Competition Between Stripes and Pairing in a $t$ -- $t'$ -- $J$ Model

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(September 22, 2018)

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 quasi-particles. Results for $n = 4$ and 6-leg ladders are discussed.

PACS Numbers: 74.20.Mn, 71.10.Fd, 71.10.Pm

Neutron scattering experiments on La\(_{1.6-x}\)Nd\(_{0.4}\)Sr\(_2\)CuO\(_4\) show evidence of a competition between static (quasi-static) stripes and superconductivity. \(^1\) Here the stripes consist of $(1,0)$ domain walls of holes separating $\pi$-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 5K. As $x$ deviates from this value, the relative intensity of the magnetic superlattice peaks decreases and the superconducting transition temperature $T_c$ increases. High field magnetization studies \(^2\) provide evidence that in this material superconducting can coexist with static (or quasi-static) 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. 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.

If the formation of static stripes could be suppressed, one might hope to find 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 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 ARPES data \(^6\). In addition, Lanczos calculations by Tolyama and Maekawa \(^7\) on $t$ -- $t'$ -- $J$ clusters and Monte Carlo calculations \(^7\) on $t$ -- $t'$ Hubbard lattices show that $t' > 0$ tends to stabilize the commensurate $(\pi, \pi)$ 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 \(^8\). Furthermore, it was concluded that a small positive $t'$ did not destabilize the stripes on these systems.

Here we will 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 will 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 will study has the form

$$H = -t \sum_{\langle ij \rangle}^\star (c_{i\uparrow} c_{j\downarrow} + c_{j\uparrow} c_{i\downarrow}) - t' \sum_{\langle ij \rangle}^\star (c_{i\uparrow}^\dagger c_{j\downarrow} + c_{j\uparrow}^\dagger c_{i\downarrow}) + J \sum_{\langle ij \rangle}^\star (\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j) \quad (1)$$

Here $\langle ij \rangle$ are near-neighbor sites, $\langle ij \rangle'$ are diagonal next-nearest-neighbor sites, $\vec{S}_i = \frac{1}{2} c_{i\uparrow}^\dagger \vec{s}_{i\uparrow} c_{i\downarrow}$, $n_i = c_{i\uparrow}^\dagger c_{i\uparrow} + c_{i\downarrow}^\dagger c_{i\downarrow}$, and $c_{i\uparrow}^\dagger (c_{i\downarrow})$ creates (destroys) an electron of spin $s$ at site $i$. No double occupancy is allowed. We will use DMRG calculations to explore the charge, spin, and pairing correlations on doped four and six leg ladders. The calculations reported below keep up to 1200 states per block, with truncation errors of about $10^{-4}$, and from six to ten finite system sweeps. We have checked the inclusion of $t'$ in our program by comparing the results for the rung hole
density on a $14 \times 4$ system with the results of Tohyama, et. al. [9]; precise agreement was found.

In a previous study of the 4-leg $t-J$ ladder, we found that four-hole diagonal domain walls formed as the doping increased. In Figure 1(a) and (b) we show the rung density

$$\langle n_r(\ell) \rangle = \sum_{i=1}^{4} \langle n_{\ell i} \rangle$$

versus $\ell$ for $J/t = 0.35$ on a $12 \times 4$ lattice with 8 holes and open boundary conditions. For $t' < 0$, we clearly see the formation of two domain walls, signaled by two broad peaks in $\langle n_r(\ell) \rangle$. As $t'/t$ is varied, one clearly sees that the static domain wall structure is suppressed for either sign of $t'$.

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

$$D(\ell) = \langle \Delta_{i+\ell} \Delta_i^+ \rangle$$

with $\Delta_i^+$ a pair creation operator which creates a singlet $d_{x^2-y^2}$ pair centered on the $i$th site of the second leg. Figure 1(b) shows a plot of $D(\ell)$ versus $\ell$ for the $4 \times 12$ ladder for $J/t = 0.35$ with 8 holes and various values of $t'/t$. As $t'/t$ initially increases, the pairing correlations are enhanced but as $t'/t$ becomes greater than $\sim 0.3$, they are suppressed. They are suppressed for $t'$ negative, with very strong suppression occuring for $t' \leq -0.2$.

Results for the charge density and spin structure of a $12 \times 6$ lattice with $J/t = 0.5$ and 8 holes are shown in Figure 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 containing 4 holes. The $\pi$-phase shifted antiferromagnetic regions which are separated by these domains are clearly visible in Figure 2 for $t' = 0$. 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.

![Figure 1](image_url)

**FIG. 1.** (a) Hole density per rung for a $12 \times 4$ system with 8 holes, $J/t = 0.35$ and open boundary conditions, with $t' = 0$. (b) Same as in (a), but with $t' = 0$. (c) and (d) $d$-wave pairing correlations for the systems shown in (a) and (b), respectively.

![Figure 2](image_url)

**FIG. 2.** Hole and spin densities on $12 \times 6$ 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 $S_z$. 
As \( t'/t \) increases, we again see a suppression of the charge order and in addition the \( \pi \)-phase shifted antiferromagnetic regions disappear. This is also true for \( t' \) negative. For \( t' = 0.3 \), we see that Néel spin order, without any \( \pi \) 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 \((\pi, \pi)\) antiferromagnetic correlations, which is consistent with our results.

The rung density shown in Figure 3(a) 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 \( L \times 6 \) 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 \( L \times 6 \) 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 \( 12 \times 6 \) 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 wavefunction 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 \( ++ ++ \). 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 \( 2 \times 2 \) \( t - J \) system, one finds that the 2-hole ground state has s-wave rotational symmetry, whereas the undoped state has d-wave rotational symmetry \[1\] \[13\]. The d-wave nature of the pairing comes from the difference in these rotational symmetries. Consequently, \( t' < 0 \), by suppressing the 2-hole \( + + ++ \) pattern, actually suppresses d-wave pairing, while \( t' > 0 \) can enhance it.

Consider the \( 2 \times 2 \) 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 \( t' \); \( E(2) = -J/2 - t^2 - (32t^2 + (J + 2t')^2)^{1/2} \). The pair binding energy is defined as

\[
E_b = 2E(1) - E(2) - E(0). \tag{4}
\]

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 \( t' \) \[4\]. 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 approximate 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 \( \frac{E_{\text{holes}}}{N_{\text{holes}}} \). 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 \( \frac{E_{\text{holes}}}{N_{\text{holes}}} \). We expect that finite size effects are not negligible, 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. [4], 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. [9] also found for \( t' \sim 0.5 \). 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 \( t' < 0 \). Note that static stripes and that for \( t' > 0 \) this can lead to an enhancement of the \( d_{x^2-y^2} \) pairing correlations, while \( t' < 0 \) we find suppression of pairing.

We thank M.P.A. Fisher, S.A. Kivelson, A. Millis, S. Sachdev, and E. Dagotto for interesting discussions. D.J. Scalapino would like to acknowledge the Aspen Center for Physics where the interplay of stripes and superconductivity in these models was discussed. S.R. White acknowledges support from the NSF under grant # DMR98-70930 and D.J. Scalapino acknowledges support from the NSF under grant # DMR95-27304.

![FIG. 4. Energy per hole of various hole configurations, as discussed in the text.](image)

\( N \)-leg, \( t-J \) ladders provide perhaps the simplest models which exhibit many phenomenologically similar characteristics to those observed in the cuprates. Here, for two different \( t-t'-J \) ladders, we find that a diagonal, next-near-neighbor hopping suppresses the formation of

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