Stripes on a 6-Leg Hubbard Ladder

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(Dated: November 12, 2018)

While DMRG 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 4 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.

PACS numbers: PACS
stripes have formed with 4 holes each separated by 
that we will discuss have periodic boundary conditions in the 
y-vertical 6-site 

boundaries on the small system mimic the presence of 
with 4 holes and $J/t = 0.35$. One can see that the open 
calculation, for which no spin symmetry has been used.

In Fig. 1, the presence of static magnetic moments 
energy per site of the system, for small applied fields,

However, we argue that the presence of these static mo-
ments has very little effect on the validity of the re-
results. To see this, we show DMRG results for an undoped 
$17 \times 6$ 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 con-
sider $\langle S_z(l) \rangle$ 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 sing-
glet, 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 superpo-
sition of all the static antiferromagnetic states with all 
possible orientations of the order parameter. The reduc-
tion 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 en-
gies only 0.0002$e$ 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,
to find values of several very accurate DMRG simulations with various $E$ in response. We minimize dependence is accurate, and for the $17 \times 6$ system were performed using a new "single-site" DMRG method[11], which performs better for the Hubbard systems 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. 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 only be able to tunnel between these configurations 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. Fig. 3(a) shows a plot of the ground state energy for a $7 \times 6$ lattice with $U/t = 12$ and 4 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 $\pi$-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 $U/t$. Fig. 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 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 1 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 sta-

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E(s, h) = E_0 + as^2 - sh
\]

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 $17 \times 6$ 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 wavefunction 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. 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 only be able to tunnel between these configurations 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. Fig. 3(a) shows a plot of the ground state energy for a $7 \times 6$ lattice with $U/t = 12$ and 4 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 $\pi$-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 $U/t = 12$.

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![Fig. 3](attachment:fig3.png)

**Fig. 3:** (a) The ground state energy of a $7 \times 6$ Hubbard model with $U/t = 12$ and 4 holes versus the number of basis states kept in the DMRG calculation. The arrow indicates the approximate point in which the stripe spontaneously forms. (b) The charge distribution $\langle n_i(l) \rangle$ seen in the DMRG calculation, labeled by the number of states kept per block $m$.

![Fig. 4](attachment:fig4.png)

**Fig. 4:** The charge and spin distribution for the system of Fig. 3

\[
E(s, h) = E_0 + as^2 - sh
\]
ble, up to the maximum 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 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). Fig. 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 ≈ 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 were 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=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 role 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.

The would like to that A. Chernyshev for useful comments. We acknowledge the support of the NSF under grants DMR98-70930 and DMR98-17242.

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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. (b) For the same set of systems the spin density \( \langle S_z(l) \rangle(-1)^l \), showing the \( \pi \) phase shift of the stripe.

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FIG. 5: (a) The hole density \( \langle n_h(l) \rangle \) of a 7×6 Hubbard model as a function of the x coordinate \( \ell_x \) for various values of U. The solid lines refer to the list of U's on the right, in order by peak height. (b) For the same set of systems the spin density \( \langle S_z(l) \rangle(-1)^l \), showing the \( \pi \) phase shift of the stripe.

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[10] Some of the reasons why our stripes are inconsistent with Friedel oscillations are: (1) the amplitude of the hole density oscillations is very large, and does not decay significantly away from the edges; (2) the hole density oscillations are largely independent of the length of an L×6 system; (3) four holes form a bound state, with a measurable binding energy to breaking up into two pairs; (4) the amplitude of the hole density oscillations do not depend significantly on local potential terms on the open edges; (5) 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 (6) suitable boundary conditions can induce longitudinal stripes.
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