Comment on “Stripes and the t-J Model”

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In a recent Letter\textsuperscript{1} Hellberg and Manousakis (HM) studied a set of 16-site t-J clusters with two holes using exact diagonalization to determine whether the 2D t-J model has a striped ground state at a doping of $x = 1/8$. Based on these diagonalizations, they concluded that the ground state of the 2D t-J model is uniform. They observed low-lying nonuniform states with stripe-like features, but argue that these could only represent ground state configurations if one applied artificial boundary conditions. In particular, (1) they concluded that there is “no physical reason for such a simplified model [the t-J model] to have a ground state with a periodic array of interfaces”\textsuperscript{2}; and (2) the striped states found in density matrix renormalization group (DMRG) calculations\textsuperscript{3} are simply an “artifact” of the boundary conditions used in DMRG. We disagree with these conclusions and believe that their analysis is flawed in several important respects.

First, there is a physical mechanism which favors stripe formation in the t-J model. As noted by HM and others\textsuperscript{4}, for $J/t$ in the relevant physical range, two holes on a t-J cluster will form a pair with $d_{x^2-y^2}$ symmetry. Now the point is the pairs can lower their energy further by forming a domain wall of holes with local pairing correlations, across which there is a $\pi$-phase shift in the antiferromagnetic background\textsuperscript{5}. Such an arrangement reduces the frustration of the antiferromagnetic background produced by the localized hopping of the holes and lowers their transverse kinetic energy, leading to a stabilization of the domain walls. The details of the correlations involved in this process have been studied extensively using DMRG and exact diagonalizations\textsuperscript{6,7,8,9}. The second point raised by HM concerned the question of boundary conditions. In using finite size clusters to study models which may have broken-symmetry ground states, it is often convenient to introduce a symmetry-breaking field and then study the limiting behavior by first letting the size of the system go to infinity and then letting the strength of the perturbation go to zero. We view the open end boundary conditions that we have used in this way and argue that far from being artificial, they are important for understanding the physics. Unfortunately, at present we are unable to carry out a finite-size scaling analysis to obtain the infinite size limit. Note that in the case of striped structures, the domain wall spacing rather than the lattice spacing enters in setting the lattice sizes required. Nevertheless, we have compared on numerous occasions systems of different lengths, and not seen any significant reduction in the stripe amplitudes. We have also compared a 12 $\times$ 6 system with the interior 12 $\times$ 6 region of a 24 $\times$ 6 system at the same doping where we found the energy per hole to be the same to within about $\pm 0.01t$. Note also that we see the stripes regardless of whether we apply a staggered field to the edges of the system. In the absence of the staggered field, it simply takes longer for the calculation to converge. Finally, we are able to observe an essentially uniform ground state even with open boundary conditions; they occur when a next-nearest neighbor hopping $t'$ is made large enough ($t' \sim 0.3t$)\textsuperscript{10}. The effect of this term is to destabilize the domain walls and favor a gas of pairs.

We also see stripes develop (without $t'$) as our DMRG calculation progresses from a starting point with all the holes in a clump in the center of a long system; the stripes appear spontaneously long before the holes have any probability amplitude of being near the open ends of the system. Such a calculation is shown in Figs. 1 and 2. Here, a 16 $\times$ 6 system with $J/t = 0.35$ and cylindrical boundary conditions, with eight holes, is studied with DMRG. No external fields were applied. In the initial DMRG sweep, all the holes were forced onto the center two columns of sites. Subsequently, as the finite system DMRG sweeps are performed, the system moves the holes in order to decrease the energy of the wavefunction. Since hole density is locally conserved, the essentially local DMRG sweeps move the holes slowly. Néel order develops spontaneously in the $z$ spin direction, since we have quantized the spins in the $z$ basis. As the calculation converges, this spontaneously broken spin symmetry slowly disappears, corresponding to an averaging of the overall spin direction over all possible directions. (This reduction in the local spin moments is not yet visible in the sweeps shown in Fig. 1.) Substantially before the hole density has approached either end of the system, two stripes appear spontaneously. The $\pi$ phase shift also appears spontaneously, and is visible in the local measurements because of the broken spin symmetry. As the calculation converges to the ground state, the $\pi$ phase shift becomes visible only through spin-spin correlations. The two stripes repel, and continue to move slowly apart as the sweeps progress until they are roughly equidistant from each other and the open left and right ends.

Turning now to the calculations reported by HM, first, it appears that by searching for the lowest energy states in a variety of 16 site clusters, they have simply found the clusters with the largest finite size effects. In this regard, it is interesting to note that the lowest-energy labeled states (a), (b), and (c) are all on the most one-dimensional clusters of the ones they studied, those with one of the primitive translation vectors being (2.2). The
fourth lowest energy state (d) is on the next most one-dimensional lattice. The authors excluded clusters which were even more one dimensional than these because of finite size effects; if they had also excluded the (2,2) clusters, their conclusions would have been quite different. The important point is that the energy differences they obtain by comparing different small clusters are far too large to relate to the subtle competition between pairing and stripes. Their lowest energy of $-0.660t$ per site translates to an energy of $-1.979t$ per hole. In an exact diagonalization, we find that the ground state energy of the ordinary $4 \times 4$ periodic cluster with two holes is $-0.628t$ per site, or $-1.72t$ per hole. From this we see that none of the states shown in Fig. 1 (which unfortunately are not labeled according to cluster) is from the $4 \times 4$ cluster—they were omitted by HM because their energy was too high. This difference of $0.26t$ per hole between these two uniform ground states of different 16 site clusters is about an order of magnitude larger than the energy difference between pairs and stripes on large systems at low doping shown in Fig. 1 of Ref. [1].

Secondly, the stripes we have found involve correlations between two or more pairs of holes, while the 16-site clusters studied by Hellberg and Manousakis have only one pair. As noted earlier by Prelovsek and Zotos [2] one needs at least 4 holes (i.e. two pairs) on a cluster to study stripe formation. In fact, using diagonalizations of clusters containing 4 holes, Prelovsek and Zotos [2] found evidence for domain wall formation. We believe that meaningful information about stripe stability cannot come from calculations which involve only one pair on a cluster. In fact, the “striped” states reported in the HM Letter have quite a different origin than the stripes in the many-hole systems we have found. Just as one can combine $p$ and $-p$ excited states of a single particle in a periodic box to create a spatial density wave oscillation, these authors have combined degenerate excited states of one pair in a cluster to create a standing density wave. The stripes we have found arise from correlations of pairs rather than the excited state of one pair.

To summarize: there is a physical mechanism for domain wall formation in the $t-J$ model and the boundary conditions used in our calculations are not artificial, but, in fact, provide a simple way of introducing a symmetry breaking field. We have seen the stripes disappear when we change the model by adding a nearest-neighbor hopping $t'$, showing that the model itself does contain a mechanism for stripe formation. We have seen little change in behavior in going to larger lattices, although we have not been able to carry out a finite size scaling analysis. We believe that the calculations reported by HM are misleading because of large finite size effects on their 16-site clusters and the fact that they only have one pair. In particular, the stripe-like patterns they observe are only standing wave patterns of the motion of a pair of holes rather than the stripes arising from correlations of many pairs of holes (e.g. in the $16 \times 8$ cluster of reference [2] there were 16 holes or 8 pairs). Finally, it is important to note that we have not argued that stripes in the 2D $t-J$ model are necessarily static, although they certainly are in our calculations. There may be low energy fluctuations of the stripes which restore translational or rotational symmetry, which require larger systems and higher accuracy than we currently can manage. However, what we do believe our calculations show is that a “uniform” many-hole state which has no manifestation of static or dynamic stripes is, in fact, not a low-lying state of the $t-J$ model near a doping $z = 0.125$. Indeed, most of the experiments which see stripes find dynamic stripes [11]; they are observable in dynamical susceptibilities, regardless of whether there are broken spatial symmetries.

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FIG. 1. A 16 × 6 t-J system, with J/t = 0.35 and eight holes, with cylindrical boundary conditions (open in the x direction, periodic in y), is studied with DMRG. The plot shows the local hole density by the diameter of the circles, according to the scales shown. The local spin moment is shown by the length of the arrows. The four pictures represent the state of the system at the end of sweeps 1, 3, 6, and 15. The number of states kept per block was increased as the sweeps progressed, with 80, 200, 600, and 1000 states kept in these four sweeps, respectively. The energy steadily decreased, taking values -42.96, -49.68, -51.890, and -52.279, in the four sweeps. The quantum numbers during the DMRG warmup sweep (sweep “0”) were manipulated to force all 8 holes onto the center two columns, in order to strongly favor a phase-separated state. However, the phase separated state is unstable, and splits into two four-hole stripes, which subsequently repel each other. Different style arrows are used to distinguish the two separate antiferromagnetic domains that form.

FIG. 2. The hole density as a function of the x coordinate is shown for the same four sweeps as in Fig. 1. Note that in sweep 6, where the striped pattern is clearly visible, the hole density on the left and right edges is still zero. Consequently, the stripes are not caused by the open boundaries. However, we find that whether the final stripe configurations are site centered or bond centered is influenced by the boundary conditions.