Stripes and the *t-J* Model

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We investigate the two-dimensional *t-J* model at a hole doping of $x = \frac{1}{8}$. The low-energy states are uniform (not striped). We find numerous excited states with charge density wave structures, which may be interpreted as striped phases. Some of these are consistent with neutron scattering data on cuprates and nickelates. Without additional terms in the *t-J* Hamiltonian, stripes can be stabilized only as ground states through the application of artificial boundary conditions.

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In the search for an understanding of the cuprate superconductors it is desirable to find a model which captures many of the essential aspects of the environment experienced by the electrons in these materials. Because these materials are born out of antiferromagnetic insulators by doping, it is somewhat urgent to decide if a simple model which begins from the strong electron correlation limit, such as the so-called *t-J* model, can explain some features which result from the electronic degrees of freedom in the cuprates [1]. Even though the progress made in trying to solve the *t-J* model may be characterized as slow, it gives some features which are present in these materials. For example, some important aspects of the calculated single-hole spectrum [2] are in agreement with the results of the photoemission data [3]. In addition, the model gives rise to a two-hole bound state [4] with the $d_{x^2-y^2}$ symmetry which is the believed symmetry of the superconducting state in these materials.

Emery and Kivelson [5] suggested that the cuprates are near an electronic phase separation instability which is prevented by the long-range part of the Coulomb interaction. In the phase-separated state, the holes cluster together, leaving the rest of the system in an antiferromagnet state with no holes. Phase separation in the *t-J* model has been studied by a number of techniques which seem to be giving conflicting conclusions [6–11]. For example, Hellberg and Manousakis [6] using a stochastic projection method, an extension of the Green's function Monte Carlo (GFMC) for lattice fermions, find that the *t-J* model has a region of phase separation at all interaction strengths. Other techniques fail to reach this conclusion. Exact diagonalization studies of small systems have been used to support [7] and reject [8] phase separation, while high temperature series expansions [9] show no phase separation in the physical region of the cuprates. In a recent calculation Calandra *et al.* [11], using the GFMC approach within the fixed node approximation, find that the phase boundary for phase separation is far from that determined by the high temperature series expansions [9] and much closer to that obtained with unconstrained GFMC [6] except in the delicate region with small hole dopings and $J/t \lesssim 0.4$. By using a uniform Fermi-liquid-type nodal structure, one disregards the possibility of a nonuniform ground state in which one component of the mixture (the antiferromagnetic phase) has no fermion degrees of freedom. In addition, in the delicate region of small J/t and low doping, spin-back-flow effects become very important resulting in the interesting structure of the hole "polaron" [12]. These effects are known to change the nodal structure of the wave function in a crucial way in strongly correlated quantum fluids. Therefore fixed-node GFMC may be inadequate in this region.

The phase separation in the *t-J* model cannot be realized in the physical system due to the Coulomb interaction [5,6,13]. Instead, such a tendency for phase separation can be satisfied locally by forming stripes or other charge density wave (CDW) structures with little Coulomb cost [14]. The coupling to lattice distortions may also encourage the formation of stripes [15].

Experimentally, stripe modulations were first observed in a doped nickelate analog of the cuprates [16]. La_2NiO_4 may be doped with holes by adding oxygen or by substituting strontium for lanthanum. The modulation seen with neutron scattering in the doped compounds is consistent with the holes forming *diagonal* domain walls separating antiferromagnetic regions of spins. Stripes with a variety of widths and hole densities along the stripes have been observed.

There is strong evidence for stripe modulations in the cuprates as well [17]. In $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$, superconductivity is suppressed at a filling of $x = \frac{1}{8}$, and neutron scattering studies reveal *vertical* domain walls of holes and spins. In these stripes, a hole density of $\rho_h = 1/2$ per lattice spacing is observed. These experiments have prompted renewed theoretical work on models for the cuprates at hole doping $x = \frac{1}{8}$.

Recently White and Scalapino (WS) found static vertical stripe order similar to that of the cuprates in the two-dimensional *t-J* model at hole doping $x = \frac{1}{8}$ using a density matrix renormalization group technique [18,19]. These results are surprising due to the fact that the *t-J* model ignores the long-range part of the Coulomb interaction and couples to no lattice distortions. One sees

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no physical reason for such a simplified model to have a ground state with a periodic array of interfaces.

In this paper we show that the t-J model at $x = \frac{1}{8}$ has a striped ground state on sufficiently small finite systems with appropriate boundary conditions, such as those used by WS. However, with more physical periodic boundary conditions, the same finite systems have lower energy states that are uniform (not striped). The striped states are present in the periodic systems, but only as excited states.

The t-J Hamiltonian is written in the subspace with no doubly occupied sites as

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

Here $\langle ij\rangle$ enumerates neighboring sites on a square lattice, $c^{\dagger}_{i\sigma}$ creates an electron of spin σ on site i, $n_i = \sum_{\sigma} c^{\dagger}_{i\sigma} c_{i\sigma}$, and $\mathbf{S}_i$ is the spin-$\frac{1}{2}$ operator. Throughout this paper, we take $t = 1$ and $J = 0.35$.

To achieve a hole doping of $x = \frac{1}{8}$, all calculations were carried out on periodic 16-site clusters with two holes. Periodic clusters may be characterized by their primitive translation vectors $\mathbf{a}_1$ and $\mathbf{a}_2$. There are a large number of possible 16-site clusters on the two-dimensional square lattice. Each cluster can support only striped phases that are commensurate with the periodicity of that particular cluster [20]. Clusters which have one particularly short translation vector are quasi-one-dimensional and behave like chains or ladders. We consider only clusters in which both translation vectors have a Manhattan length of at least $l_M = |a^x| + |a^y| \geq 4$. There are seven such clusters, shown in Table I. These clusters represent all possible quasi-two-dimensional 16-site clusters. Later in the paper, we examine six eigenstates in detail. We label these states by letters, (a) through (f), shown next to their corresponding clusters in Table I.

We studied all eigenstates with energy per site $\mathcal{E} < -0.634$ for each of the seven periodic clusters using exact diagonalization. For each cluster, we use all possible combinations of phases $\theta = 0, \pi$ along each translation vector. Several of these states are stripes or CDWs, and these are necessarily degenerate states. The density in a CDW state is characterized by an amplitude A, a wave vector $\mathbf{k}$, and an arbitrary phase ϕ. Thus the hole density $h_{\mathbf{r}} = 1 - n_{\mathbf{r}}$ on site $\mathbf{r}$ is given by

$$h_{\mathbf{r}} = \bar{h} + A\cos(\mathbf{k} \cdot \mathbf{r} + \phi), \quad (2)$$

where the average density is $\bar{h} = \frac{1}{8}$. The phase ϕ depends on the particular linear combination of degenerate states taken. A different (real) linear combination will change ϕ, moving the stripe, but A is invariant.

TABLE I. Translation vectors of the seven possible quasi-two-dimensional 16-site clusters. The letters label eigenstates examined later in the paper.

No.	$\mathbf{a}_1$	$\mathbf{a}_2$	States
1	$(0, 4)$	$(4, 0)$	
2	$(0, 4)$	$(4, 1)$	(e),(f)
3	$(0, 4)$	$(4, 2)$	
4	$(3, 2)$	$(2, -4)$	
5	$(3, 1)$	$(1, -5)$	(d)
6	$(2, 2)$	$(4, -4)$	(a),(b)
7	$(2, 2)$	$(3, -5)$	(c)

The amplitudes A of the CDW in every low-energy state are plotted in Fig. 1 as a function of energy per site. The lowest energy states are uniform and have CDW amplitude $A = 0$. For energies above $\mathcal{E} \gtrsim -0.645$ some CDW states are stabilized. The maximum CDW amplitude of these states increases with increasing energy.

We examine in detail the six labeled states in Fig. 1. State (a) is the lowest energy state and is uniform. States (b) through (f) have increasing CDW amplitude and increasing energy. Each of these states has the largest CDW amplitude of all states at or below its energy.

We plot the charge order of selected states in Fig. 2. The CDW states, (b) through (f), are degenerate, so taking a different linear combination of the eigenstates will change ϕ in (2), moving the CDW. In particular, in state (b) the maximum charge order occurs on a site, while in states (c) and (f), the maximum charge order occurs between two sites, or on a bond. All of the states have degenerate site- and bond-centered CDWs with different linear combinations [18].

States (b) and (c) have diagonal stripes with two different hole densities along the stripe. State (b) has hole density $\rho_b = 1/2$ per (1,1) step, while state (c) has $\rho_c = 1$. These states are similar to experimental results on the nickelates [17] and to the mean-field calculations of Zaanen and Littlewood [21].

States (e) and (f) exhibit vertical stripes with $1/2$ hole per (0,1) step consistent with experimental results on $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$ [17] and with the calculations of WS [18]. States (e) and (f) have the largest CDW amplitudes that we found.

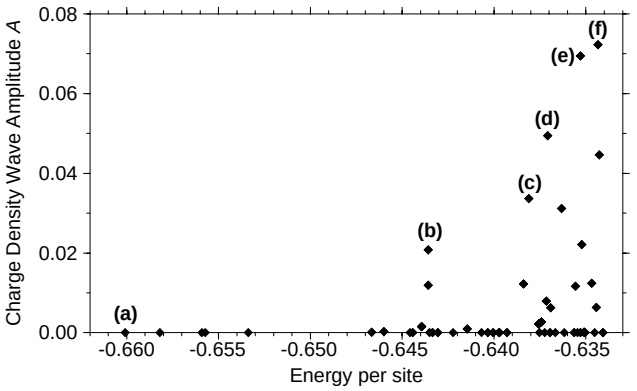

FIG. 1. Amplitude of the CDW in every state with energy per site $\mathcal{E} < -0.634$. The six labeled states correspond to states examined in detail later in the paper. The low-energy states have no CDWs.

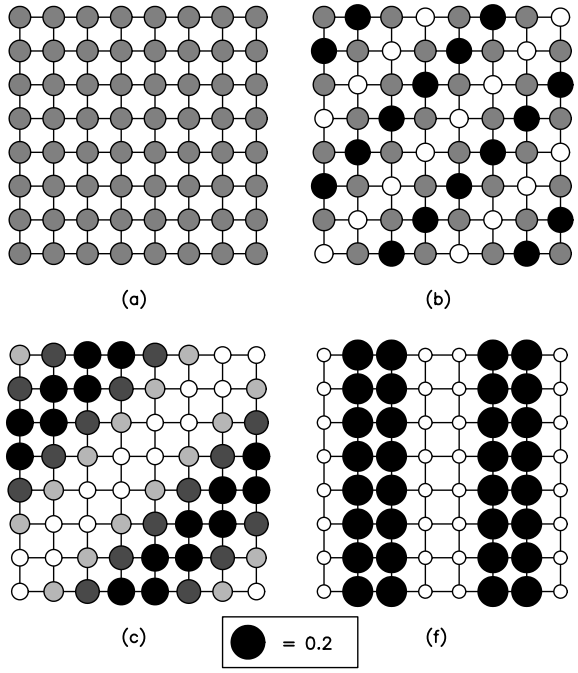

FIG. 2. Hole structures of four of the eigenstates we chose to examine in detail. The radius of each circle is proportional to the hole density on the given site. Additionally, the circles are shaded according to the relative hole density in each state: Black circles show the maximal hole density in that state while white circles show the minimum. State (*a*), which has the minimum energy, has uniform hole density. States (*b*) through (*f*) have increasing energy and show increasing CDW amplitude. Not shown are (*d*), which has a slightly diagonal stripe, and (*e*) which is nearly identical to (*f*). In all states the average spin moment on each site is zero.

Interestingly, the CDWs of the vertical stripe states are remarkably similar to the density profile obtained from the ground state of a 4×4 cluster with open boundary conditions in the $\hat{x}$ direction and periodic boundary conditions in the the $\hat{y}$ direction, the boundary conditions used by WS [18,19]. The hole density as a function of the x coordinate for these three states is shown in Fig. 3. The states (*e*) and (*f*) are excited states of the periodic cluster No. 2 in Table I. The 4×4 cluster with open boundary conditions in the $\hat{x}$ direction can be generated from the periodic cluster No. 2 by cutting all bonds along one column. In a noninteracting picture, the wave function of the holes (or electrons) vanishes at the open boundary. Since the holes are fermions, additional holes will go into higher energy states with more nodes. In this way, it becomes apparent that with open boundary conditions, one will always see density waves. Clearly, the excited states (*e*) and (*f*) essentially have an extra node along one column, resulting in a density nearly identical to the ground state of the cluster with open boundary conditions.

None of the eigenstates has a spontaneous spin density wave amplitude, but the spin correlations are affected by the CDW. One way to show the spin correlations is to apply small magnetic fields along the boundary of the simulation cell, as done by WS [18,19]. This is shown for the diagonal and vertical stripe states (*b*) and (*f*) in Fig. 4. The stripes are pinned so the sites with the fields have maximum electron density with the appropriate average polarization. In both the diagonal and vertical cases, the antiferromagnetic order in neighboring stripes is shifted by π, as in the nickelates and cuprates [17,18].

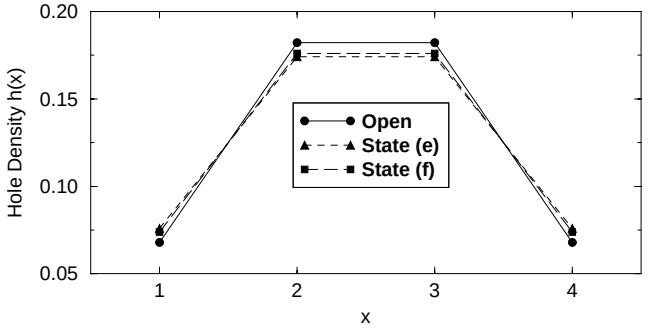

FIG. 3. Comparison of the hole density $h(x)$ as a function of x coordinate for a 4×4 cluster with open boundary conditions in the $\hat{x}$ direction and states (*e*) and (*f*). All three systems exhibit a stripe in the $\hat{y}$ direction. The state with open boundary conditions is the nondegenerate ground state.

A more accurate way to show the spin correlations is through the pair correlation functions of the eigenstates without pinning fields. Figure 5 shows the hole-hole, $H(\mathbf{r}) = \sum_{\mathbf{r}'} \langle h_{\mathbf{r}'} h_{\mathbf{r}'+\mathbf{r}} \rangle$, and spin-spin, $S(\mathbf{r}) = \sum_{\mathbf{r}'} \langle \mathbf{S}^z_{\mathbf{r}'} \mathbf{S}^z_{\mathbf{r}'+\mathbf{r}} \rangle$, correlation functions where $\mathbf{r}$ is 1 or 2 lattice spacings in the $\hat{x}$ or $\hat{y}$ directions (longer distances wrap around the periodic clusters). The averages include both the hole-rich and electron-rich regions of the striped states. In the striped states, holes are more likely to align vertically than horizontally, especially two

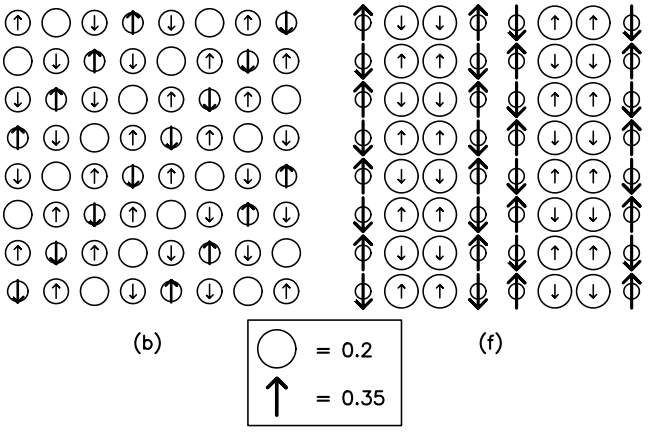

FIG. 4. Hole and spin structures of states (*b*) and (*f*) generated by applying a small staggered magnetic field of $h = 0.1$ to sites at the boundary of the simulation cell to pin the spins. The radius of each circle is proportional to the hole density on the given site, and the length of the arrows is proportional to $\langle S^z_i \rangle$. These are *not* eigenstates of the *t-J* Hamiltonian without the pinning fields, but the spin correlations pictured are similar to the correlations in the eigenstates (*b*) and (*f*).

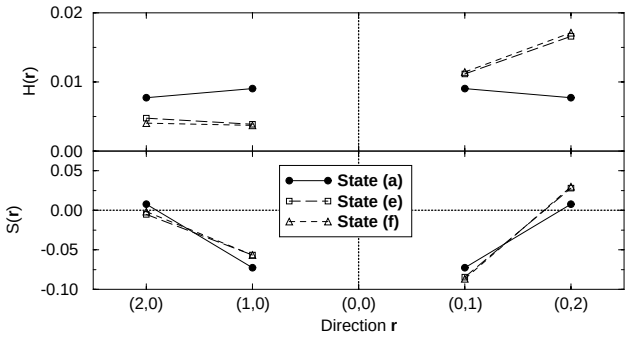

FIG. 5. Hole-hole and spin-spin correlation functions of states (a), (e), and (f) in the $\hat{x}$ and $\hat{y}$ directions.

steps vertically. Similarly the antiferromagnetic spin correlations are stronger vertically than horizontally in the stripes.

To conclude, we found stripes in the *t-J* model at a doping of $x = \frac{1}{8}$, but only as excited states in periodic systems. The ground state of the model for $J/t = 0.35$ is uniform. The energy cost per site to form diagonal stripes similar to those found in the nickelates is at least $\Delta_d \gtrsim 0.016t$, and for vertical stripes similar to those in the cuprates the energy cost is $\Delta_v \gtrsim 0.025t$. At this doping and interaction strength studies on larger systems have found that the model is nearly phase separated [6,7]. The stripes seen experimentally could be the result of phase separation frustrated by the Coulomb repulsion [13] and/or the coupling of the electrons to lattice distortions. However, the stripe states are not ground states of the simple *t-J* model, as claimed in Ref. [18]; this discrepancy may be due to the open boundary conditions used in that work.

Our findings are in agreement with the recent work of Pryadko, Kivelson, and Hone [22] who studied the interaction between localized holes in a weakly doped quantum antiferromagnet. They find that stripes are unstable due to an attractive interaction between such domain walls.

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