Hole correlation and antiferromagnetic order in the t - J model

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We study the t - J model with four holes on a 32-site square lattice using exact diagonalization. This system corresponds to doping level $x=\frac{1}{8}$. At the “realistic” parameter $J/t=0.3$, holes in the ground state of this system are unbound. They have short range repulsion due to the lowering of the kinetic energy. There is no antiferromagnetic spin order and the electron momentum distribution function resembles hole pockets. Furthermore, we show evidence that in case antiferromagnetic order exists, holes form d -wave bound pairs and there is mutual repulsion among hole pairs. This presumably will occur at low doping levels. This scenario is compatible with a checkerboard-type charge density state proposed to explain the “ $\frac{1}{8}$ anomaly” in the lanthanum cuprate family, except that it is the ground state only when the system possesses strong antiferromagnetic order.

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It is generally accepted that the physics of high temperature superconductors is the physics of a doped antiferromagnetic insulator. Although the detail mechanism is still not fully understood, it is believed that frustration due to mobile holes may lead to superconductivity as well as other competing orders¹⁻³ which may include charge-ordered and spin-ordered phases, or even more exotic phases like the staggered-flux phase. One way to examine the possibilities of these states is to start from a lightly doped antiferromagnet. The t - J model with two holes has been extensively studied using various analytical and numerical methods.⁴⁻⁹ These results indicate that two holes form a weak bound pair with $d_{x^2-y^2}$ symmetry. In addition, exact diagonalization study of the two-hole model lends support to the staggered-flux phase.¹⁰ Nevertheless there are still many open questions. In a system with two holes the electron momentum distribution function (EMDF) $\langle n_{\mathbf{k}\sigma} \rangle$ reflects the structure of the bound pair only and may not contain information on the Fermi surface in the thermodynamic limit. A system with four holes is therefore the first step in possibly extracting useful information on the system at finite doping levels. Furthermore, the two-hole system has a few low-lying excited states where the holes do not form a $d_{x^2-y^2}$ bound pair.⁴ It is therefore unclear whether d -wave hole pairing still survives when more holes are present. If so, how would hole pairs interact? And if not, what scenario replaces hole pairing?

Motivated by the above questions, we numerically diagonalize the t - J model with four holes on a 32-site lattice with periodic boundary conditions. We caution that due to the small size of our system we cannot study long-range orders. Therefore superconductivity is not the subject of this study. The doping level of this system is $x=\frac{1}{8}$ which is in the underdoped region. Incidentally this is the same doping level as the “ $\frac{1}{8}$ anomaly” in the lanthanum cuprate family where experimental signals for charge ordering are more pronounced.² The Hamiltonian of the t - J model is

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

where $\langle ij \rangle$ denotes a nearest neighbor pair. Let us consider the case $J/t=0.3$ first. This parameter is believed to be rel-

evant to high- T_c cuprates. The ground state has an energy $-18.682\,017t$, momentum $(0,0)$ and $d_{x^2-y^2}$ symmetry. (Note that this refers to the symmetry of the total wave function. It is not the pairing symmetry, nor does it imply hole pairing.) To see whether there is hole binding we calculate the hole-hole correlation function¹¹ $C(r) = \langle (1-n_r)(1-n_0) \rangle$, where n_r is the spin number operator in Eq. (1). Figure 1 shows that at $J/t=0.3$, systems with two and four holes have completely different behaviors. While holes in the two-hole system form a bound pair, in the four-hole system they are mutually repulsive— $C(r)$ increases with r and does not vary much beyond $r=2$. The root-mean-square separation between holes is $r_{\text{rms}} \equiv \sqrt{\langle r^2 \rangle} = 2.4732$. This is slightly larger than 2.3827, which is the root-mean-square separation between uncorrelated holes on the same lattice. In order to understand this repulsion, we compare $C(r)$ to the pair correlation function of four hard core bosons on the same lattice. Besides the condition of no double occupancy, hard core bosons have effective short-range repulsion due to hopping, but are otherwise uncorrelated. As shown in Fig. 1, the pair correlation function of hard core bosons is strikingly similar to $C(r)$ of our four-hole system. r_{rms} of the bosons is 2.4894, which is very close to that of the four-hole system. From this similarity we conclude that in the t - J model with four holes at J/t

FIG. 1. (Color online) Hole-hole correlation in the ground states with two and four holes. The thick shaded line is the pair correlation function of four hard core bosons on the same lattice.

FIG. 2. EMDF $\langle n_{\mathbf{k}} \rangle$ in the ground state of the four-hole system at (a) $J/t=0.3$ and (b) $J/t=0.8$. The solid line is the AFBZ boundary. Due to symmetry, only one quadrant of the Brillouin zone is shown.

$=0.3$, holes have short-range repulsion which arises from the kinetic effect due to hopping.

More information on the interaction among holes comes from the correlation in momentum space. As usual, we define EMDF as $\langle n_{\mathbf{k}\sigma} \rangle \equiv \langle \tilde{c}_{\mathbf{k}\sigma}^\dagger \tilde{c}_{\mathbf{k}\sigma} \rangle$. The result is shown in Fig. 2(a). Since the electron number is even, $\langle n_{\mathbf{k}\uparrow} \rangle = \langle n_{\mathbf{k}\downarrow} \rangle$ and we drop the spin variable σ from $\langle n_{\mathbf{k}\sigma} \rangle$. In interpreting the result it is important to realize that the general shape of the EMDF can be misleading. It features a “dome”-shape with a maximum at $(0,0)$ and slopes down towards (π, π) . This is a general feature at all doping levels and has been shown^{12,13} to result from minimizing the kinetic energy. It does not represent the true Fermi surface. Instead we should focus on those $\mathbf{k}$ points along the boundary of the antiferromagnetic Brillouin zone (AFBZ), i.e., from $(\pi, 0)$ to $(0, \pi)$. They are not affected by the kinematic effect and therefore reflect the physics of the system.⁵ Figure 2(a) shows that along the AFBZ boundary the EMDF has a minimum at $(\pi/2, \pi/2)$. Again this is in sharp contrast with the two-hole system whose EMDF has a maximum at $(\pi/2, \pi/2)$ along the AFBZ boundary.⁵ Unfortunately we do not have useful information on how the EMDF changes from $(0, 0)$ to (π, π) because kinematic effect dominates along this direction. Therefore we cannot conclude whether the minimum at $(\pi/2, \pi/2)$ implies a hole pocket or a half pocket (segmented Fermi surface). But it is not in contradiction with either one.

TABLE I. HMDF $\langle \bar{n}_{\mathbf{k}} \rangle$ in the two- and four-hole systems at $J/t=0.3$. $\mathbf{k}$ points along the AFBZ boundary are marked with $\dagger$. Numbers in parentheses are calculated using the additive assumption, Eqs. (3) and (4), where $\langle \bar{n}_{\mathbf{k}} \rangle_1$ are from Ref. 5.

$\mathbf{k}$	Two-hole system	Four-hole system
$(0,0)$	0.0031 (0.0058)	0.0041 (0.0115)
$(\pi/4, \pi/4)$	0.0042 (0.0064)	0.0103 (0.0128)
$(\pi/2, \pi/2)^\dagger$	0.0376 (0.1156)	0.1813 (0.2311)
$(3\pi/4, 3\pi/4)$	0.1234 (0.1416)	0.2565 (0.2832)
(π, π)	0.1255 (0.1316)	0.2529 (0.2633)
$(\pi, \pi/2)$	0.1360 (0.0582)	0.2454 (0.1164)
$(\pi, 0)^\dagger$	0.0497 (0.0137)	0.0594 (0.0274)
$(\pi/2, 0)$	0.0104 (0.0021)	0.0185 (0.0042)
$(3\pi/4, \pi/4)^\dagger$	0.0657 (0.0169)	0.0970 (0.0339)

The fact that the EMDF of the four-hole system has a minimum at the single-hole ground state momentum $(\pi/2, \pi/2)$ immediately suggests the relevance of the single-hole ground state to the multiple-hole one.^{13–15} If holes doped into the parent system behave like weakly interacting fermions, then it is reasonable to expect that many-hole systems can be approximated by filling up the single-hole band. This should lead to “hole-pockets” at single-hole ground state momenta.¹⁶ We would like to see how well the EMDF of the four-hole system agrees with this simple picture. For this purpose we consider the hole momentum distribution function (HMDF),

$$\langle \bar{n}_{\mathbf{k}\sigma} \rangle \equiv \langle \tilde{c}_{\mathbf{k}\sigma}^\dagger \tilde{c}_{\mathbf{k}\sigma} \rangle = (N_\sigma + N_h)/N - \langle n_{\mathbf{k}\sigma} \rangle, \quad (2)$$

where N_σ and N_h are numbers of σ spins and holes, respectively. If multiple-hole states can be built up from single-hole states, we expect their HMDFs to be additive,

$$\langle \bar{n}_{\mathbf{k}} \rangle_2 \simeq \langle \bar{n}_{\mathbf{k}\uparrow} \rangle_1 + \langle \bar{n}_{\mathbf{k}\downarrow} \rangle_1, \quad (3)$$

$$\langle \bar{n}_{\mathbf{k}} \rangle_4 \simeq 2(\langle \bar{n}_{\mathbf{k}\uparrow} \rangle_1 + \langle \bar{n}_{\mathbf{k}\downarrow} \rangle_1), \quad (4)$$

where $\langle \bar{n}_{\mathbf{k}\sigma} \rangle_{N_h}$ is the HMDF of the N_h -hole system. Table I shows the HMDF in the two- and four-hole systems together with the approximations from Eqs. (3) and (4), respectively.¹⁷ Note that Eq. (3) and (4) lead to very prominent maxima at $(\pi/2, \pi/2)$ along the AFBZ boundary. This, of course, does not agree with our exact results in the two-hole system. Even in the four-hole system, the maximum is too sharp compared to the exact result. Therefore a simple additive model as given in Eqs. (3) and (4) does not work in the t - J model. We remark that such a simple additive picture holds in the extended t - J model with parameters chosen to represent electron-doped cuprates.¹⁸ We conclude that although the EMDF of the four-hole system exhibit minima that suggests the relevance of the single-hole ground state to the multiple-hole one, there must still be appreciable correlation among the holes.

Next we look at a subtle form of correlation that is believed to reflect hole binding. A staggered pattern in the current correlation function $\langle j_{kl} j_{mn} \rangle$, where $j_{kl} = it(\tilde{c}_k^\dagger \tilde{c}_l - \tilde{c}_l^\dagger \tilde{c}_k)$ is

FIG. 3. Current correlation in the ground state of the four-hole system at $J/t=0.3$. The reference bond mn is indicated by a shaded line. Except for the reference bond, linewidths are proportional to $\langle j_{kl} j_{mn} \rangle / x$, where $x = \frac{1}{8}$ is the doping level. For reference purposes, the numerical values of $\langle j_{kl} j_{mn} \rangle / x$ are shown next to two horizontal bonds.

the hole current on the nearest neighbor bond kl , was suggested as a manifestation of the staggered flux phase.¹⁹ Although there exists another explanation in terms of the spin polaron theory,²⁰ both theories point to the fact that such staggered correlation reflects hole binding in the d -wave channel. The current correlation at $J/t=0.3$ is shown in Fig. 3. We note that the direction of the correlation function on many bonds deviate from a staggered pattern. It certainly does not have the clear staggered pattern that exists in the two-hole system.¹⁰ Another way to display the overall pattern is through the vorticity correlation, $C_{VV}(r) \equiv \langle V(r)V(0) \rangle / x$. The vorticity $V(\mathbf{r})$ of a square plaquette centered at $\mathbf{r}$ is defined by summing up the current correlations around it in the counterclockwise direction.¹⁹ We plot $C_{VV}(r)$ in Fig. 4. It clearly shows that the vorticity correlation is weak and decays rapidly, leading to deviation from a staggered pattern at large distances. Hence from the current correlation we conclude that there is no sign of d -wave pairing in the four-hole system at $J/t=0.3$.

Up to now we have shown that when the number of holes in a 32-site lattice is increased from two to four, d -wave pairing no longer exists. We note that at the same time antiferromagnetic (AF) correlation in the spin background is also lost. Evidence comes from Fig. 5 which shows the spin correlation function $\langle \mathbf{S}_0 \cdot \mathbf{S}_r \rangle$ and static structure factor $S(\mathbf{k})$. At $J/t=0.3$, when we increase the number of holes from two to four, the spin correlation decreases very rapidly and has large fluctuations. The sign of the correlation at larger distances shows deviation from the Néel order. In the momentum space this leads to a strong suppression of the AF peak in $S(\mathbf{k})$ at (π, π) , leaving no sign of AF correlation at all. Note that this is consistent with the phase diagram of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, where a small doping level of a few percent is

FIG. 4. The vorticity correlation $C_{VV}(r)$ in the ground state of the four-hole system at $J/t=0.3$. The reference plaquette at $r=0$ is indicated by a cross inside it. Because of symmetry, only a quarter of the cluster is shown.

enough to destroy the AF phase. This partially answer the question we posed at the end of the first paragraph in this paper—when the doping level is large enough to destroy AF correlation, holes do not form bound pairs. Instead they become mutually repulsive. Then how about at lower doping levels where the AF correlation still exists? Do our two-hole results really represent the behavior of a lightly doped system, or are they just due to the artifact that there is only one hole pair? To answer this question directly one has to solve the t - J model with a few hole pairs on a larger lattice. But this is currently not feasible. In order to mimic a lightly doped system with a few hole pairs, we put two hole pairs on a 32-site lattice with an AF spin background. For this purpose we increase J/t to 0.8. The ground state at this parameter has energy $-31.917\,820t$, momentum $(0,0)$, and s symmetry. Figure 5(a) shows that its spin correlation decays almost as a power law, showing that it has at least local antiferromagnetic order. Its static structure factor clearly has

FIG. 5. (Color online) (a) Spin correlation function $\langle \mathbf{S}_0 \cdot \mathbf{S}_r \rangle$ and (b) static structure factor $S(\mathbf{k})$. Empty and filled symbols in (a) represent positive and negative correlations, respectively.

FIG. 6. Same as Fig. 3 except at $J/t=0.8$.

a peak at (π, π) . We therefore believe that the four-hole system at $J/t=0.8$ possesses AF order. Next we are going to investigate the possibility of d -wave pairing in this system.

A first sign of d -wave pairing at $J/t=0.8$ comes from the current correlation shown in Fig. 6. Except for a few bonds at or near the edge of the lattice, the directions of the current correlation at all other bonds show the correct staggered pattern. Compared to the result at $J/t=0.3$ (Fig. 3), the current correlation is much stronger in the present case, especially at small distances. When we sum up the current correlation around plaquettes to obtain the vorticity correlation, a clear staggered pattern emerges. Figure 7 clearly shows that the vorticity correlation has a staggered pattern with a characteristic π phase shift,¹⁹ i.e., the sign of $\langle V(r)V(0) \rangle$ is $(-1)^{r_x+r_y+1}$. Note that the vorticity correlation decays quite fast, which is a characteristic of strong hole-binding at $J/t=0.8$.¹⁰ This shows that the four-hole system at $J/t=0.8$ possesses at least short-range staggered current correlation. A second sign of d -wave pairing at $J/t=0.8$ comes from the hole correlation $C(r)$ in Fig. 1. It consists of two regions with different behavior. At $r \leq 2$ it resembles that of a two-hole

FIG. 7. Same as Fig. 4 except at $J/t=0.8$.

TABLE II. HMDF in systems with two holes ($\langle \bar{n}_{\mathbf{k}} \rangle_2$) and four holes ($\langle \bar{n}_{\mathbf{k}} \rangle_4$) at $J/t=0.8$. $\mathbf{k}$ points along the AFBZ boundary are marked with $\dagger$.

$\mathbf{k}$	$2\langle \bar{n}_{\mathbf{k}} \rangle_2$	$\langle \bar{n}_{\mathbf{k}} \rangle_4$
(0,0)	0.0037	0.0028
$(\pi/4, \pi/4)$	0.0027	0.0046
$(\pi/2, \pi/2)^\dagger$	0.0728	0.0823
$(3\pi/4, 3\pi/4)$	0.2222	0.2196
(π, π)	0.2226	0.2179
$(\pi, \pi/2)$	0.2463	0.2340
$(\pi, 0)^\dagger$	0.1395	0.1176
$(\pi/2, 0)$	0.0301	0.0218
$(3\pi/4, \pi/4)^\dagger$	0.1498	0.1618

system which shows a decaying trend and with a maximum at $r=\sqrt{2}$. The latter feature has been shown to be due to the d -wave nature of the two-hole bound state.^{21,22} At $r > 2$, $C(r)$ remains almost constant, showing that holes at larger distances are uncorrelated or even repulsive. This suggests that holes form d -wave bound pairs, and the two hole-pairs repel each other. Further evidence for this scenario comes from the EMDF. First of all, we note the qualitative similarity between the EMDFs of the four-hole [Fig. 2(b)] and two-hole systems (Fig. 8 of Ref. 5)—along the AFBZ boundary they are largest at $(\pi/2, \pi/2)$ and smallest at $(3\pi/4, \pi/4)$. If the two-hole pairs like to stay away from each other, then their mutual influence will be a minimum. Consequently we expect that the EMDF of a system with two hole-pairs can be built up from that with one pair in an additive manner. This is demonstrated in Table II, which shows that the HMDF of the four-hole system along the AFBZ boundary is roughly twice that of the two-hole system.

To summarize, our results indicate a close relation between d -wave pairing and AF correlations. They favor the scenario that holes in the lightly doped t - J model form weak d -wave bound pairs when the spin background has AF order, and there is an effective repulsion among the d -wave pairs. In this case the system has all the characteristics previously reported for a system with two holes^{4,5,10}—the hole correlation function has a maximum at $r=\sqrt{2}$, and the EMDF is a maximum at $(\pi/2, \pi/2)$ along the AFBZ boundary. The current correlation function exhibits a staggered pattern. All these characteristics reflect the d -wave nature of the bound state. At higher doping levels where AF correlation disappears, holes no longer form bound pairs and they become mutually repulsive. This repulsive behavior is very similar to that of hard core bosons where the repulsion is short-ranged and is due to the lowering of kinetic energy. The EMDF exhibits dips at $(\pi/2, \pi/2)$ along the AFBZ boundary. This agrees with mean-field theory predictions,^{23,24} although we cannot determine whether the dips are hole pockets or segmented Fermi surfaces. We emphasize once more that since we cannot study long-range correlations in our small system, we do not know whether those d -wave hole pairs can lead to superconductivity. Therefore, although our result indicates the coexistence of AF order and d -wave pairing, it *does not*

necessarily imply the coexistence of AF order and superconductivity.

One popular candidate of a charge-ordered phase in a doped antiferromagnet is the stripe phase where charge carriers form one-dimensional strips. It is used to explain the “ $\frac{1}{8}$ anomaly” which, incidentally, is at the same doping level as our four-hole system. But since the model we use is isotropic in the x - y plane, we are not able to detect any anisotropic correlation. Therefore our results are inconclusive regarding stripe phase. Another possible charge-ordered phase that can give rise to enhanced charge order at $x=\frac{1}{8}$ is the checkerboard-type ordering of hole pairs.^{25,26} This ordering emphasizes the two-dimensional nature of the spin system in contrary to the one-dimensional nature of the stripe phase. In the checkerboard-type picture, holes form d -wave bound pairs which in turn form charge-ordered states at a series of magic doping levels. At $x=\frac{1}{8}$ these bound pairs are arranged in a square lattice of sides 4. Incidentally this configuration is compatible with our results when there is AF correlation—the long distance correlation of hole pairs in the checkerboard-type order will make hole pairs appear to be repulsive on a small lattice. As a result the hole correlation will have characteristics of d -wave pairs at small distances and becomes repulsive at larger distances, very much like the one at $J/t=0.8$ in Fig. 1. But according to our results the system must possess at least local AF order in order for this

to be possible. At $x=\frac{1}{8}$ and realistic value of J/t , AF correlation no longer exists and such a charge-ordered phase should not be the ground state. Nevertheless, this charge-ordered phase may exist as an excited state. Therefore our results can be interpreted as providing indirect evidence for the checkerboard-type charge ordering. But we caution that this does not mean that our results favor the checkerboard-type ordering to stripe phase. Due to its isotropic nature, the model we use naturally favors a two-dimensional ordering to a one-dimensional one unless other effects (such as lattice distortion) play a role in selecting the ground state. Finally we remark that our results do not seem to support phase separation at this doping level because we do not see evidence that four holes tend to cluster together even when the spin exchange integral J is as large as $0.8t$.

Note added in proof. After this work was finished we learned that A. Laeuchli had independently solved the t - J model with four holes on a 32-site lattice using exact diagonalization.

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¹¹ $C(r)$ is normalized such that $\sum_{r>0} N_E(r)C(r) = N_h - 1$, where $N_E(r)$ is the number of equivalent sites at distance r from the origin. See Eq. (2) of Ref. 5.

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