Density Matrix Renormalization Group Study of the Striped Phase in the 2D t-J Model

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Using the density matrix renormalization group, we study the 2D t-J model at a hole doping of $x = \frac{1}{8}$ on clusters as large as 19×8. We find a striped phase consistent with recent neutron scattering experiments. We find that bond-centered and site-centered stripes have nearly the same energy, suggesting that in the absence of pinning effects the domain walls can fluctuate. [S0031-9007(97)05257-5]

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In the low temperature tetragonal (LTT) phase of $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$, the tilt pattern of the CuO_6 octahedra form lines of displaced oxygens parallel to the Cu-O bond directions. These lines are rotated by 90° between adjacent layers. At a filling of $x = \frac{1}{8}$, superconductivity is suppressed, and neutron scattering studies [1,2] reveal a striped domain wall ordering of holes and spins which is believed to be commensurately locked by the tilt distortion of the lattice. One model for this striped order [1,2] is illustrated in Fig. 1(a). Here the charge domain walls are shown running vertically and centered along the Cu-O-Cu legs, although the phase information required to determine whether the domains should be leg centered or bond centered (centered between two legs) is not known. As shown, the domains are separated by four Cu-O-Cu spacings and, for $x = \frac{1}{8}$, contain one hole per two 4×1 domain wall unit cells. This latter feature is at odds with one-electron Hartree-Fock calculations [3] which predict a domain wall filling of one hole per domain wall unit cell. The spins in the regions between the walls are antiferromagnetically correlated with a π phase shift across a domain wall. When $x \neq \frac{1}{8}$, superconductivity is found to coexist with a weakened domain wall ordering, suggesting a close connection between the two.

Here we present the results of numerical density matrix renormalization group (DMRG) [4] calculations for a t-J model with a hole doping $x = \frac{1}{8}$. We find evidence for domain walls with π phase-shifted antiferromagnetic regions separating the walls, and with a filling of one hole per two 4×1 domain wall unit cells. Kivelson and Emery [5] have suggested that domain walls arise when phase separation of the holes into uniform hole-rich and hole-poor regions is frustrated by long-range Coulomb forces. The question of whether, in fact, the t-J model exhibits phase separation for the relevant physical values of J/t and doping x remains controversial [6,7]. Our present results show that long-range Coulomb forces are not necessary for the formation of domain walls.

Depending on the size and boundary conditions (BCs) of the cluster we study, the domain walls may be site centered, as shown in Fig. 1(a), bond centered, or in between. In contrast to Fig. 1(a), however, the site-centered domain walls have substantial hole densities over three rows of sites, rather than one. Previous attempts to understand the charge degrees of freedom of the striped phase have focused on single chain models [5,8]. We consider another approach, in which coupled ladders are used to model the 2D system. In particular, in order to understand bond-centered stripes, we consider an array of two-leg ladders which are coupled antiferromagnetically via a mean field. We find that the π phase-shifted magnetic order of the bond-centered striped phase can be understood within this mean field picture.

The t-J Hamiltonian in the subspace of no doubly occupied sites is given by

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

Here $\langle ij \rangle$ are near-neighbor sites, s is a spin index, $\vec{S}_i = c_{i,s}^{\dagger} s_{s,s'} c_{i,s'}$, and $n_i = c_{i\uparrow}^{\dagger} c_{i\uparrow} + c_{i\downarrow}^{\dagger} c_{i\downarrow}$, with $c_{is}^{\dagger}$ (c_{is}) being an operator which creates (destroys) an electron at site i with spin s. The near-neighbor hopping interaction is t and the near-neighbor exchange interaction is J. We refer to the Cu-Cu lattice spacing as a and measure energies in units of t. We consider only $J/t = 0.35$ here.

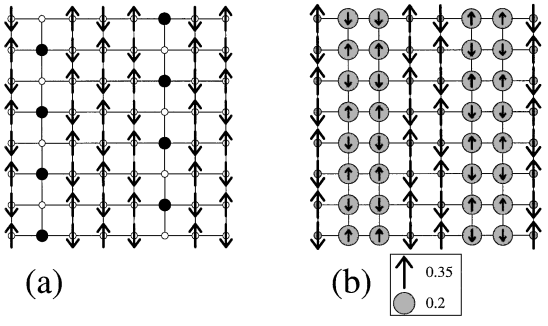

FIG. 1. (a) Spin and hole structure suggested in Ref. [1] to account for neutron scattering experiments. (b) Hole density and spin moments for the central 8×8 region of a 16×8 t-J system. The diameter of the gray holes is proportional to the hole density $1 - \langle n_i \rangle$, and the length of the arrows is proportional to $\langle S_i^z \rangle$, according to the scales shown. The domain wall order shown in (b) depends on the boundary conditions as discussed in the text.

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We present results here for $L \times 8$ clusters, with L as large as 19. As first discussed by Liang and Pang [9], the truncation errors in a DMRG calculation typically rise *exponentially* with the width of a large two-dimensional system (while only linearly with the length). However, the errors also tend to *fall* exponentially with the number of states kept per block. Consequently, while studies of doped $L \times 8$ clusters are quite difficult, by keeping from 1000–2000 states per block, we can obtain useful results, with truncation errors of 0.0002–0.0001. We are able to keep this many states because of recent improvements in the DMRG finite-system algorithm [10].

The nature of the ground state of the 2D t-J systems causes additional numerical difficulties. Rather than an approximately homogeneous phase, we find that the system tends to have inhomogeneous charge and spin distributions (such as domain walls), which can be pinned by the open BCs usually used in DMRG. Usually more than one such low-energy configuration is possible: For example, one could have horizontal as opposed to vertical stripes. A DMRG calculation involves sweeps through the sites of the lattice, and the energy of the approximate DMRG ground state of the system is decreased mostly through "local" improvements of the wave function. We find that, in a large 2D system, DMRG is usually unable to tunnel between two substantially different low-energy configurations. Even when a low-energy tunneling path exists between two very different configurations, the calculation may move along the path slowly. To deal with these difficulties, we usually perform several simulations for each system. These systems differ in the charge and spin configurations in the first few sweeps. Later sweeps drive the system to a local energy minimum. One can then compare the total energy of different simulations to find which configuration is the ground state. The charge and spin configurations can be controlled in two ways: (1) by adjusting the total quantum numbers of the system at each step as the lattice is first built up from a few sites, and (2) by applying local chemical potentials and magnetic fields for the first few sweeps. Unfortunately, it is possible to miss the true ground state configuration if it is substantially different from what one expects. However, unlike an ordinary variational calculation, only the crudest overall features of the wave function, such as the general location of the domain walls, are specified in the initial sweeps. These various runs can give substantial insight into what types of low-energy configurations can possibly occur under slightly different BCs or small perturbations to the Hamiltonian [11].

Figure 1(b) shows the charge and spin density in the ground state for the central 8×8 section of a 16×8 system with $J/t = 0.35$ and 16 holes, corresponding to a filling $x = \frac{1}{8}$. Periodic BCs were used in the y direction, and open BCs were used in the x direction. Along the left and right edges of the system a small staggered magnetic field of $0.1t$ was applied. The BCs and the edge staggered field serve to orient and pin the domain walls in the configuration shown. In an LTT phase, the domain walls are oriented, and possible pinned, by the lattice distortion. The staggered edge field further acts to pick a direction for the spin order, which allows direct measurement of the spin configurations and reduces truncation errors in the DMRG calculation. Previous to this calculation, dozens of simulations were performed, mostly on 8×8 clusters, to find the nature of the ground state and the effect of various BCs. Included were several initial conditions corresponding to phase separation, with the hole cluster either on the edge or in the center of the system. These phase-separated configurations were unstable, with the hole cluster tending to split or lengthen into domain walls. A single eight-hole vertical domain wall was also unstable, even when initial conditions and boundary staggered magnetic fields favored one. Objects resembling diagonal domain walls have been observed in three chain and four chain ladders [12,13], but attempts to stabilize a diagonal domain wall on an 8×8 system instead yielded a bent domain wall with the central part aligned in the (1,0) direction. Periodic BCs in the y direction tend to favor vertical domain walls; open BCs in the direction of the stripes tend to suppress them.

In the simulation shown in Fig. 1(b), eleven sweeps were performed, and in the final sweep 1400 states were kept. A local chemical potential was applied to confine the holes to the width-two stripes shown for the first six sweeps, and then removed. No initial magnetic field was needed away from the left and right edges to orient the π-shifted antiferromagnetic domains as shown.

Figure 2 shows the domain wall structure in a different way. With the solid circles, we show the local hole density, $n_h(\ell) = 1 - \langle c^\dagger_{\ell\uparrow} c_{\ell\uparrow} + c^\dagger_{\ell\downarrow} c_{\ell\downarrow} \rangle$, as a function of the x-coordinate ℓ_x. The bond-centered nature of these domain walls is evident. To show the spin structure, we define

$$S_\pi(l_x) = 1/L_y \sum_{l_y=1}^{L_y} (-1)^{l_x + l_y} \langle S_z(l_x, l_y) \rangle . \qquad (2)$$

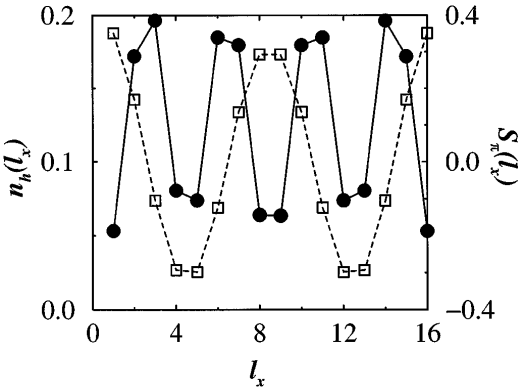

FIG. 2. Average hole density $n_h(\ell_x)$ (solid circles) and spin structure function $S_\pi(\ell_x)$ (open squares) for the 16×8 system of Fig. 1(b).

With the open squares, we show $S_\pi(l_x)$. The period-8 spin structure is clearly evident.

The boundary conditions have a strong effect on the structure of the domain walls which appear. Bond-centered domain walls tend to form one lattice spacing away from an open boundary. This initially led us to believe that site-centered domain walls were not stable, but subsequent simulations showed that site-centered walls also occur. In Fig. 3 we show the local hole density and spin structure function $S_\pi(l_x)$ for a 19×8 cluster with 20 holes. The same BCs and edge magnetic field as for the system shown in Fig. 2 were applied. A system such as this, with an odd number of domain walls and open BCs in the x direction, is forced by symmetry under reflection about a vertical line to have a site-centered domain wall in the center if L_x is odd, and a bond-centered wall if L_x is even. In the calculation shown, reflection symmetry is used explicitly, which ensures that a site-centered domain wall appears in the center. Note that the second and fourth domain walls, which are not so constrained by geometrical effects, are more site centered than bond centered. We have compared the local energies averaged over 4×4 regions covering site-centered and bond-centered walls; the difference in energy per site between these was within our numerical errors for local energies, with both giving $E/N \approx 0.62t \pm 0.01t$. In addition to bond-centered and site-centered walls, asymmetrical walls can occur. The close energy differences between these different types of walls suggests that a large 2D t-J system at $x = \frac{1}{8}$ might have fluctuating domain walls.

The π phase-shifted antiferromagnetic regions reduce the energy for transverse hopping of holes within a domain wall. To understand in more detail the bond-centered striped structure, we consider a model of antiferromagnetically coupled two-leg ladders. Ladders doped with $x = 0.25$ are alternated with undoped ladders, and no hopping is allowed between ladders. Ladders are exchange coupled via a mean field, which is staggered along a ladder, but which may or may not have a π phase shift across a doped ladder. The properties of a single ladder are calculated with DMRG, with a static magnetic field with wave vector (π,π) or $(0,\pi)$. In Fig. 4 we show the magnetic response $|\langle S_z\rangle|$ to an applied field with magnitude h. As expected, an undoped ladder has a much greater response at the Néel wave vector (π,π). A doped ladder, in contrast, shows a substantially greater response at $(0,\pi)$. Hence the mean field treatment shows the π phase shift seen in the 2D calculations. The mean field self-consistency conditions are

$$h_{d,u} = J|\langle S_z\rangle_{u,d}|, \tag{3}$$

where u and d stand for doped and undoped ladders. From the results shown in Fig. 3, we find $|\langle S_z\rangle_u| = 0.32$ and $|\langle S_z\rangle_d| = 0.15$. The results from the 16×8 system, in contrast, are $|\langle S_z\rangle_u| = 0.29$ and $|\langle S_z\rangle_d| = 0.13$. As one expects, the mean field treatment overestimates the magnetic order. (We expect that correction for truncation errors and finite size effects would further decrease the DMRG results.) The energy of this mean field striped phase (with $x = 0$ and $x = 0.25$), including the exchange coupling between ladders, is about 2% higher than the energy of an array of uncoupled ladders at uniform density ($x = 0.125$). Hence the mean field approach does not predict the charge ordering of the striped phase. Nevertheless, these results suggest that coupled ladders are natural starting points for understanding striped phases.

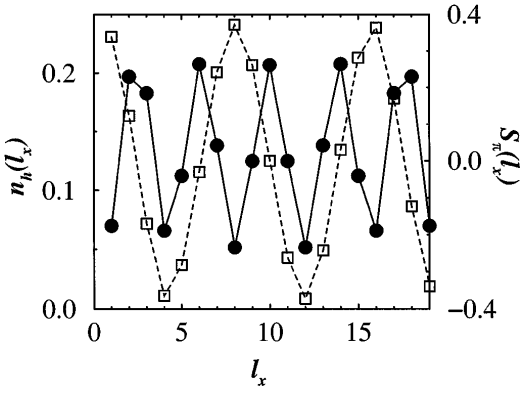

FIG. 3. Average hole density $n_h(\ell_x)$ (solid circles) and spin structure function $S_\pi(\ell_x)$ (open squares) for a 19×8 system.

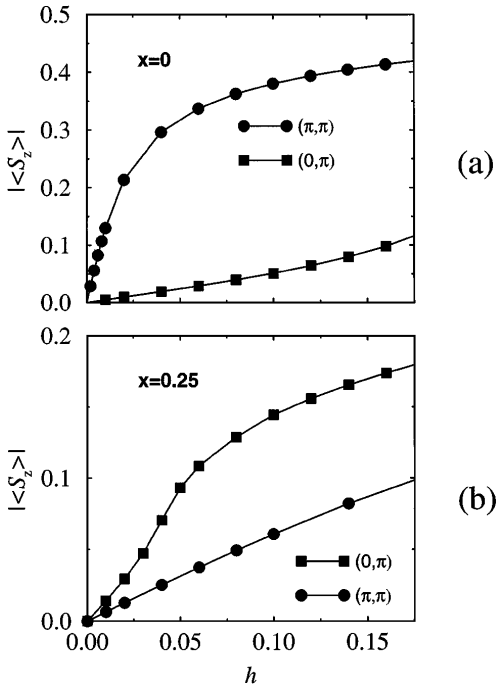

FIG. 4. Magnetization per site $|\langle S_z\rangle|$ induced by an applied magnetic field h at wave vectors (π, π) and $(0, \pi)$ on a 2×32 ladder. (a) An undoped ladder. (b) A ladder with doping $x = 0.25$.

A similar mean field treatment can be made for site-centered domain walls, coupling doped three-leg ladders with undoped single chains. This also yields π phase-shifted antiferromagnetism, with reasonable magnitudes for $|\langle S_z \rangle|$. We will present these results elsewhere.

According to the Maxwell construction, phase separation results in a linear dependence of the energy on the filling over a range of fillings. While there has been disagreement in previous studies about whether phase separation occurs in the low-doping region for $J/t = 0.3-0.5$, it is clear that the curvature in the energy versus filling curve is small [6,7]. The possibility of a striped phase, which has generally not been considered in these studies, makes the analysis more difficult. If we assume that, at low doping, holes go into a single domain wall, then it would appear from the energy alone that one has phase separation up to a filling of $\sim N^{-1/2}$, where N is the number of sites in the system. At higher dopings, an array of weakly repulsive, widely spaced domain walls would show a nearly linear energy versus filling dependence. In fact, we have observed exactly this scenario on a 12×6 system at $J/t = 0.5$, with periodic BCs in the y direction and open BCs in the x direction. Two holes bind into a pair, with a binding energy of $0.26t \pm 0.01t$. Two pairs bind into one vertical domain wall, with binding energy $0.10t \pm 0.03t$. Both site-centered and bond-centered walls are seen. The linear hole density along the wall, however, is $\frac{2}{3}$ rather than $\frac{1}{2}$. Eight holes form two widely spaced domain walls; twelve holes form three domain walls.

Why is superconductivity suppressed specifically at $x = \frac{1}{8}$ in $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$? We can only make some general statements. First, viewing the stripes as coupled two-leg ladders, there does not appear to be any anomalous feature in an isolated two-leg ladder at $x = 0.25$, such as a charge gap, which would suggest that domain walls must occur with exactly this doping. In any case, the charge on the domain walls spills out onto the rows of adjacent sites; our bond-centered domain walls have a hole density of $x \approx 0.18$ on the walls and $x \approx 0.07$ on the adjacent sites. This suggests, along with our results on the 12×6 system, that domain walls can occur with a range of dopings.

The period of charge density wave (CDW) correlations, however, is insensitive to the broadening of the walls. We have observed this effect on width-four models of domain walls. The CDW can be viewed as a one-dimensional line of hole pairs. The pairs extend beyond the two-site width of the wall, but the period is set by the one-dimensional hole density. This period is $4a$ at $x = 0.25$, the same as the transverse period of the stripes. In the LTT phase, the CuO_6 tilt structure causes the domain walls to be perpendicular in adjacent planes [1]. This suggests that a coupling between planes, such as through an electrostatic potential [5] or thorough a lattice distortion, could induce a static CDW order along the domain walls. This CDW order would tend to suppress superconductivity.

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[11] One might wonder if the broadened, bond-centered domain walls of Fig. 1(b) simply represent a superposition of the configuration shown in Fig. 1(a) and an equivalent with the domain walls shifted to the right by one lattice spacing. We have examined this by applying a chemical potential pinning field along the columns of sites containing the holes in Fig. 1(a). For this large cluster, the tunneling energy mixing of the two states would be expected to be very small, allowing even a small pinning field to eliminate the superposition. We found no evidence for a superposition even with the pinning potential as large as J.
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