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Competition between stripes and pairing in a t-t'-J model

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As the number of legs n of an n-leg, t-J ladder increases, density-matrix renormalization group calculations have shown that the doped state tends to be characterized by a static array of domain walls and that pairing correlations are suppressed. Here we present results for a t-t'-J model in which a diagonal, single-particle, next-nearest-neighbor hopping t' is introduced. We find that this can suppress the formation of stripes and, for t' positive, enhance the $d_{x^2-y^2}$-like pairing correlations. The effect of $t'>0$ is to cause the stripes to evaporate into pairs and for $t'<0$ to evaporate into quasiparticles. Results for $n=4$ and 6 n-leg ladders are discussed. [S0163-1829(99)51326-X]

Neutron-scattering experiments on $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$ show evidence of a competition between static (quasistatic) stripes and superconductivity.[1] Here the stripes consist of (1,0) domain walls of holes separating π phase shifted, antiferromagnetic regions. For $x=0.12$ ($x\approx 1/8$), the intensity of the charge and spin superlattice peaks is largest and T_c is less than 5 K. As x deviates from this value, the relative intensity of the magnetic superlattice peaks decrease and the superconducting transition temperature T_c increases. High-field magnetization studies[2] indicate that in this material superconductivity can coexist with quasistatic stripe order. However, the fact that T_c is a minimum where the superlattice peaks are most intense suggests that static stripe order competes with superconductivity.

We are interested in understanding whether a t-J-like model can exhibit this type of behavior. In studies of n-leg, t-J ladders we have previously found evidence for stripe formation. In particular, for $n=3$ and 4 legs we have found evidence for both stripes and pairing.[3,4] These systems have open boundary conditions in both directions, and the stripes are open ended. Of particular interest is the result that the pairing is enhanced in both of these systems when increased doping induces the stripes, compared with unstriped lower doped phases. However, in wider ladders ($n=6$ and $n=8$) with cylindrical boundary conditions, where the stripes close on themselves rather than having free ends, the stripes appeared to be more static and the pairing correlations were found to be suppressed.[5] This suppression of the pairing correlations was also observed when an external potential was applied to further pin the stripes. Thus there appears to be a tendency for pairing to favor strongly fluctuating stripes.

If the formation of static stripes could be suppressed by an additional term in the Hamiltonian, one might hope to find generally enhanced pairing correlations. It is not clear whether the complete elimination of stripes or only a slight destabilization would be more favorable to pairing correlations. We have been investigating various interaction terms which could destabilize stripes. Here we focus on the effect of a next-nearest-neighbor diagonal hopping t'. Effective hopping parameters have been evaluated from band-structure calculations and finite CuO cluster calculations. For the hole-doped cuprates t' is found to be negative while for the electron-doped cuprates it is positive. Both t' and the one-electron hopping t'', which connects next-nearest-neighbor sites along the (0,1) or (1,0) axis, have been used in t-t'-t''-J models to fit angle-resolved photoemission spectroscopy (ARPES) data.[6] In addition, Lanczos calculations by Tohyama and Maekawa[7] on t-t'-J clusters and Monte Carlo calculations[8] on t-t' Hubbard lattices show that $t'>0$ tends to stabilize the commensurate (π,π) antiferromagnetic correlations. Recently, exact diagonalization and density-matrix renormalization group (DMRG) calculations on small clusters and four-leg ladders have found that $t'<0$ destabilizes stripes.[9] Furthermore, it was concluded that a small positive t' did not destabilize the stripes on these systems.

Here we consider the effect of t' on both open four-leg and cylindrical six-leg ladders. In addition to considering the effect of t' on stripe stability, we measure its effect on pairing correlations. We find that stripes are destabilized for either sign of t', and that pairing is suppressed for $t'<0$, and enhanced for $t'>0$. This latter effect is surprising, since superconducting transition temperatures are generally higher for hole-doped cuprates ($t'<0$) than for electron-doped ($t'>0$).

The t-t'-J Hamiltonian which we have studied is

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

Here $\langle ij\rangle$ are nearest-neighbor sites, $\langle ij\rangle'$ are diagonal next-nearest-neighbor sites, $\vec{S}_i=\frac{1}{2}c_{is}^{+}\sigma_{ss'}c_{is}$, $n_i=c_{i\uparrow}^{+}c_{i\uparrow}+c_{i\downarrow}^{+}c_{i\downarrow}$, and $c_{is}^{+}(c_{is})$ creates (destroys) an electron of spin s at site i. No double occupancy is allowed. We use DMRG calculations to explore the charge, spin, and pairing correlations on doped four- and six-leg ladders. The pairing correlations were found to be especially slowly converging with the number of states kept per block. Therefore, long runs were made,

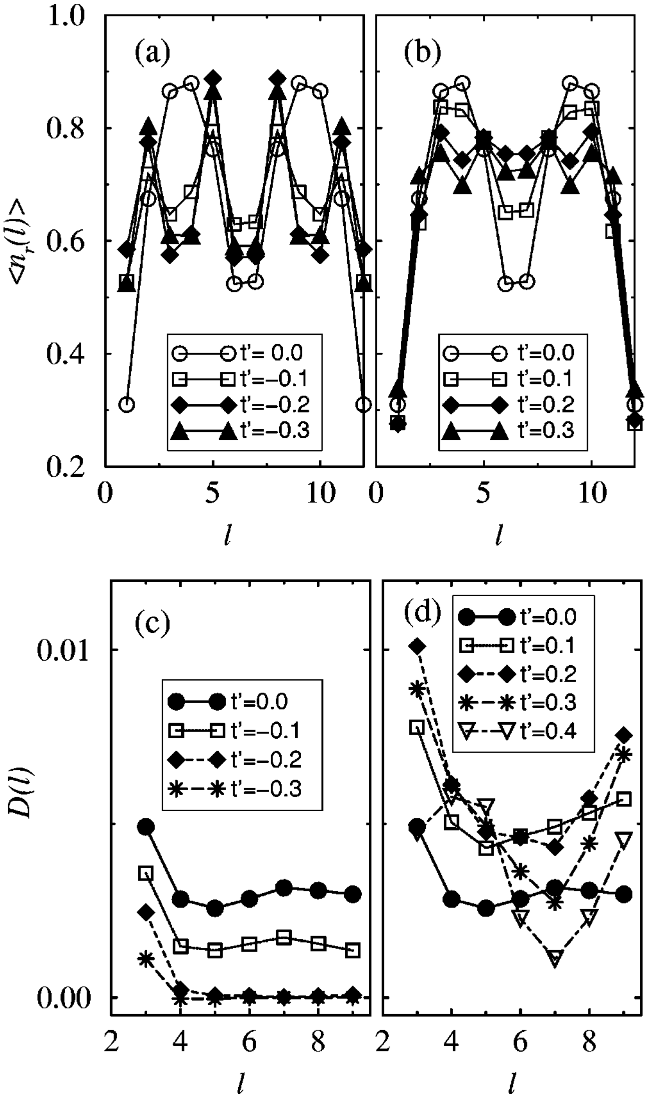

FIG. 1. (a) Hole density per rung for a 12×4 system with eight holes, $J/t=0.35$, and open-boundary conditions, with $t'\leqslant 0$. (b) Same as in (a), but with $t'\geqslant 0$. (c) and (d) d-wave pairing correlations for the systems shown in (a) and (b), respectively.

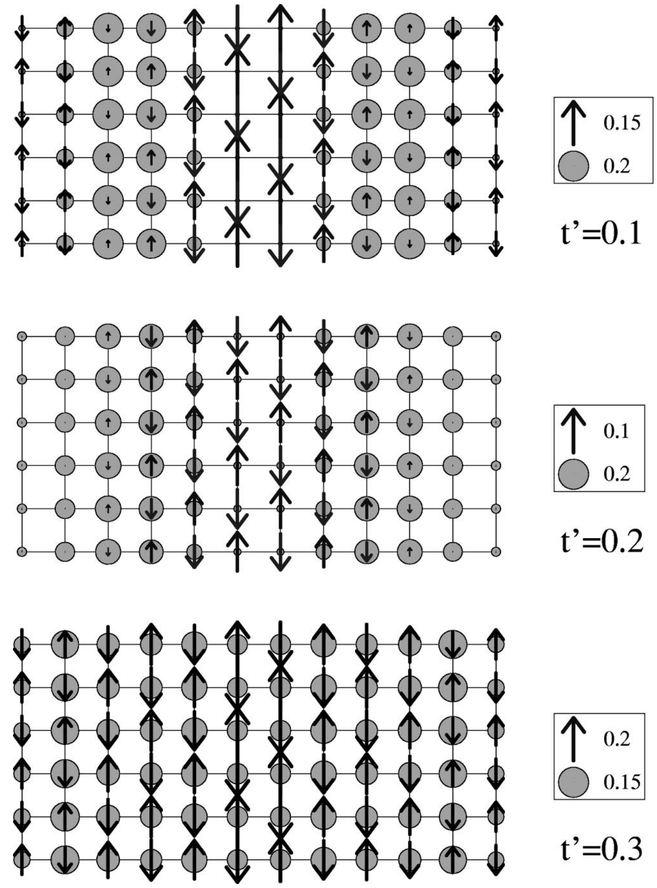

FIG. 2. Hole and spin densities on 12×6 systems with cylindrical boundary conditions. The hole density is proportional to the diameter of the circles, according to the indicated scale, and similarly the length of the arrows gives the expectation value of S_z.

keeping up to 2400 states per block for the 12×4 systems and up to 2200 states per block for the 12×6 systems, with from 10 to 12 finite system sweeps, giving truncation errors of about 4×10^{-5} and 10^{-4}, respectively. Even so, uncertainties in the pairing amplitudes at the largest distances remained in the neighborhood of 10−30%. These uncertainties do not affect the qualitative nature of our results. We have checked the inclusion of t' in our program by comparing the results for the rung hole density on a 14×4 system with the results of Tohyama *et al.*;[9] precise agreement was found.

Previously, we found that in the four-leg t-J ladder, four-hole diagonal domain walls form as the doping increased. In Figs. 1(a) and (b) we show the rung density

$$\langle n_r(l)\rangle = \sum_{i=1}^{4} \langle n_{li}\rangle \tag{2}$$

versus l for $J/t=0.35$ on a 12×4 lattice with eight holes and open-boundary conditions. For $t'=0$, we clearly see the formation of two domain walls, signaled by two broad peaks in $\langle n_r(l)\rangle$. As t'/t is increased, one clearly sees that the static domain wall structure is suppressed.

For $t'<0$, the four-hole domain-wall density oscillation is suppressed, but equally large density oscillations occur which appear to be pairs of holes. However, our results below indicate that pair formation is suppressed for $t'<0$. Consequently, the nature of the density oscillations for $t'<0$ is unclear.

For this same 12×4 lattice, we have studied the pair-field correlation function

$$D(l) = \langle \Delta_{i+l}\Delta_i^+\rangle \tag{3}$$

with Δ_i^+ a pair creation operator which creates a singlet $d_{x^2-y^2}$ pair centered on the ith site of the second leg. Figures 1(c) and (d) show a plot of $D(l)$ versus l for the 12×4 ladder for $J/t=0.35$ with eight holes and various values of t'/t. As t'/t initially increases, the pairing correlations are enhanced but as t'/t becomes greater than ~0.3, they are suppressed. They are suppressed for t' negative, with very strong suppression occurring for $t'\leqslant -0.2$.

Results for the charge density and spin structure of a 12×6 lattice with $J/t=0.5$ and eight holes are shown in Fig. 2. Here we have taken cylindrical boundary conditions, i.e., periodic in the y direction, open in the x direction. In this case, for $t'/t=0$, the holes form two transverse domains each

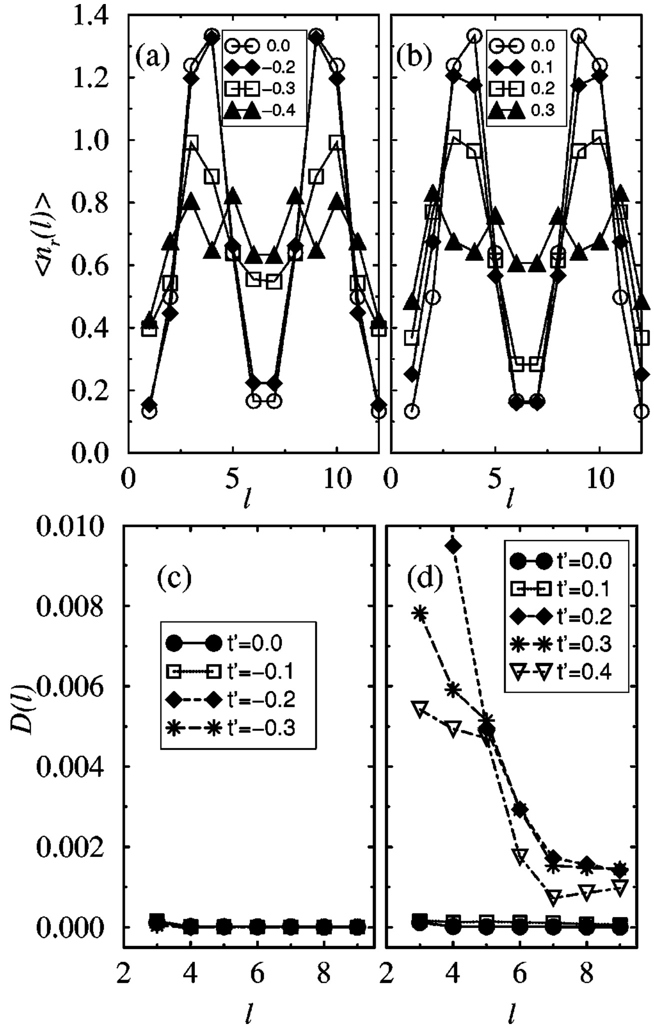

FIG. 3. (a) and (b) Density of holes per rung for the 12×6 ladder systems shown in Fig. 2. (c) and (d) d-wave pairing correlations for the same systems.

containing four holes. The π phase shifted antiferromagnetic regions which are separated by these domains are clearly visible in Fig. 2 for $t'=0.1$; the results for $t'=0.0$ look almost identical. The DMRG calculation has selected a particular spin order, breaking symmetry; as the number of states kept per block increases, the magnitude of this spin order decreases, and the exact ground state would have no net spin on any site. However, here the spin order serves to illustrate the underlying spin correlations in the exact ground state, which we expect to be a superposition of the broken symmetry state rotated to all possible directions.

As t'/t increases, we again see a suppression of the charge order and in addition the π phase shifted antiferromagnetic regions disappear. This is also true for t' negative. For $t'=0.3$, we see that Néel spin order, without any π phase shifts, is now the broken symmetry state. As previously noted, Lanczos[7] and Monte Carlo[8] calculations indicated that a positive t' tended to stabilize the commensurate (π,π) antiferromagnetic correlations, which is consistent with our results.

The rung density shown in Figs. 3(a) and 3(b) provides a more quantitative display of the suppression of the charge domains walls. In this case, a finite magnitude of t' seems to be necessary to substantially reduce the charge-density structure. The domain walls in $L\times6$ ladders at $t'=0$ are stable bound states of two-hole pairs, and a finite change in the parameters of the systems is needed to break them up. We believe that $L\times6$ cylindrical systems have unusually stable domain walls, and that more generally a smaller value of $|t'|$ would destabilize the stripes. Here, we see that the stripes are suppressed for $t'=0.2$, and completely destabilized for $t'=0.3$.

Figures 3(c) and (d) show the pair-field correlations $D(l)$ versus l for various values of t'/t for the 12×6 ladder. We see when the stripes are weakened by a positive t', pairing correlations are strongly enhanced. The optimal t' appears to be near $t'=0.2$. Pairing is once again suppressed for negative t', even when the domain walls are destabilized.

From a weak coupling point of view, our results on the effect of t' on pairing are surprising. In weak coupling, the effect of $t'<0$ is to shift the Van Hove singularity in the density of states away from half filling, so that the singularity may occur near the Fermi level in a doped system. Thus, one might have expected to find an enhancement in pairing for $t'<0$. However, in the t-J model, we find a suppression of the pairing. In strong coupling, one can understand this effect. Consider a pair of holes, and imagine we fix one hole and let the other hole hop around it. Consider the phase of the wave function of the second hole on the four sites next to the first hole. It appears that $t'<0$ will directly favor a $+-+-$ d-wave phase pattern as the second hole hops around the first, whereas $t'>0$ would favor the s-wave pattern $++++$.[10] However, the actual phase of a pair is a relative phase between a system with N holes and one with $N+2$ holes. If one considers a 2×2 t-J system, one finds that the two-hole ground state has s-wave rotational symmetry, whereas the undoped state has d-wave rotational symmetry.[11–13] The d-wave nature of the pairing comes from the difference in these rotational symmetries, with the crucial minus sign coming from the undoped system. Assuming this situation generalizes to larger systems, $t'<0$, by suppressing the two-hole $++++$ pattern, actually suppresses d-wave pairing, while $t'>0$ can enhance it.

Consider the 2×2 system.[13] The energy of the undoped system is independent of t'; we find $E(0)=-3J$. The energy of the one hole system depends only weakly on t'; for t' small, we find $E(1)=-J-1/2(J^2+12t^2+4Jt'+4t'^2)^{1/2}$. For $J=0.35$, $t=1$, this varies with t' as $E\approx-2.09087-0.1005t'$. The energy of the two-hole system, in contrast, depends strongly on t': $E(2)=-J/2-t'-[32t^2+(J+2t')^2]^{1/2}$. The pair binding energy is defined as

$$E_b=2E(1)-E(2)-E(0). \quad (4)$$

The dependence of the pair binding energy on t' is dominated by $E(2)$, and we find that $t'>0$ strongly enhances the pair binding.

On larger systems, the detailed energetics are more complex, but a similar effect occurs. In Fig. 4, we show the energy per hole of several systems as a function of t'.[14] The systems allow us to compare the stability of paired states, striped states, and states with isolated holes. The first system is a single hole in an 8×8 open system, with a staggered antiferromagnetic field of strength 0.1 on the edges to ap-

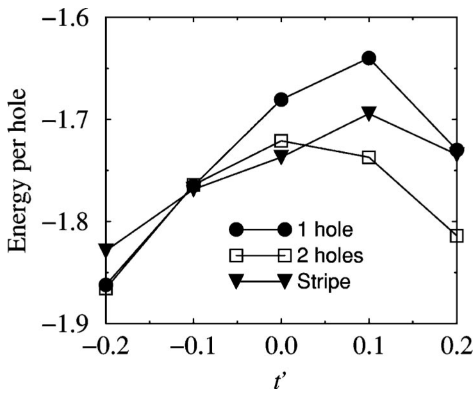

FIG. 4. Energy per hole of various hole configurations, as discussed in the text.

proximate the magnetic coupling to the rest of the system, which is assumed to be undoped. The second system is similar, but has two holes. We plot the energy difference between these systems and the same system without holes, divided by the number of holes.[14] The third system is a 16×6 system, with open-boundary conditions, and staggered fields of magnitude 0.1 with a π phase shift applied on the first and last chain. These boundary conditions favor the development of a stripe down the center of the ladder. Then we subtract the energy of an undoped 16×6 system, also with staggered fields, but without the phase shift.[14] We expect that finite-size effects are not neglible, and these could shift the striped phase curve relative to the other two curves. However, we believe the general trends are reliable. That is, the striped system is lowest in energy near $t'=0$, but becomes unstable as t' becomes less than -0.1, or as t' increases above a value slightly greater than 0.0. Thus, the striped region is quite narrow as a function of t'. This conclusion differs somewhat from that of Ref. 9, where it was found that stripes were enhanced for $0<t'<0.2$, but were suppressed for larger values of t'. For positive t', the new stable state has pairs of holes, as Tohyama, *et al.* (Ref. 9) also found for $t'\sim0.5$. For $t'<-0.1$, the near degeneracy between one and two holes indicates that the holes are not bound into pairs: instead, the stripes break up into quasiparticles. These observations are consistent with enhanced pairing correlations for $t'>0$, and suppressed pairing correlations for $t'<0$.

In summary, we have studied two different t-t'-J ladders: one, an open four-leg ladder which exhibits diagonal stripes when $t'=0$ and a second, periodic six-leg ladder which exhibits (0,1) stripes when $t'=0$. We find that a diagonal, next-nearest-neighbor hopping suppresses the formation of static stripes and that for $t'>0$ this can lead to an enhancement of the $d_{x^2-y^2}$ pairing correlations, while for $t'<0$ there is suppression of pairing.

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