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Pairing on striped t-t'-J lattices

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Results are given from a density-matrix renormalization-group study of pairing on a striped t-t'-J lattice in the presence of boundary magnetic and pair fields. We find that pairing on a stripe depends sensitively on both J/t and t'/t. In the strong-pairing model-parameter regime, the stripes are easily coupled by the pair field and have a uniform phase. There is a small but measurable energy cost to create antiphase superconducting domain walls.

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Experimental studies are providing insight into the interplay of the charge, spin, and d-wave pairing correlations in the underdoped cuprates. Scanning tunneling microscopy measurements[1] on $Ca_{1.88}Na_{0.12}CuO_2Cl_2$ and $Bi_2Sr_2Dy_{0.2}Ca_{0.8}Cu_2O_{8+8}$ suggest that at low temperatures, as the doping increases, superconducting correlations develop on a glassy array of $4a_0$ wide domains oriented along the Cu-O x- or y-bond directions. Neutron[2] and x-ray scattering[3] experiments on $La_{1.873}Ba_{0.125}CuO_4$ find charged stripes with a $4a_0$ period separated by π phase shifted antiferromagnetic regions. Moreover, when the temperature decreases below the spin ordering temperature, the planar ρ_{ab} resistivity shows evidence of a Kosterlitz-Thouless-like[4] behavior consistent with the development of two-dimensional (2D) pairing correlations.[5] Remarkably, ρ_{ab} follows the Halperin-Nelson[6] 2D prediction over an extended temperature range, implying a decoupling of the pair phase between the CuO_2 planes. In underdoped $La_{2-x}Sr_xCuO_4$, superconductivity and static spin-density waves coexist,[7] and recent far-infrared measurements[8] find that the Josephson plasma resonance is quenched by a modest magnetic field applied parallel to the c axis. An applied c-axis magnetic field is known to stabilize a magnetically ordered state[7] for a range of dopings near $x=1/8$. This is believed to be a striped state and Schafgans[8] argued that just as in $La_{1.873}Ba_{0.125}CuO_4$, the establishment of antiferromagnetic stripes leads to a suppression of the interlayer Josephson coupling. To explain this suppression, it has been suggested that antiphase domain walls in the d-wave order parameter locked to the spin-density wave stripes are stabilized in the striped magnetic state.[9,10] In this case, the 90° rotation of the stripe order between adjacent planes would lead to a cancellation of the interlayer Josephson coupling.

Early mean-field calculations[11] found striped states in t-J and Hubbard models. However, these stripes had a hole filling which was twice that which was observed in the cuprates. While arguments[12] were made that this problem could be overcome by including a next-near-neighbor hopping t', an alternative view suggested that it reflected the importance of underlying $d_{x^2-y^2}$ pair field correlations.[13] Density-matrix renormalization-group (DMRG) calculations found half-filled hole stripes, π-phase shifted antiferromagnetism, and short-ranged $d_{x^2-y^2}$ pairing correlations.[14] This interplay of oscillating hole density, spin density, and $d_{x^2-y^2}$ superconductivity was also found in Gutzwiller-projected variational Monte Carlo (VMC) calculations.[10] In certain parameter ranges, these VMC calculations found a stable striped state in which the $d_{x^2-y^2}$ pair field had π phase shifts between the stripes, i.e., antiphase domain walls. A recent renormalized mean-field theory (RMFT) treatment found a similar small energy difference, with the uniform phase d-wave state lying slightly lower in energy.[15] A π-phase shifted d-wave pair field would provide a natural explanation for the observed suppression of the interlayer Josephson coupling.[9,10] A similar, low-lying, and modulated superconducting state was also found in VMC resonating valence bond calculations.[16,17] Here, however, no incommensurate antiferromagnetic order was assumed.[18]

We have carried out a series of DMRG calculations on underdoped t-t'-J lattices with a Hamiltonian

$$H = -t\sum_{\langle ij\rangle}(c_{is}^{\dagger}c_{js} + \text{H.c.}) - t'\sum_{\langle ij\rangle'}(c_{is}^{\dagger}c_{js} + \text{H.c.}) + J\sum_{\langle ij\rangle}\left(\vec{S}_i\cdot\vec{S}_j - \frac{n_i n_j}{4}\right). \quad (1)$$

Doubly occupied sites are excluded from the Hilbert space, $\vec{S}_i$ and $c_{i,s}^{\dagger}$ are electron-spin and creation operators, respectively, and $n_i = c_{i\uparrow}^{\dagger}c_{i\uparrow} + c_{i\downarrow}^{\dagger}c_{i\downarrow}$ is the electron number on site i. There is a near-neighbor $\langle ij\rangle$ hopping t, a next-near-neighbor $\langle ij\rangle'$ hopping t', and an exchange coupling J. We set $t=1$. Using boundary magnetic and pair fields, we have explored how a pair field is established over a magnetically striped array at low doping.

Figure 1 shows two 12×8 ladders (tubes) with cylindrical boundary conditions (CBCs). In Fig. 1(a), a weak staggered magnetic field is applied to the open ends and the number of holes is fixed at 12, corresponding to a doping $\delta=0.125$. The end boundary conditions break the translational and spin symmetries in the x direction, giving rise to finite varying values of $\langle n_i\rangle$ and $\langle S_i^z\rangle$; but the basic stripe pattern, with antiferromagnetic order between stripes and with π phase shifts in the magnetic order across stripes is intrinsic and the

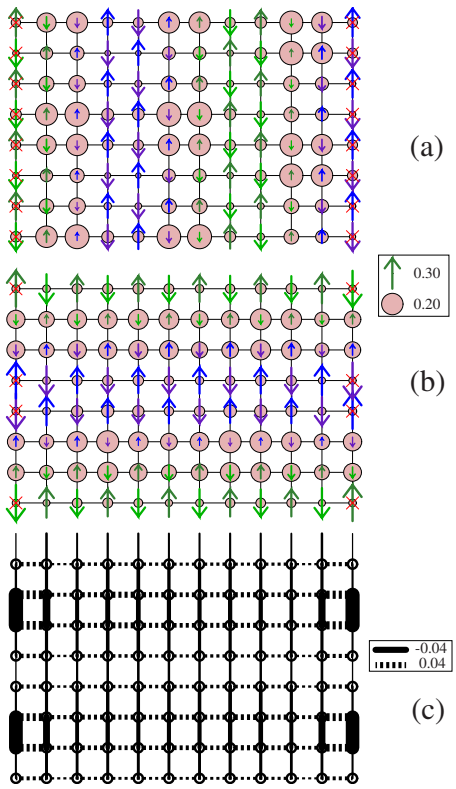

FIG. 1. (Color online) (a) Hole $\langle 1-n_i\rangle$ and spin densities $\langle S_i^z\rangle$ for a 12×8 lattice with 12 holes and $J=0.5$ and $t'=0$, with cylindrical boundary conditions: periodic in the y direction and open in the x direction. A staggered magnetic field of magnitude $h=\pm 0.05$ has been applied to the ends (red X's). (b) A similar lattice with $J_x=0.55$, $J_y=0.45$, and $t'=0.0$ such that the stripes run along the x axis. Here we use $h=\pm 0.2$ on the sites with a red X, and a pair field $\Delta_0=1.0$ to the edge links without X's. A chemical potential $\mu=1.23$ was used to give a doping of $x=0.127$. (c) The pair field strength $\langle D_{ij}\rangle$ on each link for the system shown in (b).

open ends and boundary h field only act to pin the stripes. Up to $m=4000$ states per block were kept.

In this cluster, there are four holes per stripe, and DMRG calculations on longer stripes have shown that this linear stripe filling of 0.5 holes per unit length is the preferred filling.[14] Fluctuations in which a pair of holes are exchanged between the stripes are energetically unfavorable for this short a stripe, and the local $d_{x^2-y^2}$ pair field correlations are short ranged and pair field coupling between stripes is negligible.

Previous DMRG calculations have not found ground states with both extended pairing correlations and stripes. There are two reasons. First, it has been difficult to construct limited-size clusters allowing significant particle number fluctuations on a stripe and second, as we show below, the model parameters which strongly favor pairing (e.g., $J/t\sim 0.5$, $t'/t\sim 0.2$) are different from the values usually taken to represent the cuprates (e.g., $J/t\sim 0.3$, $t'/t=-0.2$). In Fig. 1(b), we show results for a cluster which does have both stripes and pairing. In order to allow hole fluctuations, a slightly anisotropic exchange interaction ($J_x=0.55$, $J_y=0.45$) was chosen to favor orienting the stripes along the x direction, overcoming an opposite tendency due to the cylindrical geometry. Then, in addition to the magnetic fields at the open left and right ends, a pair field coupling has been applied to the ends of the stripes. Defining the link pair-creation operator

$$\Delta_{ij}^\dagger = \frac{1}{\sqrt{2}}(c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger + c_{j\uparrow}^\dagger c_{i\downarrow}^\dagger) \tag{2}$$

on specified links, we add to the Hamiltonian boundary region terms of the form $\Delta_0 D_{ij}$, where

$$D_{ij} = \frac{1}{2}[\Delta_{ij}^\dagger + \Delta_{ij}], \tag{3}$$

and we measure D_{ij} on each link in the resulting (approximate) ground state. For this system, we took $\Delta_0=1.0$ for the four thickest lines of (c) and also $\Delta_0=0.5$ for the four vertical links adjacent to them. With the pair field boundary conditions, total particle number is only conserved modulo two, and the average number of holes is controlled by a chemical potential μ. Up to $m=6000$ states were kept per block during 23 sweeps in this calculation. As shown in Fig. 1(c), a proximity d-wave pair field is established throughout the lattice.

In order to understand the system in more detail, it is useful to separate questions dealing with (a) pairing on a stripe from (b) pairing between stripes. First, can a single stripe support strong pairing, and if so, for what model parameters? Second, do stripes with pairing couple their pair fields, and if so, is the coupling in phase or antiphase? To answer these questions, we will study clusters somewhat smaller than shown in Fig. 1 to ease the computational burden and increase the accuracy.

To look in more detail at the pairing correlations associated with a stripe, we have studied a single stripe on the 16×5 lattice with CBCs shown in Fig. 2. In this case, boundary conditions were used to force the presence of a stripe similar to those shown in Figs. 1(b) and 1(c). Here a strong pair field was applied to only one end of the stripe. The proximity-induced pairing response $\langle D_{ij}\rangle$ is shown in Fig. 2(b) for a case with strong pairing. The strength of the induced pair field depends upon J, t', and the doping x. As a measure of this response, its magnitude on the 12th $y=2-3$ rung is plotted in Fig. 2(c) versus the hole doping for various values of t' and J. As previously found in both DMRG and VMC calculations, a positive value of t' favors pairing while a negative value suppresses it. Here, one also sees that when the pairing is strongest, the response peaks for a linear filling $\rho\sim 0.5$ holes per unit length but shifts to higher doping for smaller t'. We see a strong dependence on J/t, with pairing when $J/t=0.3$ quite weak and when $J/t=0.5$ quite strong. Also, as shown in Fig. 3, the compressibility, which is related to the slope of the curves, for $\rho=0.5$ increases as t' increases, consistent with the observed enhancement of the pairing response for positive values of t'. The increased pairing for larger J/t may be due to a reduced repulsion between pairs, leading to an enhanced compressibility.

Next we turn to the question of antiphase domain walls in the pair field. For values of t' and doping where there is a significant pair field response, we find that the pair field re-

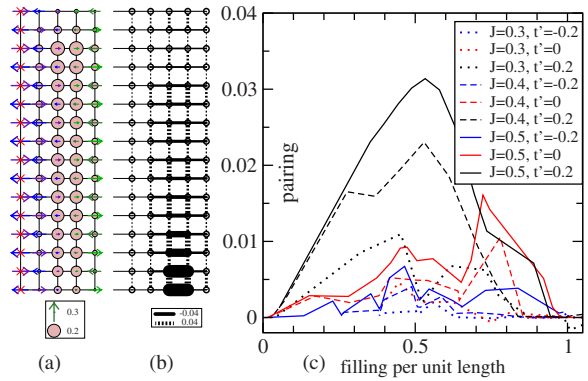

FIG. 2. (Color online) A cluster with a single forced stripe on a 16×5 ladder with CBCs, with the x direction oriented vertically. For all dopings, on the $y=5$ leg, a staggered field $(-1)^x h$ with $h=0.05$ was applied, along with a chemical potential of 2.0. On the other four legs, a chemical potential μ was applied to vary the doping; in the case shown in (a) and (b), $\mu=1.41$, $J=0.5$, and $t'=0.2$, yielding a doping of $x=0.106$, which corresponds to a linear doping of 0.53. In each case, a strong pair field was applied to four rungs ($x=1-4$, connecting $y=2$ and $y=3$) visible as the four thickest links in (b). The magnitude of the applied field in the four rungs was 1.0, 1.0, 0.5, and 0.25. (a) The hole density $\langle 1-n_i\rangle$ and spin density $\langle S_i^z\rangle$. (b) The measured pair field $\langle D_{ij}\rangle$. (c) The measured pair field at the $x=12$ and $y=2-3$ rung versus the number of holes per unit length. The maximum value for $\langle D_{ij}\rangle$ in (c) is on the order half of what one would find for a BCS ground state with $\Delta_0/t=0.1$.

mains in phase across the stripes, as shown in Fig. 1(b). This implies that the energy to create an antiphase domain wall is positive. To probe this, we have studied 12×6 ladders with open boundary conditions in both the x and y directions, and with magnetic and chemical-potential fields applied to force two stripes. Figure 4 shows such a system where each stripe has a linear doping of 0.6. Then by applying pair fields on every link on the outermost legs ($y=1$ and $y=6$), a pair field is established. When the applied pair fields are in phase, the induced pair field is shown in the middle figure of Fig. 4. The right-hand side shows what happens when the applied pair fields are out of phase. The energy per unit length versus the DMRG sweep number for the in-phase and antiphase configurations is plotted in Fig. 5 for different values of t'. Although the energy difference is small, it varies little with the sweep as the number of states in increased up to $m=3000$ for sweep 17. Here, one sees that it costs energy to create an antiphase domain wall and the energy per unit length increases as the overall strength of the induced pair field increases. For $t'=0.2$, the energy per unit length of the antiphase domain wall is on the order of $0.01t$.

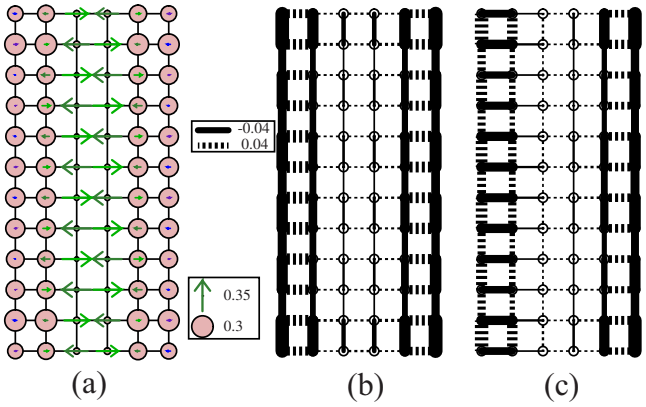

FIG. 4. (Color online) (a) Hole and spin densities for a 12×6 ladder (plotted with x oriented vertically) with $J=0.5$ and $t'=0$ and with open boundary conditions in both directions with fields applied to force two stripes. The center two legs have an applied staggered field $(-1)^x h$ with $h=0.05$, along with a chemical potential of 1.3. The outer four legs have a chemical potential of 0.9, leading to a doping of $x=0.198\,1$, corresponding to a linear doping per stripe of 0.594. The outermost two legs have applied pair fields of 0.5 on each horizontal rung. In (a), the pair fields are applied in phase. (b) Measured pair fields for the in-phase case. (c) Measured pair fields when the applied fields have opposite sign.

There are both similarities and differences between our DMRG results and those from VMC.[10] Both approaches find evidence for low-lying-striped states with $d_{x^2-y^2}$ pair fields, as seen experimentally. However, we find that negative values of t' suppress the d-wave pair field. Thus the parameter regime where we have studied the interplay of the stripes and the pair field differs from the $t'<0$ region of the VMC study. Our DMRG calculations also find that the energy to form an antiphase d-wave domain wall is positive.

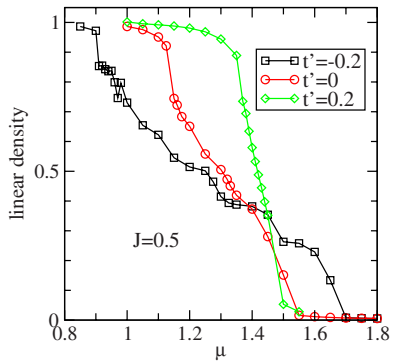

FIG. 3. (Color online) The linear density versus μ for different values of the next-nearest-neighbor hopping t' for $J=0.5$ for the systems of Fig. 2.

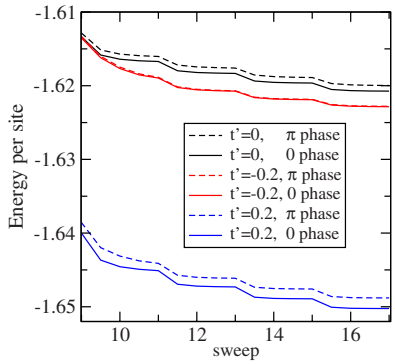

FIG. 5. (Color online) Energy per site for the 12×6 ladder of Fig. 4 versus sweep number for the in-phase and antiphase applied fields. The runs all had $J=0.5$ and had the values of t' indicated.

In comparing to experiments for the cuprates, the puzzle raised by our calculations, as well as the RMFT (Ref. 15) results, is the positive energy required to create an antiphase domain wall in the *d*-wave order. Because this is a small energy, one can imagine that effects missing from the t-t'-J model could lead to antiphase domain walls. However, we believe that there could be an alternate explanation of the suppression of the interlayer Josephson coupling observed in the underdoped regime. It could be that the decoupling arises from the lack of overlap of the Fermi surfaces of the adjacent layers. There are a number of experiments[19,20] which imply that a Fermi-surface reconstruction occurs for hole doping near $x=1/8$. The resulting Fermi surface is characterized by electron pockets and open orbits whose location in the Brillouin zone depends upon the stripe orientation.[21] In this case, since the stripes alternate their orientation by 90° from one plane to the next, the lack of overlap between the Fermi surfaces can lead to a suppression of the interlayer pair transfer processes.[22]

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