Phase separation and stripe formation in the two-dimensional *t-J* model: A comparison of numerical results

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We make a critical analysis of numerical results for and against phase separation and stripe formation in the *t-J* model. We argue that the frustrated phase separation mechanism for stripe formation requires phase separation at too high a doping for it to be consistent with existing numerical studies of the *t-J* model. We compare variational energies for various methods, and conclude that the most accurate calculations for large systems appear to be from the density-matrix renormalization group. These calculations imply that the ground state of the doped *t-J* model is striped, not phase separated.

The recent discovery of stripes in the underdoped cuprates[1] has brought renewed interest to the question of the existence of phase separation in the *t-J* and Hubbard models. Interest in this question began a decade ago, when evidence for phase separation in $La_2CuO_{4+\delta}$ was found.[2] In particular, Emery *et al.* argued that rather than stemming from the chemistry of the mobile oxygen atoms in this material, the phase separation reflected a universal tendency for doped holes in antiferromagnets to phase separate.[3] They argued that this phase separation is not seen in the absence of mobile dopants because it is frustrated by the long-range Coulomb repulsion between holes. This led to a number of studies using analytical arguments and numerical simulations to find out whether the *t-J* and Hubbard models (which do not have long-range Coulomb interactions) exhibit phase separation[4] and to the related question of the mechanism responsible for stripe formation in the cuprates.

There are, in fact, currently two main views regarding the origin of stripes. In the first, stripes form because of a competition between kinetic and exchange energies in doped antiferromagnets. In this approach, long range Coulomb interactions are not important. Indeed, a decade ago Hartree-Fock solutions of the two-dimensional (2D) Hubbard model showed that domain walls were present in mean field solutions of the Hubbard model.[5] However, the stripes in the Hartree-Fock solution are characterized by a filling of one hole per domain wall unit cell, while the incommensurate spin susceptibility peaks seen in experiments require a filling of half this. Subsequently, numerical studies of the *t-J* model by Prelovsek and co-workers[6] showed that indeed, stripelike correlations are an important ingredient in the ground state of small *t-J* clusters. This work also made clear that stripes act as domain walls in Néel antiferromagnets. However, because of the limited size of the systems studied, only filled stripes were found. Recently, using density-matrix renormalization group methods (DMRG) (Ref. 7) to study much larger systems numerically, we have found evidence for striped ground states for a wide range of dopings in the *t-J* model.[8,9] Significantly, we have found that stripes with a linear doping of one hole per two domain wall unit cells are the lowest energy configurations at low doping.

The second approach starts with the assumption that without long-range Coulomb interactions, doped antiferromagnets phase separate. Stripe formation arises in this approach because the long-range Coulomb repulsion frustrates the phase separation, leading to an inhomogeneous charge density state.[10] The π phase shift characteristic of a domain wall arises in this ''frustrated phase separation'' approach from a secondary effect, namely, from the same reduction of the transverse kinetic energy of hopping which *drives* domain wall formation in the first approach. In support of this approach, studies of classical spin models of competing long and short range interactions have been shown to have a variety of inhomogeneous ground states, including striped states.[11] Unfortunately, the difficulty associated with the long-range Coulomb interactions has so far prevented more realistic microscopic calculations. However, as a minimum requirement for the viability of the frustrated phase separation scenario, one clearly must have phase separation in relevant models of doped antiferromagnets which lack the long-range Coulomb interaction, such as the *t-J* or Hubbard models. Extensive numerical studies of the Hubbard model have failed to find convincing evidence of phase separation[4] and interest has shifted to the *t-J* model which does exhibit phase separation in certain regions of J/t-doping parameter space. In this case, the question becomes one of determining whether the phase separation takes place in the physical parameter range. More generally, the question becomes one of whether more elaborate models such as, for example, three-band models or models which include electron-phonon interactions will exhibit phase separation in the physical region of parameter space. Here we will not address this more general question, but rather focus on the *t-J* model because it has often been used in the discussion of stripe formation.

The proposal that the doped *t-J* model phase-separates in physically relevant parameter and doping regimes has been supported by variational arguments,[3] diagonalizations of small clusters,[3] Green's function quantum Monte Carlo (QMC) calculations,[12] and the recent analysis of the Casimir force arising from fluctuating spin waves in the antiferro-

magnetic regions separating widely spaced stripes.[13] On the other hand, a substantial body of other QMC calculations,[14] series expansions,[15] exact diagonalizations,[16] and our DMRG calculations[8,9] have yielded results contradicting these claims. In this paper, we will review some of these calculations and arguments. However, we will pose a slightly different, and easier question regarding phase separation than has generally been addressed in previous studies. Rather than asking, ''does the t-J model phase separate at arbitrarily low doping?,'' we will ask, ''does the t-J model phase separate at high enough doping to allow the frustrated phase separation mechanism to yield stripes consistent with those found in the cuprates?'' We will conclude that the answer to this question is that it does not.

We will also compare the variational energies of several of the numerical approaches. In this comparison, we find that the DMRG calculations yield energies in excellent agreement with exact diagonalization, but can be extended to much larger systems. On the other hand, we find that the best Green's function QMC calculations to date are slightly higher in energy, and that this energy difference is close to the stabilization energy of stripes over pairs. Our DMRG calculations give striped ground states directly, without long range Coulomb interactions included in the model and without phase separation. Note that formation of a uniform array of stripes is *not* phase separation.

Most of the numerical work on doped antiferromagnets has centered on the t-J model, with a Hamiltonian given by

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

where doubly occupied sites are explicitly excluded from the Hilbert space. Here $\langle ij \rangle$ are near-neighbor sites, s is a spin index, $\vec{S}_i$ and $c_{i,s}^{\dagger}$ are electron spin and creation operators, and $n_i = c_{i\uparrow}^{\dagger} c_{i\uparrow} + c_{i\downarrow}^{\dagger} c_{i\downarrow}$. The near-neighbor hopping and exchange interactions are t and J. We measure energies in units of t.

We begin with a review of previous arguments and numerical data concerning phase separation. Emery, Kivelson, and Lin[3] used a combination of variational arguments for large and small J/t and exact diagonalization for moderate values of J/t to argue for the occurence of phase separation at all values of J/t. The variational arguments show that for small enough J/t (roughly $J/t < 10^{-2}$), and low enough doping, a uniform paramagnetic phase of independent holes has higher energy than a phase-separated state in which the hole-rich state is ferromagnetic. Emery *et al.* pointed out that this variational argument would not rule out other phase-separated states which might have even lower energy and be more physical than the ferromagnetic state. However, these hypothetical states might also be uniform.[15] In particular, Putikka *et al.* suggested[15,17] that a uniform ferrimagnetic state might have lower energy than the phase-separated ferromagnetic state. In any case, the ''Nagaoka-like'' ferromagnetic state which was shown to have low energy is of limited relevance to the cuprates.

The exact diagonalization of Emery *et al.* showed, at $J/t = 0.1$ and 0.4, that two holes on a 4×4 system bind into a pair, but that two pairs do not bind. Emery *et al.* argued that the pair formation was a sign of phase separation at low doping. However, others argued that the binding of two pairs, rather than pair formation, signals the onset of phase separation.[18] The possibility of striped ground states makes even the binding of two pairs an unreliable indicator of phase separation: the two pairs may form a short ''stripe,'' but if stripes do not attract, there is no phase separation.

Larger systems have subsequently been studied using several different types of QMC and related techniques. Almost all of these studies concluded that there was no phase separation in the parameter regimes relevant to the cuprates.[14,15,18-20] In contrast, using Green's function Monte Carlo, Hellberg and Manousakis (HM) (Ref. 12) concluded that phase separation occurs at all values of J/t at low enough doping, and in particular that for $J/t = 0.3$ it occurs for hole-doping levels less than about $x \sim 0.12$. Although in these various studies the possibility of striped ground states was usually not considered, and thus was not specifically excluded, the results obtained were generally uniform. Our DMRG calculations represent a third possibility, namely that stripes form in the t-J model, without any phase separation into uniform hole-rich and undoped regions, and without the need to add long-range Coulomb terms. Consequently, there are three broad possibilities for the charge ordering of the ground state of the lightly-doped, pure t-J model at $J/t \approx 0.3$: phase separated, uniform, or striped.

The question of what happens in the limit of very low doping is quite difficult for numerical methods, requiring increasingly larger systems as the doping is reduced. Most of the controversy has centered on the very low doping range. Fortunately, if one is interested in the mechanism of stripe formation at dopings x relevant to the cuprates, say, from $0.07 \leq x \leq 0.25$, one need not be concerned with extremely low doping. The frustrated phase separation scenario, in fact, appears to put rather strong constraints on the dopings required to produce phase separation. First, note that according to this scenario, phase separation must occur at all dopings in which stripes are found. Furthermore, note that the long-range part of the Coulomb interaction between holes makes the hole density distribution more uniform. Consider, therefore, as in Ref. 3, a phase-separated system, in the absence of long-range Coulomb forces, which has all of the holes in one region at a density x_{ps} and no holes in the other region. Then, turning on the Coulomb interaction will tend to drive the holes apart, possibly elongating the hole-rich regions into stripes, if the long-range repulsion is not too weak and not too strong. Under these circumstances, the local hole density in the stripes x_s is lower or, at most, the same, as the original hole density x_{ps}: $x_s \lesssim x_{ps}$. If this is true, then the known lower limits for x_s from experiments imply lower limits on x_{ps}. Note that x_{ps} is simply the critical doping at which phase separation first occurs, for any particular value of J/t.

Neutron scattering shows that the hole doping per unit length of the stripes for $x \leq 0.125$ is about 0.5. The neutron scattering experiments currently cannot determine whether the stripes are centered on copper sites (site-centered) or on the oxygen sites between them (bond centered). If one assumes the stripes are site-centered, with nominal width 1 in the t-J model, then the local doping *within* a stripe is $x_s = 0.5$. If one takes them as bond centered, with nominal width 2, then the doping within a stripe is $x_s = 0.25$. Of course, the hole density is not strictly zero in the antiferro-
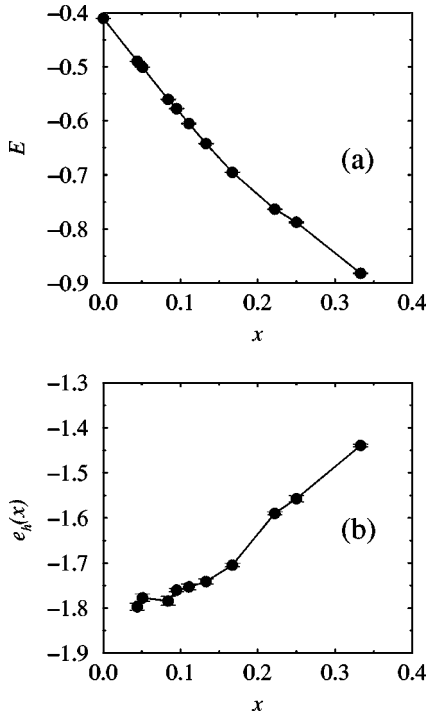
FIG. 1. (a) Energy per site in $L \times 6$ t-J systems, with J/t $=0.35$ for a variety of lengths L up to $L=19$. Cylindrical boundary conditions were used, along with extrapolation to reach zero truncation error. (b) Energy per hole $e_h(x)$ for the same systems as in (a).

magnetic regions between stripes. On the other hand, there are some signs of stripes well above $x=0.125$, and one would expect some suppression of x_s relative to x_{ps}. Furthermore, if stripes are necessary for superconductivity, one certainly needs them for the whole superconducting doping range. Therefore, for the sake of argument, we will assume that experiments require $x_{ps} \gtrsim 0.25$. However, our conclusions would not change if a somewhat smaller limit (say $x_{ps} \gtrsim 0.2$) were used.

Although there is disagreement about the behavior at smaller doping, there is general agreement among the various approaches on the lack of phase separation at $x=0.25$. For example, HM report the critical doping level for J/t $=0.3$ to be about $0.12(2)$, implying the density of the hole-rich regions is also $0.12(2)$, far from $x=0.25$. Kivelson *et al.* interpreted the lack of binding of two pairs in Ref. 3 as indicating the critical doping was less than $x=3/16$ $=0.1875$.[21] We are not aware of any interpretations of quantitative numerical calculations finding phase separation above this value. What value of J/t can give phase separation near $x=0.25$? According to HM, one would need J/t ~ 0.9. Other calculations find higher values of J/t. For example, Calandra, Becca, and Sorella find $J/t \sim 1.0$, and series expansion techniques produce an even higher valuec of J/t ~ 1.5.

Although the calculations seem in reasonable agreement regarding the lack of phase separation near $x=0.25$, it is still important to compare them carefully in order to assess their descriptions of the ground states, as well as possibly put even lower limits on the possible dopings having phase separation.

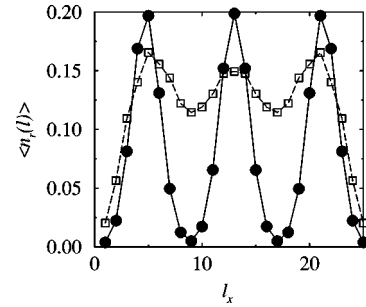In Fig. 1(a), we show DMRG results for the energy per

FIG. 2. Density of holes per site as a function of the x coordinate l_x in a 25×6 t-J system (filled circles), with 12 holes, compared with the hole density in a 25×1 system, with 3 holes (open squares).

site, as a function of overall doping, for $L \times 6$ t-J lattices, with $J/t=0.35$ for a variety of lengths L up to $L=19$. Note the near linearity of the data for $x \lesssim 0.12$. If our uncertainties were much larger, we might have been tempted to claim phase separation based on this data. This near linearity of the data illustrates the numerical difficulty of the problem— precise linearity in an exact calculation in the thermodynamic limit is an indication of phase separation, whereas deviations may be finite size effects, numerical errors, or they may indicate the absence of phase separation. In this case, as we will discuss, the near linearity reflects the weak repulsion of the four-hole domain walls which form in these lattices, wrapping around the $L \times 6$ cylinder. With DMRG, we are able to resolve the energy quite precisely and reliably on these $L \times 6$ systems. The major constraint for DMRG is the system's width—the accuracy falls off rapidly for wider systems. Green's function Monte Carlo can treat wider systems, but the presence of the fermion sign problem makes the result depend, perhaps strongly, on a trial or guiding wavefunction which is usually chosen to have uniform hole density. Thus it is essential to assess the relative importance of finite size effects versus the approximations used to control the fermion sign problem.

In Fig. 1(b) we show the same data plotted as the energy per hole $e_h(x)$ (following Ref. 3), relative to the undoped system

$$e_h(x) = \frac{E(N_h) - E(0)}{N_h}, \quad (2)$$

where N_h is the number of holes, and $E(N)$ is the energy of the system with N holes. In this case, phase separation would be seen as a minimum away from $x=0$. We see no evidence for such a minimum, but the results are far from conclusive for $x \lesssim 0.1$. At $x \sim 0.25$, however, the results clearly indicate the absence of phase separation. The energy per hole is about $0.25t$ higher at $x \sim 0.25$ than at small x. As we discuss below, this energy difference is about an order of magnitude higher than typical finite size effects at this width. Therefore, we conclude, in agreement with other simulations, that there is no phase separation near $x \sim 0.25$.

In fact, the systems shown in Fig. 1 with $x < 0.25$ are striped, with four-hole stripes wrapping around the cylindrical systems. In Fig. 2 we show the average hole density per site as a function of the x coordinate on a 25×6 system with 12 holes. For comparison, so that one can judge the effects of

the open boundary conditions, we show a 25×1 system with 3 holes. In the case of a single chain, the charge density oscillations decay as a power law away from the open ends, but in the thermodynamic limit the system is uniform. In the case of the $L \times 6$ systems, however, the amplitude of the oscillations is much larger and much more anharmonic at this doping. Using DMRG, we have found evidence for striped ground states for a wide range of dopings in the t-J model.[8,9] Importantly, we have found that stripes with a linear doping near $1/2$ on long domain walls are the lowest energy configurations at low doping.

The striped nature of the ground state tells us why the energy shown in Fig. 1(a) is so nearly linear: adjacent stripes repel, but only very weakly at large distances. The repulsion appears to be due to overlap of the hole densities in the adjacent stripes, and falls off roughly exponentially with the separation at short to intermediate distances. Thus, the system at low doping becomes almost infinitely compressible, making the energy per site as a function of doping nearly linear, and suggesting phase separation.

As mentioned above, our results showing the presence of stripes disagree with most Green's function Monte Carlo work. This may be because the uniform trial wave functions used to date in these calculations bias the calculations towards uniform states. Note also that all that is necessary to generate false signals of phase separation is that one's trial wave function be substantially worse for low doping than for high doping. Fortunately, it is possible to compare the various calculations because most are variational—if a trial wave function is poor, it will produce a higher energy result than it should. Even in cases where the calculation is not variational, a poor calculation will often result in an energy above the true ground state energy. In the case of DMRG, two results are available: a variational energy, and a more accurate but nonvariational energy coming from extrapolating the truncation error to zero. However, we find that the shift in energy in DMRG coming from this extrapolation is small compared to the differences in energies between different methods.

In Fig. 3, we compare the energies per hole from DMRG and exact diagonalization calculations for a number of systems with $J/t = 0.5$. We see that the DMRG results agree nicely with exact diagonalization,[22] within finite size effects. Note that perhaps the largest finite size effect in the energy per hole comes from how the reference undoped energy $E(0)$ is defined. For the $N = 20$ and $N = 26$ lattices studied with the Lanczos method, the undoped Heisenberg system is unfrustrated, and the ground state energy per site is lower than in an infinite system. This results in a higher energy per hole (Lanczos-I) than if one uses the infinite-system energy per site $-1.16944(4)J$ (Ref. 23) as reference (Lanczos-II). This effect is much less pronounced on the larger $N = 26$ site system. However, the corresponding doped systems are not necessarily unfrustrated. In particular, formation of a single stripe would be frustrated by these boundary conditions. This would make it very difficult to draw any conclusions about stripe stability from the Lanczos data alone. However, the Lanczos data provide an important check on the accuracy of the calculations on larger systems. For the DMRG with cylindrical boundary conditions, one cannot use the infinite-system reference energy, so the same undoped system is
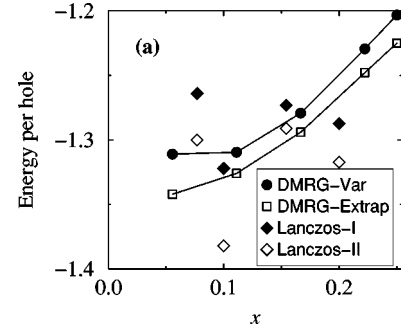

FIG. 3. Energy per hole e_h, in units of t, using DMRG and exact diagonalizations. The points labeled DMRG-Var are from DMRG calculations performed with cylindrical boundary conditions on 12×6 systems, and are variational. The points labeled DMRG-Extrap are extrapolated to zero truncation error. Here, the energies are defined relative to the DMRG energy of an undoped system on the same lattice. These calculations for undoped systems are much more accurate than for the doped systems, and we ignore any errors in these energies in claiming that the DMRG-Var results are variational. Two different types of exact diagonalization results are shown, for systems with $N = 20$ and $N = 26$ sites, with two or four holes. For the points labeled Lanczos-I, the energy is defined relative to the exact undoped energy on the same lattice. For the Lanczos-II points, we used as the undoped energy the energy per site for an infinite Heisenberg lattice, multiplied by the number of sites.

used. Using the same system as reference results in a cancelation of exchange energies associated with the open sides, reducing the finite size effects. Note that with cylindrical boundary conditions, striping is not frustrated.

In Fig. 4, we compare DMRG and Green's function Monte Carlo results. The results of Hellberg and Manousakis are based on unpublished data[24] which was summarized in Ref. 12. The points shown are a representative subset of the results used in Ref. 12. A fit to all the data, showing a minimum near $x = 0.14$, was the basis for the conclusion of phase separation at $J/t = 0.5$ in Ref. 12. For the 6×6 system with 4 holes and the 7×7 system with 7 holes, the results of HM and Calandra et al.[25] are in fairly good agreement. The DMRG energy on a 12×6 system is lower. We attribute this energy difference to the energy associated with the formation of stripes. Note that the 6×6 system with 4 holes would be frustrated if the holes formed a single stripe. To study a similar, frustrated 6×6 system with DMRG, we have applied frustrating staggered magnetic fields to the open ends of a 6×6 system with cylindrical BCs. The points labeled "AF" have this field, which would favor Néel order, but frustrate the π phase shift of a stripe. Two field strengths were used, $h = 0.1$ (the lower energy point) and $h = 0.2$. The calculation labeled π had a π phase shift (with $h = 0.1$) favoring a stripe in the applied staggered fields. As reference energies, the equivalent undoped, unfrustrated Heisenberg system was used in all cases. Application of the frustrating fields brings the energy of the 6×6 system very close to the QMC results. We interpret this to mean that the stabilization energy of the stripe is nearly balanced by the frustration of the boundary conditions. Thus the QMC energy of Calandra et al.[25] on the 6×6 system may be quite accurate, even if it does not have a stripe. (We note that their results for the N
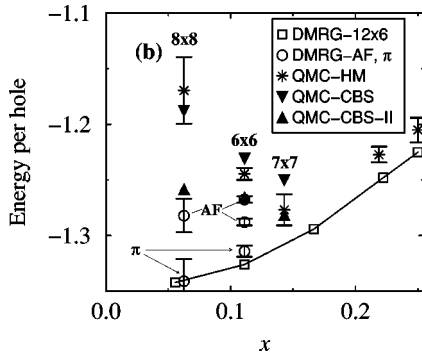
FIG. 4. Energy per hole e_h, in units of t, comparing DMRG and Green's function Monte Carlo data. The points labeled DMRG-12$\times$6 are the DMRG-Extrap points from Fig. 3. The QMC points are from a variety of periodic lattices, some of which are labeled. In this case, the energies are defined relative to the identical undoped system, as in the Lanczos-I data. However, for the 7$\times$7 system, the undoped system would be frustrated, and therefore an extrapolation using the 6$\times$6 and 8$\times$8 undoped systems and the known finite size dependence on system size was used to obtain a reference energy for this case. The points labeled QMC-CBS are variational fixed node quantum Monte Carlo calculations provided to us by Calandra, Becca, and Sorella. The points labeled QMC-CBS-II are from their stochastic reconfiguration method ($p=6$), which is not variational. The points labeled QMC-HM are from the calculations of Hellberg and Manousakis, which use a released-node procedure and are not strictly variational. The DMRG-AF, π calculations are described in the text. Where not shown, error bars are smaller than the symbols.

=26 sites system compare well with Lanczos.) On a 7$\times$6 system with 4 holes (not shown) Calandra *et al.* obtain an energy per hole of about $-1.26t$, very close to their result for the 6$\times$6 system. However, in this case, where a single stripe is not frustrated, we believe that the energy should be about the same as in the 12$\times$6 system near this doping, namely about $-1.31t$. In general, on $L\times6$ systems which do not frustrate stripes, we expect the QMC results to be too high by a stripe stabilization energy of $\sim0.05t$ per hole near $x\sim0.1$.

Measurements of the hole-hole correlation function by Calandra *et al.* in Ref. 20 were made using the less accurate fixed node approximation. Even in these measurements, they found some signs of incommensurate correlations indicating incipient fluctuating stripes.

The data point for the 8$\times$8 system with four holes of HM appears to be anomalously high. Our results with frustrating and nonfrustrating fields (all with $h=0.1$) on the 8$\times$8 system give results very similar to those of the 6$\times$6 system, and with much lower energy than found by HM. The stochastic reconfiguration result of Calandra *et al.* for the same system is also much lower. The high energy on the 8$\times$8 systems appears to have been important for the conclusion of phase separation near $x=0.14$ at $J/t=0.5$ of HM. The best data of Calandra *et al.* also show a slight minimum near $x=0.14$, but in Ref. 20 calculations on larger systems showed this to be only a finite size effect. Note that aside from the small systems studied by Lanczos, and cases where issues of frustration arise, typical finite size effects are rather small in the energy per hole. Systems with about 50 sites were found in Ref. 20 to have finite size effects of about $0.01t-0.02t$

per hole, when compared to much larger systems. Similar finite size effects were reported in Ref. 9. These finite size effects may be important for the determination of phase separation, but they are small enough to allow us to compare the various methods on slightly different lattices. We also find that the energy per hole is insensitive to the use of open boundary conditions on the two short ends of our $L\times6$ systems. For example, in comparing a 12$\times$6 system and the central 12$\times$6 region of a 24$\times$6 system, keeping the doping constant, we find a difference of less than $0.01t$ in the energy per hole.

A recent analysis[26] of Casimir forces involving spin-wave modes has found that in the limit of low doping, in the absence of Coulomb interactions, static stripes attract with an interaction decaying as r^{-2}. One can also estimate the coefficients in front of the leading decay terms; for stripes, the behavior is roughly $10^{-2}Jr^{-2}$ per unit length, with r in lattice spacings, for large r. At all length scales this force is a small correction to Coulomb interactions, which decay as r^{-1} with a larger coefficient, assuming dielectric screening. This means that the Casimir effect cannot have a role in frustrated phase separation. However, the Casimir force is potentially relevant to the issue of phase separation in the pure t-J model, since it would induce an attraction between stripes, causing an unusual form of true macroscopic phase separation into regions having widely spaced stripes, and regions without stripes.[21] It is important to estimate at what dopings this force can come into play.

Our simulations automatically include the Casimir effects as well as other short range effects. At distances between stripes in our $L\times6$ systems of up to about 10–12 lattice spacings, we have found only pure repulsion. We believe this is because the wave functions of the holes in the stripes extend beyond the stripe in exponentially decaying tails, and the overlap of these tails apparently causes higher hole kinetic energy. At larger separations the energies are too small to resolve. This distance puts a limit on the maximum doping, for the Casimir effect to be important, of about 0.06. We have also fit the short range repulsion in $L\times6$ striped systems to an exponential form;[9] we find the potential is roughly $0.6t\exp(-r/1.8)$ per unit length. If this repulsion is assumed, the Casimir effect becomes dominant at distances of about $r=20$ between stripes, corresponding to dopings of less than 0.025. The temperature at which such small energies could be relevant would be less than 1 K, assuming $J\approx1500$ K. Despite its limited applicable doping range, the Casimir effect illustrates the extreme difficulty of resolving the issue of phase separation in the t-J model in the limit of small doping, using only numerical simulations. However, this question is of very limited relevance physically.

These comparisons indicate that the DMRG calculations are quite reliable, at least in terms of the ground state energies. Based on this, we conclude that the short distance behavior and correlations of these systems, which affect the energy most strongly, are reliably determined by DMRG. However, we would like to address the question of the boundary conditions used by DMRG in somewhat more detail. It has been suggested that the stripes we see with DMRG may be due to the use of cylindrical boundary conditions, that they are artifacts which would not appear in "more realistic" periodic boundary conditions. We disagree with this
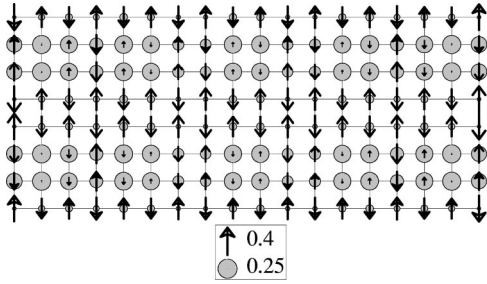
FIG. 5. Hole density and spin moments showing longitudinal stripes on a 18×8 t-J lattice with cylindrical boundary conditions, $J/t = 0.35$, and 20 holes. The diameter of the circles is proportional to the hole density $1 - \langle n_i \rangle$ on the ith site and the length of the arrows is proportional to $\langle S_i^z \rangle$, according to the scales shown. Differently styled arrows are used to show the two different antiferromagetic domains. This structure depends on the boundary conditions as discussed in the text.

position. In using finite size clusters to study models which may have broken-symmetry ground states, one often introduces a symmetry-breaking field and then studies 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 in the DMRG calculations in this way. Far from being artificial, they are important for understanding the physics. Of course, at present we are unable to carry out a proper finite-size scaling analysis to obtain the infinite size limit. Such a study would require very large lattices, since the domain wall spacing rather than the lattice spacing sets the lattice sizes required. Nevertheless, we have compared on numerous occasions systems of different lengths, and not seen significant reduction in the stripe amplitudes. Furthermore, while we have seen various arrangements of stripes depending on boundary conditions, we have been *unable* to stabilize any uniform states. In contrast, 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 $(t' \sim 0.3t)$.[27] The effect of this term is to destabilize the domain walls[28] and favor a gas of pairs.

As an illustration of the robustness of the striped state, we have made an effort to stabilize *longitudinal* half-filled stripes in $L \times 8$ systems with cylindrical boundary conditions. This is somewhat difficult, because the transverse stripes appear to have slightly lower energy. Furthermore, we have found that domain walls do not like to end on open boundaries, which seem to repel wall ends. However, we have found that we can stabilize the ends nicely by increasing the hopping slightly on a single edge link at which we wish the domain wall to end. In Fig. 5 we show the hole and spin densities in an 18×8 system with two longitudinal stripes. We used a hopping of $1.2t$ on the second and sixth

vertical edge links on both the left and right edges, and we also applied staggered fields with a π phase shift built in on sites $(1,1)$, $(1,4)$, $(1,5)$, and $(1,8)$, and the equivalent sites on the right edge. To stabilize the stripe configuration it was also necessary to apply pinning fields throughout the system during the warmup sweep and first several finite system sweeps. Because of the mapping of the sites in the 2D system onto an effective 1D chain in DMRG, during these first sweeps the system is much better equilibrated in the y direction than the x direction, and the system is unstable to the formation of transverse stripes. After these sweeps, all of the interior fields were turned off and about a dozen more sweeps were performed, with the final number of states kept per block equal to 1600. This calculation shows that with pinning terms applied only at the edges, a rather long cylinder supports longitudinal stripes. These stripes cannot be regarded as simple charge density oscillations induced by boundaries, as one could argue one has in the single chain system shown in Fig. 2. Of course, on a long system the state with longitudinal stripes might have higher energy than a state with the bulk having transverse stripes. DMRG is unable to tunnel between two states which differ so much over large length scales. However, we believe that DMRG would have no trouble making the system shown in Fig. 5 uniform if the correct ground state was uniform, simply by smearing out the stripes in the central region.

Thus, while we are unable to carry out a rigorous finite size scaling analysis, we believe our results imply that the pure 2D t-J model, in the small-J/t regime most relevant to the cuprates, and with dopings near $x \sim 0.1$, has a ground state which is striped.[29] By this, we mean that dynamical spin and charge susceptibility measurements will show either divergences or sharp peaks characteristic of static or fluctuating stripes, respectively. Furthermore, we believe that there are no low-lying states which do not have some signs of such stripes. Specifically, for $J/t = 0.5$ we estimate the lowest energy stripeless states are about $0.05t$ per hole higher in energy than the ground state. We believe that if one tries to write down variational wave functions for the ground state, and omits the striping behavior, one will not achieve a low energy state, even in cases where the stripes in the true ground state fluctuate. Finally, the energy scales involved suggest that a proper description of superconductivity requires taking these stripes into account.

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[29] We consider it to be a separate issue whether the stripes are static or dynamic. In our calculations, the stripes are static. In particular, at low doping, the half-filled stripes show no signs of significant fluctuations. On the other hand, at higher dopings, we find some signs that filled stripes may fluctuate (Ref. 9). However, even at low doping, it would require a very careful finite size scaling analysis on very large systems to rule out low energy dynamic quantum fluctuations.