the largest probability of finding two holes occurs at a separation of $\sqrt{13}a$ (a is the lattice constant of the square CuO_2 plane) when $J/t < 0.18$, $\sqrt{2}a$ for $0.18 < J/t < 1.0$, and a for $J/t > 1.0$ — the ratio of $J/t = 0.3 \sim 0.4$ is believed to be appropriate to CuO_2 planes.⁴

We have also calculated the hole-hole correlation function for two holes on a 16-site $\sqrt{8} \times \sqrt{32}$ lattice and a 24-site $\sqrt{18} \times \sqrt{32}$ lattice using an exact diagonalization technique. For realistic values of the antiferromagnetic superexchange ($J/t \sim 0.4$), we have found that the holes tend to stay as far apart as possible (for these clusters, that distance is $\sqrt{10}a$). Clearly, these results are in disagreement with those found in Refs. 5–8, and here we explore why supposedly exact results can be in disagreement with one another.

To begin, let us define the Hamiltonian that we are studying, and the correlation functions that we calculate. The t - J model⁴ is defined as

$$H_{tJ} = -t \sum_{\langle i,j \rangle, \sigma} (\tilde{c}_{i,\sigma}^\dagger \tilde{c}_{j,\sigma} + \text{H.c.}) + J \sum_{\langle i,j \rangle} (\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j), \quad (1)$$

where the i and j label the sites of a two-dimensional square lattice, $\tilde{c}_{i,\sigma} \equiv c_{i,\sigma}(1 - n_{i,-\sigma})$, $\vec{S}_i$ is an $S=1/2$ spin operator, $c_{i,\sigma}$ is the true electron annihilation operator, n_i is the electron number operator, and the notation $\langle i,j \rangle$ implies near-neighbor pairs. The spatial correlation function that is the focus of this report is the hole-hole correlation function, defined as^{9,10}

$$P_{hh}(d) = \frac{1}{N_h N_E(d)} \sum_{i,j} \langle (1 - n_i)(1 - n_j) \delta_{|i-j|,d} \rangle, \quad (2)$$

where N_h is the total number of holes, and $N_E(d)$ is the number of equivalent sites a distance d from some chosen site.

Exact diagonalization calculations were performed using a Lanczos method¹¹ for small clusters. As mentioned above, the clusters studied were a nonsquare 16-site $\sqrt{8} \times \sqrt{32}$ lattice and a 24-site $\sqrt{18} \times \sqrt{32}$ lattice (see Fig. 1 of Ref. 10 for a picture of these types of clusters). As elaborated in Ref. 10, and more recently in Ref. 12, we believe that the lack of square symmetry is not detrimental to our attempts to mimic a bulk two-dimensional plane. Instead, our main reason for choosing these nonsquare clusters is the fact that both of them contain the $(\pm\pi/2, \pm\pi/2)$ wave vectors, something that we believe to be more important than maintaining the square symmetry. (Note that although the square 4×4 cluster has square symmetry, for the t - J model it has the sym-

FIG. 1. The hole-hole correlation function for $J/t=0.4$ on both our 16-site and 24-site clusters. The separation between holes (d) is given in units of the lattice constant, and the solid lines are only guides to the eye.

metry of a four-dimensional hypercube, thus leading to unwanted degeneracies.) In order to allow for a direct comparison with Ref. 5 in the parameter regime thought to be relevant to the high- T_c superconductors, the ground state was calculated for $J/t=0.4$. The hole-hole correlation function was calculated for both of these lattices, the results of which are presented in Fig. 1. From this figure it is evident that the holes tend to stay as far apart as the lattice will let them; however, the binding energy⁹ for the two holes is negative, implying that the holes are still weakly bound together. The tendency for the holes to stay far apart from one another is completely different than the behavior found in Ref. 5. It is to be stressed that these results are both exact diagonalization data, and thus it is important to understand what is causing this difference.

We believe the reason behind this difference is associated with the fact that our clusters have the important $(\pm\pi/2, \pm\pi/2)$ wave vectors present. Many theories predict that the wave vector(s) of the single-hole ground state for this model is in fact found at $(\pm\pi/2, \pm\pi/2)$.⁴ Further, recent photoemission data for $\text{Sr}_2\text{CuO}_2\text{Cl}_2$ (Ref. 13) involve the study of a single hole propagating in an antiferromagnetic background. For this compound, indeed the valence band maximum was found to occur at $\vec{k}=(\pm\pi/2, \pm\pi/2)$, stressing the importance of including such wave vectors in any theoretical study of carriers in the CuO_2 planes.

The above argument can only be correct if the multiply-doped ground states of our clusters are composed of $\vec{k}=(\pm\pi/2, \pm\pi/2)$ quasiparticles. To demonstrate that this is indeed true, we have calculated the electron momentum distribution function, defined as

$$\langle n_\sigma(\vec{q}) \rangle = \langle \tilde{c}_{\vec{q}\sigma}^\dagger \tilde{c}_{\vec{q}\sigma} \rangle = \langle c_{\vec{q}\sigma}^\dagger c_{\vec{q}\sigma} \rangle. \quad (3)$$

FIG. 2. The electron momentum distribution function for the t - J model with two holes on our 16-site cluster and with $J/t=0.4$. The filled circles represent occupied electron states, the unfilled circles unoccupied states, and the dashed line is the antiferromagnetic Brillouin zone.

[This quantity has been used by many authors (see, e.g., Refs. 14, 15, 10, 16, and 17) to discuss the possibility of rigid-band filling,¹⁸ but the answer to this problem is still an outstanding question.] Since we always consider an even number of holes, and all of these ground states are singlets,

$$\langle n_\uparrow(\vec{q}) \rangle = \langle n_\downarrow(\vec{q}) \rangle \equiv \langle n(\vec{q}) \rangle. \quad (4)$$

For the two clusters on which we performed exact diagonalization results, $\langle n(\vec{q}) \rangle$ is shown in Figs. 2 and 3. The solid circles represent filled states (such as defined, e.g., in Refs. 14, 15, and 10), the open circles unfilled states, and the dashed line represents the antiferromagnetic Brillouin zone. Clearly, in both clusters all states within the antiferromagnetic Brillouin zone are occupied *except* for those at $\vec{k}=\pm(\pi/2, \pi/2)$ (thus supporting our view¹⁰ of rigid-band

FIG. 3. The electron momentum distribution function for the t - J model with two holes on our 24-site cluster and with $J/t=0.4$. The symbols have the same meaning as in Fig. 2.

filling in these lattices). It is also interesting to note that even though we find hole pockets, Luttinger's theorem is still satisfied for these ground states.

The importance of finding these quasiparticles in the two-hole ground state to the spatial correlation function shown in Fig. 1 follows from the nature of the spin distortions induced by such carriers.¹⁹ To be specific, these carriers generate long-ranged spin distortions of dipolar symmetry. In order for the energy of the two-hole ground state to be minimized, the spin distortions apparently do not wish to overlap, and thus the two holes try to remain distant from one another. Clearly, the extension of this idea to nonzero densities of carriers is an important problem.

So, for our clusters, in which the carriers in the two-hole ground state tend to stay as far apart as possible, $\vec{k}=(\pm\pi/2,\pm\pi/2)$ quasiparticles are present. These results should be contrasted with the spatial distribution of holes for the square 16-, 18-, 20-, and 26-site lattices⁵⁻⁸—for these clusters, the holes tend to stay close together and studies of $\langle n(\vec{q}) \rangle$ always show the lack of $\vec{k}=(\pm\pi/2,\pm\pi/2)$ quasiparticles^{14,15} for multiply doped ground states. Both semiclassical theories¹⁹ and self-consistent Born approximation formulations of the $\vec{k}=(\pi,0)$ quasiparticles^{12,20} predict that the spin distortions induced by these mobile holes are very short ranged. Thus, it is perhaps not surprising that such carriers cluster together. Thus, we have found a clear correlation between the electron momentum distribution function, the spin distortions generated by such carriers, and the spatial distribution of carriers.

Our results are obtained from exact diagonalization studies of small clusters, and thus at present we cannot extend our conclusions to bulk systems. However, there is evidence suggesting that this result extends to larger numbers of mo-

bile holes. In Ref. 10 we found that even for four holes doped into our nonsquare 16-site cluster, the electron momentum distribution function displayed that the quasiparticles in the system were located at the four wave vectors $\vec{k}=(\pm\pi/2,\pm\pi/2)$ —see Fig. 10 of Ref. 10. If, as we have suggested above, the spin distortions generated by such quasiparticles tend to force the holes apart, then perhaps the physics discussed above applies to even larger carrier densities.

In summary, we have displayed an interesting relationship between the spatial distribution of carriers and the quasiparticles present in a two-carrier system for the t - J model: when hole pockets are formed at the wave vectors $[\vec{k}=(\pm\pi/2,\pm\pi/2)]$ of the single-hole ground state the carriers tend to want to remain as far apart as possible. It is interesting to note that we have recently found similar differences between the spatial correlations and the electron momentum distributions when comparing the electron- and hole-doped 214 superconductors¹²—we believe that a clustering together of carriers is much more likely to occur in the electron-doped materials (e.g., Nd-Ce-Cu-O) than in the hole-doped systems (e.g., La-Sr-Cu-O) for which we expect well separated holes. The discrepancies between our exact diagonalization results and those of others⁵⁻⁸ will most likely be resolved when two holes can be doped into a square 32-site lattice, a (hopefully manageable) cluster that includes all of the important wave vectors [e.g., $\vec{k}=(\pm\pi/2,\pm\pi/2)$, and $\vec{k}=(\pm\pi,0),(0,\pm\pi)$] and yet still maintains full square symmetry.

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¹P.W. Anderson, *Science* **235**, 1196 (1987).

²F.C. Zhang and T.M. Rice, *Phys. Rev. B* **37**, 3759 (1988).

³H. Eskes, G.A. Sawatzky, and L.A. Feiner, *Physica C* **160**, 424 (1989).

⁴For a recent review of the application of these models to the high- T_c compounds, see E. Dagotto, *Rev. Mod. Phys.* **66**, 763 (1994).

⁵D. Poilblanc, *Phys. Rev. B* **49**, 1477 (1994).

⁶J. Bonča, P. Prelovšek, and I. Sega, *Phys. Rev. B* **39**, 7074 (1989).

⁷Y. Hasegawa and D. Poilblanc, *Phys. Rev. B* **40**, 9035 (1989).

⁸P. Prelovšek and X. Zotos, *Phys. Rev. B* **47**, 5984 (1993).

⁹J.A. Riera and A.P. Young, *Phys. Rev. B* **39**, 9697 (1989).

¹⁰R.J. Gooding, K.J.E. Vos, and P.W. Leung, *Phys. Rev. B* **49**, 4119 (1994).

¹¹P.W. Leung and P.E. Oppenheimer, *Comput. Phys.* **6**, 603 (1992) and the references contained therein.

¹²R.J. Gooding, K.J.E. Vos, and P.W. Leung, *Phys. Rev. B* **50**, 12 866 (1994).

¹³B.O. Wells *et al.*, *Phys. Rev. Lett.* **74**, 694 (1995).

¹⁴W. Stephan and P. Horsch, *Phys. Rev. Lett.* **66**, 2258 (1991).

¹⁵H.-Q. Ding, *Physica C* **203**, 91 (1992).

¹⁶R. Eder and Y. Ohta, *Phys. Rev. Lett.* **72**, 2816 (1994).

¹⁷S. Haas, *Phys. Rev. B* **51**, 11 748 (1995).

¹⁸See, e.g., S.A. Trugman, *Phys. Rev. Lett.* **65**, 500 (1990).

¹⁹B.I. Shraiman and E.D. Siggia, *Phys. Rev. Lett.* **61**, 467 (1988).

²⁰R.J. Gooding (unpublished).