Stripes on a 6-Leg Hubbard Ladder

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While density matrix renormalization group calculations find stripes on doped n-leg t-J ladders, little is known about the possible formation of stripes on n-leg Hubbard ladders. Here we report results for a 7×6 Hubbard model with four holes. We find that a stripe forms for values of U/t ranging from 6 to 20. For $U/t \sim 3$–4, the system exhibits the domain wall feature of a stripe, but the hole density is very broadened.

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The nature of the ground state of the two dimensional t-J model continues to be controversial, even if one restricts one's attention to numerical simulations. Density matrix renormalization group (DMRG) calculations [1] for n-leg t-J ladders (with n ranging from 2 to 8) with J/t in the physical region of interest for the cuprates, find that stripes are formed when the ladders are doped with holes [2]. In contrast, the Green's function Monte Carlo (GFMC) results of Sorella *et al.*, on square, periodic t-J lattices find a $d_{x^2-y^2}$-wave superconducting ground state [3]. The aspect ratio of an n-leg lattice and the open boundary conditions used in the DMRG calculations may be sufficient to favor a striped state. Alternatively, the choice of the guiding trial wave function for the GFMC may bias the system towards a superconducting state [4]. It is clear that the t-J model is a delicately balanced system. Thus it is interesting to go back one step and study the underlying Hubbard model in which the on site Coulomb interaction U is a parameter.

Much less is known about the nature of the ground state of the 2D Hubbard model, which is computationally more demanding. Previous DMRG calculations [5] on 3-leg Hubbard ladders found that diagonal three-hole stripes with a linear filling density of unity formed when U/t was greater than 5. Early mean-field Hartree-Fock calculations for the 2D Hubbard model found that vertical stripes were favored for U/t less than of order 4 and diagonal stripes formed at larger values of U/t [6]. These Hartree-Fock stripes have a linear filling density of 1 and their width is set by a coherence length $\xi_0 \sim t/\Delta_0$ with Δ_0 the gap of the half-filled system. As U increases, ξ_0 decreases, approaching a lattice spacing at larger values of U/t. Eventually, when U exceeds twice the bandwidth, the mean-field stripes disappear [7]. Note, however, that the Hartree-Fock treatments do not include pairing and that their energy per hole is of order $1t$ too high. Here, we extend the DMRG study of stripe formation in the Hubbard model and, in particular, examine the question of whether stripes form on a 6-leg Hubbard ladder and how their structure depends upon U/t. Our results represent the first reliable ground state results for a Hubbard cluster large enough to exhibit an unambiguous stripe. From this single cluster we are not able to make conclusions about the infinite 2D lattice; on the other hand, our results strongly suggest that stripes are low-lying states in the Hubbard model, as they are in the t-J model.

The cluster geometry was chosen with some care. Stripelike behavior involving only two holes can be suggestive [8,9] but may represent only a feature of hole pairs. One would like at least four holes in a stripe, which makes the system size beyond the current reach of exact diagonalization. Periodic boundary conditions, when the dimensions of the cluster are even, *frustrate* a single stripe [7,9]. Making one of the dimensions odd tends to *force* a single stripe. We choose a 7×6 cluster, with cylindrical boundary conditions, periodic in the y direction and open in the x direction, and with four holes. Our previous calculations on the t-J model show that cylindrical $L \times 6$ systems have ground states with four-hole stripes wrapped around the cylinder. The open boundaries neither frustrate nor force the stripes, although if they form, the boundaries serve to pin them. One may worry that Friedel oscillations in the charge density, induced by the open boundaries, mimic stripes, but we find, for a number of reasons, that our stripes in the t-J model are inconsistent with the Friedel oscillation scenario [10]. Sorella *et al.* compared GFMC and DMRG on a 6×6 cylindrical t-J cluster with six holes [3]; however, we expect six holes to split into a stripe and a pair, with resonance between them, obscuring any obvious signs of a stripe in the charge or spin densities. (A stripe having an odd number of holes would be frustrated in the y direction.)

Here we begin by looking at the t-J model and then turn to the Hubbard model. A typical result for a 17×6 t-J lattice with $J/t = 0.35$ and 12 holes, with cylindrical boundary conditions, is shown in Fig. 1. A maximum of $m = 5000$ states were kept, for a discarded weight of

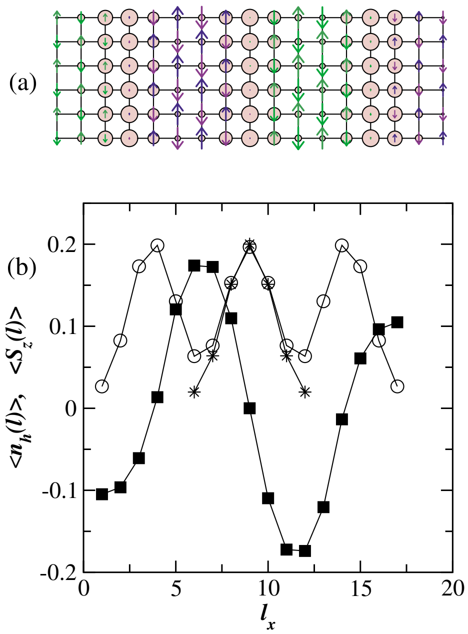

FIG. 1 (color online). (a) Charge and spin distribution on a doped 17×6, t-J lattice with 12 holes and $J/t = 0.35$. All the lattices that we discuss have periodic boundary conditions in the vertical 6-site y direction and have open boundary conditions in the x direction. Here, on the 17×6 lattice, three charge stripes have formed with four holes each separated by π-phase-shifted antiferromagnetic regions. (b) The same results, plotted differently. The open circles show the hole density $\langle n_h(l)\rangle$ and the squares show the spin density $\langle S_z(l)\rangle(-1)^l$. In addition, the asterisks show results for a 7×6 system with four holes, shifted to the center of the system.

7×10^{-5}. One can see in Fig. 1 that three charged stripes have formed and the spins form π-phase-shifted regions between the stripes. For an $L \times 6$ ladder, the linear charge density along a stripe is 2/3. Studies of longer stripes find that the preferred density on a long stripe is 1/2. Competing with the four-hole stripe, but higher in energy per hole, is a single pair, which also exhibits some stripe-like features. As seen in Fig. 1, there are two types of four-hole stripes: the stripes on the ends are (mostly) bond centered, and the stripe in the middle is site centered. The energy per unit length of these two configurations is extremely close. The charge and spin density profiles along the x direction are plotted in a more conventional fashion in Fig. 1(b). Since later we consider a 7×6 ladder for the Hubbard model, also shown is the local hole density on a 7×6, t-J ladder with four holes and $J/t = 0.35$. One can see that the open boundaries on the small system mimic the presence of the other stripes on the larger system.

In Fig. 1, the presence of static magnetic moments makes the π-phase shift in the antiferromagnetic spin density as one crosses a stripe clearly visible. No external magnetic fields were applied to the system, and these static magnetic moments are artifacts of the DMRG calculation, for which no spin symmetry has been used. However, we argue that the presence of these static moments has very little effect on the validity of the results. To see this, we show DMRG results for an undoped 17×6 system in Fig. 2. The undoped system converges very rapidly with the number of states m, allowing us to study the convergence in detail. In particular, we consider $\langle S_z(l)\rangle$ versus the error in energy for a particular number of states kept m. The exact ground state of this system, by the Lieb-Mattis theorem, is a spin singlet, which is spin-rotationally invariant, and therefore $\langle S_z(l)\rangle = 0$ for all sites l. However, as measured by the spin-spin correlation function, this state has long-range antiferromagnetic order. The ground state is a superposition of all the static antiferromagnetic states with all possible orientations of the order parameter. The reduction in energy due to the macroscopic superposition of the states is very small. We see from Fig. 2 that there exist states with static moments of order 0.2 with energies only $0.0002t$ per site above the ground state. In a doped system with some form of magnetic order, the behavior of the holes in each of the states with different spin orientations would be identical. It is reasonable to assume that the effect of the superposition on the hole behavior is slight.

We can also analyze this effect in the undoped system by applying a staggered magnetic field. We assume the energy per site of the system, for small applied fields, varies as

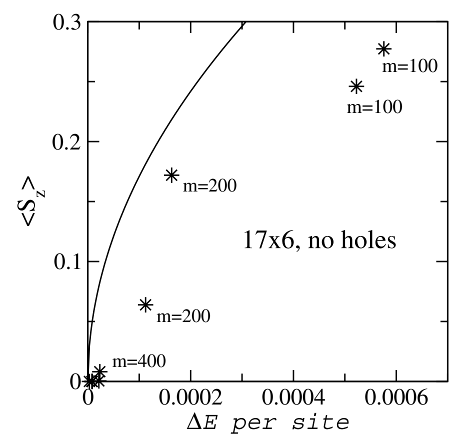

FIG. 2. Expectation value of the spin $|\langle S_z(l)\rangle|$ at a site in the center of an undoped 17×6 t-J system, as a function of the error in the total energy per site. The error in the total energy per site is measured relative to a nearly fully converged DMRG calculation, accurate to about 10^{-6}. Each symbol corresponds to a particular DMRG sweep, for which the number of states kept was m. Two sweeps were performed for each value of m. Although the exact ground state has $S_z(l) = 0$, states with substantial static antiferromagnetic order can have energies only slightly above the ground state. The solid curve was generated by applying a staggered magnetic field to the system, and it represents the maximum value of $|\langle S_z(l)\rangle|$ possible for a given error in the energy (see text).

$$E(s, h) = E_0 + as^2 - sh, \tag{1}$$

where h is the magnitude of the applied staggered field in the z direction and s is the average magnitude of $\langle S_z(l)\rangle$ in response. We minimize $E(s, h)$ over s, keeping h fixed, to find $s(h) = h/(2a)$, and hence $E(s) = E_0 - as^2$. From several very accurate DMRG simulations with various values of h, we find that for $s < 0.1 - 0.2$, this energy dependence is accurate, and for the 17×6 system $a \approx 0.0034$. To describe the case where there is no applied field, and a finite value of s is considered an error, we define $\Delta E = as^2$, yielding $s(\Delta E) = (\Delta E/a)^{1/2}$, which is shown as the solid line in Fig. 2. This should be considered to be an upper bound on the $s(\Delta E)$ obtained from DMRG, for which there are other sources of error in the wave function besides a finite value of s.

We turn now to the Hubbard model. Our results for the Hubbard systems were performed using a new "single-site" DMRG method [11], which performs better than the standard DMRG algorithm having two sites in the center when the number of states per site is more than two or three. Using this method, we have been able to keep up to 7500 states per block in some cases. Unfortunately, discarded weights are not informative, and we do not report them. Otherwise, single-site and two-site DMRG differ primarily in calculation time, and results can be compared directly. When performing DMRG calculations on 2D clusters, one must deal with the possibility that the calculation will get stuck in a metastable state. For example, a striped state may be lower in energy than a state with two widely separated pairs, but the calculation may be able to tunnel between these configurations only when keeping very large numbers of states per block. In this case, one must repeat the calculations with constrained initial configurations and compare final energies. On the other hand, a calculation is particularly robust if one sees that it does tunnel between very different states. Figure 3(a) shows a plot of the ground state energy for a 7×6 lattice with $U/t = 12$ and four holes as a function of the number of basis states m. The hole density distribution obtained at a number of sweeps, labeled by the value of m, is shown in Fig. 3(b). The initial configuration consisted of two separate pairs. As the number of basis states increases and the ground state energy converges, one clearly sees the stripe develop, with the "tunneling" occurring for about $m = 1200$ states. From Fig. 4 we see that, just as for the t-J model, there is a π-phase shift in the magnetization density across a stripe. One can see that as the stripe develops, the DMRG ground state energy decreases and that just as for the t-J model, doped holes on 6-leg Hubbard ladders can form striped ground state structures for $U/t = 12$.

We have performed a limited study of the behavior of this system as a function of U/t. Figure 5 shows the charge and spin densities for U/t ranging from 3 to 20. For $U/t = 8$, we started the system with the holes as two

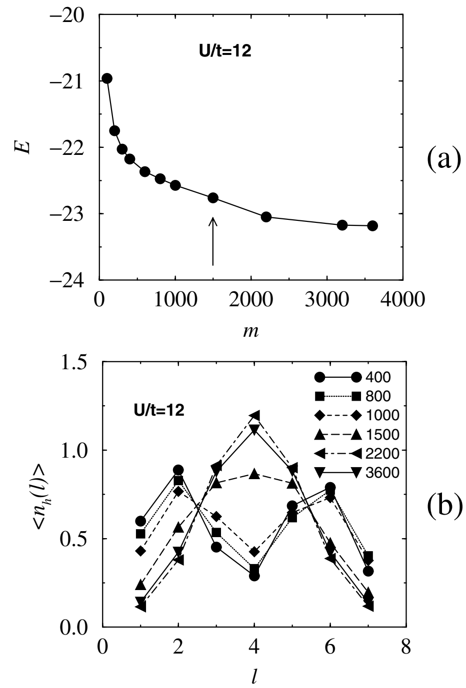

FIG. 3. (a) The ground state energy of a 7×6 Hubbard model with $U/t = 12$ and four holes versus the number of basis states kept in the DMRG calculation. The arrow indicates the approximate point at which the stripe spontaneously forms. (b) The charge distribution $\langle n_h(l)\rangle$ seen in the DMRG calculation, labeled by the number of states kept per block m.

separate pairs. We observed tunneling to the stripe state near $m = 3600$, considerably later than for $U/t = 12$. We let this calculation continue until it used all the available memory (3 Gb), taking about one week of computer time, on an Athlon MP 1800+ processor. In this case, further sweeps reached a maximum of $m = 7500$, with little change in the charge and spin distributions. For $U/t = 6$, we observed tunneling to the stripe state near $m = 4000$, again with a maximum of $m = 7500$. For $U/t = 4$ and $U/t = 3$, we did not try to observe the tunneling, instead starting with the four holes together in the center. Here, we found that a broadened striped configuration was stable, up to the maximum

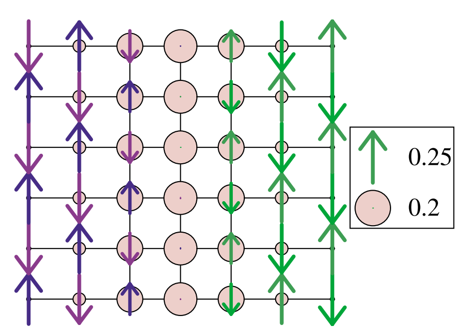

FIG. 4 (color online). The charge and spin distribution for the system of Fig. 3.

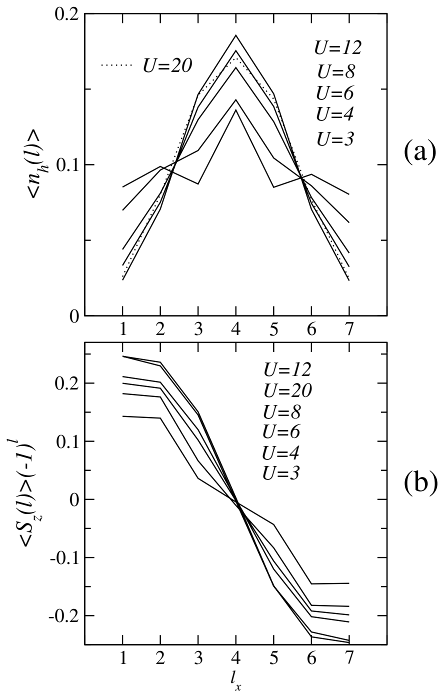

FIG. 5. (a) The hole density $\langle n_h(l)\rangle$ of a 7×6 Hubbard model as a function of the x coordinate ℓ_x for various values of U. The solid lines refer to the list of U's on the right, in order by peak height. The dotted line refers to $U = 20$, which is out of order by peak height. The data are taken from the final sweep in each run, with m values ranging from 3600 to 7500 (see text). Because of the different m values, differences between curves of less than about 5% are not significant. (b) For the same set of systems the spin density $\langle S_z(l)\rangle(-1)^l$, showing the π phase shift of the stripe. Here, we estimate that differences of less than about 10% are not significant.

number of states kept ($m = 6000$ and $m = 4000$, respectively). For $U/t = 3$, the charge distribution is perhaps too broad to consider it a stripe, but the domain wall nature of the spin configurations is still fairly robust. However, since, as noted above, the spin expectation values are (useful) artifacts of the DMRG procedure, we do not attach much significance to the specific magnitudes shown in Fig. 5(b). Figure 5 also shows results for $U/t = 20$. For this run, we started it in a state with the four holes together, but during the first several sweeps, keeping only $m \approx 200$, the holes partially split apart. Subsequently, near $m = 1000$, a definite stripe formed along with the antiferromagnetic domain wall. A maximum of $m = 6000$ states was kept. For this large value of U/t, the stripe appears somewhat less stable than at $U/t = 12$. We observe a very similar weakening in the stripe in the t-J model, as the value of J/t is reduced from 0.35 to 0.2 [the peak height in $\langle n_h(l)\rangle$ drops from 0.21 to 0.18].

In conclusion, we have found that on a moderately sized Hubbard cluster, with cylindrical boundary conditions and doped with four holes, the ground state has a stripe. The stripe is narrow and well-defined for $U/t = 8$–12. For smaller values of U, starting at $U/t \approx 6$, the stripe broadens, until at $U/t = 3$ the width of the stripe is the size of the system. At $U/t = 20$, the stripe is somewhat broadened compared to $U/t = 12$. The overall behavior is very similar to that seen in the t-J model. Although the open ends in one direction may encourage the stripe to form, the same roll may be played by neighboring stripes in larger systems. We find nearly the same hole density profile for a stripe in a 7×6 t-J system as in the central portion of a t-J 17×6 t-J system. For small U/t, the broad stripes we obtain are probably strongly influenced by the open boundaries.

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[10] Some of the reasons why our stripes are inconsistent with Friedel oscillations are (i) the amplitude of the hole density oscillations is very large and does not decay significantly away from the edges; (ii) the hole density oscillations are largely independent of the length of an $L \times 6$ system; (iii) four holes form a bound state, with a measurable binding energy to breaking up into two pairs; (iv) the amplitude of the hole density oscillations does not depend significantly on local potential terms on the open edges; (v) stripes form in the early sweeps of DMRG calculations in long systems, even when the hole density near the edges is still precisely zero; and (vi) suitable boundary conditions can induce *longitudinal* stripes.
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