Why do stripes form in doped antiferromagnets and what is their relationship to superconductivity?

Steven R. White\textsuperscript{1} and D.J. Scalapino\textsuperscript{2}

\textsuperscript{1}Department of Physics and Astronomy, University of California, Irvine, CA 92697

\textsuperscript{2}Department of Physics, University of California, Santa Barbara, CA 93106

Abstract

Experiments show evidence for stripe formation in the underdoped cuprates. Here we discuss recent numerical calculations on the $t$-$J$ model which tell us about the mechanism responsible for stripe formation and the relationship between stripes and superconductivity.

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It is clear from a variety of experiments\cite{1} that stripes appear as important low-energy configurations in the underdoped cuprates. However, the basic questions of why stripes form and what role they play in superconductivity remain controversial. A decade ago Hartree-Fock solutions of the Hubbard model showed that stripes—one-dimensional domains of increased hole density forming anti-phase Néel boundaries—were present in mean field solutions of the Hubbard model\cite{2}. Here the stability of the stripe structure arises from the reduction in kinetic energy that the holes experience in moving transverse to the stripes. However, the stripes in the Hartree-Fock solution are characterized by a filling of one hole per domain wall unit cell, while experiments on the cuprates at low doping find a filling of half this. In addition, within the Hartree-Fock framework, it is not clear how superconductivity enters.

An alternative view argues that stripe formation arises from competition between phase
separation and long-range Coulomb interactions. Central to this “frustrated phase separation” picture is the assumption that lightly doped $t-J$ or Hubbard models, with parameters in the relevant physical regime, will, in the absence of a long-range Coulomb interaction, globally phase separate into uniform hole-rich and undoped regions. In this approach, it is argued that the formation of stripes is governed by a larger charge energy scale and that pairing arises as a secondary effect associated with the transfer of a spin gap from the undoped regions to the stripes and a subsequent pair transfer between stripes, leading to a Josephson coupling and superconductivity. The fact that stripes act as antiferromagnetic domain walls is also a secondary “kinetic” effect in this picture.

Recently we have carried out numerical density matrix renormalization group (DMRG) calculations on various $t-J$ systems which suggest a third view. These calculations show that low-lying striped states occur in the $t$-$J$ model in the absence of long-range Coulomb interactions. Furthermore, unlike the Hartree-Fock solutions, the domain walls are characterized at low doping by a filling of one hole per two domain wall unit cells. The short-range structure of the domain wall contains strong antiferromagnetic singlet bond correlations crossing the holes. Just as in the case of the two-hole bound state, these spin correlations around and across the holes form in order to maximize the hopping overlap with other hole configurations, which lowers the kinetic energy, while at the same time minimizing the disturbance of the AF background. For this reason it is not surprising that the binding energy per hole of a domain wall is only slightly greater than that of a hole in a $d_{x^2-y^2}$ pair. When an additional next-nearest-neighbor, one-electron hopping term is added, the tendency to form stripes is weakened and we find that the domain walls become unstable with respect to the $d_{x^2-y^2}$ pairing state. These calculations suggest:

1. When two holes are added to the undoped system, a pair forms as the holes locally arrange themselves so as to satisfy the competing requirements of minimizing their kinetic energy and minimizing the disturbance of the background exchange interactions. At finite doping, domain walls form for similar local reasons and to support $\pi$
phase-shifted regions on either side as a way of further reducing the disturbance of the exchange interactions and to lower the transverse kinetic energy of the holes.

2. The domain walls have a minimum energy for a linear filling of $\rho_\ell = 0.5$, corresponding to one-hole per two domain-wall unit cells. Domain walls form at this linear filling for hole dopings $x < 1/8$, at which point the repulsion between domain walls becomes large enough so that additional holes cause walls with $\rho_\ell > 0.5$ to form.

3. Stripes compete with superconductivity, and by changing the parameters of the system, a pairing state can be obtained as the stripes evaporate. In particular, a change in parameters which enhances pair mobility can destabilize the stripes, leading to a stronger pairing state.

In the following we will discuss numerical results for the $t$-$J$ model which lead us to this view.

The Hamiltonian of the basic $t$-$J$ model is

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

where doubly occupied sites are explicitly excluded from the Hilbert space. Here $\langle ij \rangle$ are nearest-neighbor sites, and $s$ is a spin index. The operator and $c_{is}^\dagger$ creates an electron of spin $s$ on site $i$ and $\vec{S}_i = \frac{1}{2} c_{is}^\dagger \vec{\sigma}_{ss'} c_{is'}$ and $n_i = c_{i\uparrow}^\dagger c_{i\uparrow} + c_{i\downarrow}^\dagger c_{i\downarrow}$ are the electron spin moment and charge density operators at site $i$. The nearest-neighbor hopping and exchange interactions are $t$ and $J$, and the average site occupation $\langle n \rangle = 1 - x$ is set by the hole doping parameter $x$.

In the absence of hole doping ($x = 0$) the $t$-$J$ model reduces to a Heisenberg $S = 1/2$ antiferromagnet and the 2D ground state has long range antiferromagnetic order. The question is, what happens when it is doped? At sufficiently large values of $J/t$, the doped system will globally phase separate into a hole-free antiferromagnetic region and a hole rich region. However, in the physically relevant regimes of $J/t$ and doping discussed here, the system does not exhibit global phase separation. Rather, the DMRG calculations for the
$t$-$J$ model which we will discuss here have striped ground states. On various hole-doped $t$-$J$ lattices we have observed bond-centered and site-centered domain walls which run along the (1,0) or (0,1) direction as well as diagonal domain walls which run along the (1,1) direction, depending upon the nature of the boundary conditions. In all cases, these domain walls separate $\pi$-phase shifted AF regions, and exhibit antiferromagnetic bonds crossing the holes. The (1,0) and (0,1) walls have a lower energy with the bond-centered and site-centered walls very close in energy. Figure 1(a) shows a typical bond-centered (0,1) domain wall structure. Here the charge density and spin structure on a centered $8 \times 8$ section of a $16 \times 8$ lattice is shown. For the results shown in Fig. 1, $J/t = 0.35$, $x = 0.125$, and the lattice has periodic boundary conditions in the $y$-direction and open boundary conditions in the $x$-direction with a staggered magnetic field of strength $h = 0.1t$ applied to the open ends. On the full $16 \times 8$ lattice there are four vertical bond-centered stripes separating $\pi$-phase shifted antiferromagnetic regions. Two of these stripes on the central $8 \times 8$ section of the lattice are shown in Fig. 1(a). Each of the stripes contains 4 holes corresponding to a linear filling of 1 hole per two-domain wall unit cells. Fig. 2(a) shows a $13 \times 8$ lattice with 12 holes and with a $\pi$-phase shift in the staggered magnetic field which is applied at the ends. In this case, domain walls form which are site centered. Just as for the bond-centered domains, the site-centered domains shown in Fig. 2(a) have a linear filling of one hole per two domain wall unit cells.

To understand why such stripes form in the $t$-$J$ model, it is useful to examine these domain walls in more detail. In Fig. 1(b), we show results from a smaller system, of size $8 \times 8$, with the same hole doping and boundary conditions as in (a). The spin and hole densities for this system (not shown) are almost identical to those shown in (a). The blue circles show the most probable configuration of the eight holes in the system. The thickness of the lines connecting various sites denotes the strength of the exchange field $\langle \vec{S}_i \cdot \vec{S}_j \rangle$ for this configuration of the holes. The maximum strength of this exchange field corresponds to a singlet bond with $\langle \vec{S}_i \cdot \vec{S}_j \rangle = -3/4$. A similar construction for the site-centered case is shown in Fig. 2(b). Note the numerous frustrating valence bonds crossing the holes, most of which
connect opposite sides of each domain wall. In fact, we find that a tendency for frustrating valence bonds to form across mobile holes is universal in doped antiferromagnets, coming directly from the local competition between the kinetic and exchange energies. A domain wall allows most of these exchange bonds to form in a way which cooperates, rather than competes, with the background spin configuration. The configurations shown for these two cases in Figures 1(b) and 2(b) are, of course, only one out of the huge number which form the ground states, but they provide a local strong coupling picture of the type of correlations which are present in the domain walls.

It is interesting to compare the domain wall configuration of Fig. 1(b) with the two most probable configurations of two holes on an $8 \times 8$ lattice shown in Fig. 3(a). In the unphysical regime $J > t$, the most probable configuration for the two holes would tend to be near neighbors to reduce the number of broken exchange bonds. In the physical region, $J < t$, the kinetic energy plays an increasingly important role so that the diagonal configuration of the holes shown on the left-hand side of Fig. 3(a) is the most probable. When the holes sit on diagonal sites, there is also a large diagonal singlet correlation. As shown in Fig. 3(b), four of the eight one-electron hops from this diagonal configuration lead to a configuration in which the diagonal singlet becomes a nearest-neighbor exchange bond. The phasing of the near neighbor hole configurations has $d_{x^2-y^2}$ symmetry as does the diagonal site configuration when the background spins are taken into account. Thus, in this strong coupling picture the pairing arises from a compromise in which the holes locally arrange themselves so as to minimize the disturbance of the background exchange energy while at the same time lowering their kinetic energy by the hopping between configurations such as those shown in Fig. 3(b).

In a similar way, the site-centered domain wall configuration of Fig. 2(b) reminds one of the valence bond-like region that forms around holes in the one-dimensional $t$-$J$ model. Again, to maximize the hopping overlap with adjacent hole configurations one expects there to be strong antiferromagnetic correlations between next-nearest-neighbor sites across a hole. Such a valence bond-like correlation becomes a nearest-neighbor link after one hop of the
hole to either neighboring site, since moving the hole also moves the bond.

We see that the domain walls *locally* share a number of the same features as the two-hole pairing state, which accounts for the fact that the energy per hole for a domain wall is close to the energy per hole of a pair. In addition, however, by lining up to form a domain wall, the holes can support a $\pi$-phase shift in the surrounding antiferromagnetic background, lowering the energy further. For the site-centered wall this reflects the reduction in the kinetic energy that holes experience in moving transverse to the domain walls across which there are strong antiferromagnetic bonds (see Fig. 2(b). A similar effect occurs for the bond-centered domain wall shown in Fig. 1. In this case it is useful to think of local pairs lined up to support the $\pi$-phase-shift in the surrounding antiferromagnetic background. The stabilization energy of a $\pi$-phase shifted field on a pair can be calculated for the simple case of two holes on $2 \times 2$ $t$-$J$ lattice, such as that shown in Fig. 3(b). Representing the exchange field which runs along both sides of the stripe by a mean field of magnitude $h$, and numbering the site counterclockwise around the plaquette, the perturbation added to the $t$-$J$ Hamiltonian for the $\pi$-phase-shifted antiferromagnetic domain wall is

$$H_{\pi AF} = h (S_z^1 + S_z^2 - S_z^3 - S_z^4)$$

while if there were no phase shift

$$H_{AF} = h (S_z^1 - S_z^2 + S_z^3 - S_z^4).$$

In second order, one finds that either perturbation lowers the energy per hole by a term of order $h^2/t$ when $J/t$ is small, but the coefficient in the $\pi$-phase-shifted field case is about four times larger. The $\pi$-phase-shifted antiferromagnetic field at the edges of the domain mixes in a spin-triplet contribution to the local pairing correlations, lowering both the exchange and kinetic energies. This is similar to the effect that Krotov et. al. discussed, for the case of a 2-leg ladder, within a weak coupling renormalization group approach. There, because they neglected Umklapp processes, which may lead to a charge density wave (CDW) for $\rho_e = 0.5$, they found that a $\pi$-phase-shift field on the edges of a two-leg ladder enhanced the
pairing correlations. Here we find that the energy per hole of such a domain wall is lowered, but there are only short range pairing correlations.

In order to examine the properties of a domain wall in more detail, we have studied a single long domain wall which forms down the center of $16 \times 4$ and $16 \times 6$ lattices which have a $\pi$-phase shifted staggered magnetic field $0.1t$ applied to the top and bottom edges. The energy per hole for this system defined relative to an undoped ladder of the same size with $AF$ edge boundary conditions is shown in Fig. 4 versus the linear domain wall filling $\rho_\ell = N_{\text{holes}}/L$ with $L = 16$. One sees that the energy is a minimum on the $16 \times 6$ lattice for a linear filling of one hole per two-domain wall unit cells, $\rho_\ell = 0.5$, and is concave for this size system for $0.5 < \rho_\ell < 1.0$. On a longer $40 \times 6$ lattice we have seen phase separation into segments with $\rho_\ell \approx 1.0$ and $\rho_\ell \approx 0.5$ when the average filling is between 0.5 and 1.0. Similar results are found for the site centered domain wall. Additional simulations have shown that domain walls repel each other at short distances so that at low doping ($x < 1/8$) one has an array of half-filled domain walls with a spacing $d = (2x)^{-1}$. At $x = 1/8$, the repeat distance for the walls is four lattice spacings as seen in Fig. 1. At fillings greater than 1/8, the wall repulsion is sufficiently strong that, rather than reduce the wall spacing further, some domain walls with $\rho_\ell = 1.0$ are added leading to a change in the $d$ versus $x$ relation at $x = 1/8$.

We have also measured the pair field correlations along the $\rho_\ell = 0.5$ domain wall in the $16 \times 4$ lattice. Fig. 5 shows the pair-field correlations along the central two legs with

$$D_{yy}(\ell) = \langle \Delta_y(i + \ell)\Delta_y^\dagger(i) \rangle$$  \hspace{1cm} (4)

and

$$D_{xy}(\ell) = \langle \Delta_x(i + \ell)\Delta_y^\dagger(i) \rangle$$  \hspace{1cm} (5)

Here

$$\Delta_y^\dagger(i) = c_{i,2\uparrow}^\dagger c_{i,3\downarrow}^\dagger - c_{i,2\downarrow}^\dagger c_{i,3\uparrow}^\dagger$$ \hspace{1cm} (6)

is an operator that creates a singlet pair on the $i^{\text{th}}$ rung between leg 2 and leg 3, and
\[ \Delta_x(i) = c_{i+1,2\downarrow}c_{i,2\uparrow} - c_{i,2\downarrow}c_{i+1,2\uparrow} \] (7)

destroys a singlet pair on leg 2 between the \( i \) and \( i + 1 \) rungs. The short range \( d_{x^2-y^2} \)-like structure of the pairing correlations is seen in the sign change between \( D_{yy}(\ell) \) and \( D_{xy}(\ell) \). The pair-field correlations are clearly suppressed at larger distances.

The suppression of pairing along a domain wall can be understood as arising from a suppression of charge fluctuations induced by the \( \pi \)-shifted antiferromagnetic background. Strong local charge fluctuations are essential for superconductivity. In a domain wall with \( \rho_\ell = 0.5 \), as two adjacent holes or hole pairs move away from each other, the resulting region in which the two \( \pi \)-phase shifted domains are in contact result in a restoring potential which grows linearly with the separation. This strongly suppresses such charge fluctuations, and leads to the decay of the longer-range pairing correlations. Further suppression of pairing correlations may come from a tendency for CDW formation at \( \rho_\ell = 0.5 \). We have found that a 2-leg ladder with a filling \( x = 0.25 \), corresponding to a linear filling \( \rho_\ell = 0.5 \), has a small charge gap and long range CDW order in its ground state.

We have recently studied systems with a next nearest neighbor hopping term \( t' \) added to Eq. (1). Although a variety of terms can be added to the basic \( t-J \) Hamiltonian to improve its applicability to experimental systems, \( t' \) is particularly interesting because it directly affects the competition between pairing and stripe formation. Fig. 6(a) shows the hole and spin density for different values of \( t' \) for a \( 12 \times 6 \) system with periodic boundary conditions in the \( y \)-direction. As \( t' \) increases, the static stripe structure is smeared out and, as shown in Fig. 6(b), the pairing correlations are enhanced. We have measured the density-density CDW correlations for the lattices with the smeared out domain walls and find them to be negligible, implying that the smearing out of the charge density is not due to fluctuations of the domain walls, but rather a reduction in their ability to bind holes which eventually leads to the complete evaporation of the stripes into pairs. The effect of \( t' \) is to enhance the pair mobility, leading to a lowering of the stabilization energy of the domain walls. As this happens, the pairing correlations increase and the stripes disappear. For \( t' = 0.3t \) the
antiferromagnetic response driven by the staggered field at the open ends is peaked at \((\pi, \pi)\) and \(d_{x^2-y^2}\)-pairing correlations are dominant. Fig. 6 clearly shows that the striped domain-wall state and the superconducting pairing state compete for \(t' > 0\). However, there does appear to be an overlap region in which pairing is significant but weakly bound domain walls remain.

Thus, in the nearest-neighbor \(t-J\) model, domain walls are energetically favored over pairs and we see only weak pairing correlations. Turning on \(t' > 0\) enhances the pair mobility, tipping the balance towards a \(d_{x^2-y^2}\)-pairing state. Phenomenologically, \(t'/t > 0\) models the electron-doped materials, with \(x = \langle n_i \rangle - 1\) the electron doping rather than the hole doping. Thus, one might have expected to see even stronger pairing correlations for \(t'/t < 0\), corresponding to the hole doping case. However, as discussed in\(^6\), in this case the domain walls evaporate into quasi-particles and the \(d_{x^2-y^2}\)-pairing correlations remain weak\(^{15}\).

In summary, these results lead to the conclusions that in the \(t-J\) model, stripes and pair formation are driven by the same basic mechanism, the competition between kinetic and exchange energies, and that they compete with each other. In the nearest-neighbor \(t-J\) model, domain-wall/stripe formation is slightly favored over \(d_{x^2-y^2}\) pairing. At low doping the stripes are characterized by a linear filling \(\rho_\ell = 0.5\) and the repulsion between the stripes give a stripe spacing \(d = (2x)^{-1}\). For a hole doping \(x \geq 1/8\), some of the stripes switch to a filling \(\rho_\ell = 1.0\) giving rise to a change of behavior at this doping. In the nearest-neighbor \(t-J\) model, domain walls are energetically favored over pairs, and the pairing correlations are weak. As the next-nearest-neighbor hopping \(t'\) is turned on, one goes continuously from a situation in which the stripe correlations dominate to one in which the pairing correlations are dominant. Similar effects should be seen for other changes in the model which enhance pair mobility or act to destabilize the stripes. The regime where the pairing is strongest is broad, and includes the case where the static stripes are completely absent as well as the case where weak, smeared-out stripes are still present. In this regime there is no evidence of stripe fluctuations in the density-density correlation function; rather, the stripes have completely or nearly evaporated into pairs.
Our conclusions differ from those of previous approaches in several respects. Contrary to the frustrated phase separation scenario, we do not have global phase separation; stripe formation is not driven by competition with long range coulomb interactions; and stripes and pairing compete, although there is a region in which both coexist. In this coexistence regime, the pairing correlations are two-dimensional rather than one-dimensional. A key difference between the view we have presented and the Hartree-Fock approach is that the local structure of the domain wall we have discussed involves short-range antiferromagnetic singlet bond correlations across the holes rather than the mean-field, single-particle correlations of the Hartree-Fock solution. Furthermore, we find domain walls with a linear filling of $\rho_\ell = 0.5$ rather than $\rho_\ell = 1$.

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We believe that one needs a finite onsite Coulomb repulsion $U$, rather than the infinite repulsion of the $t$-$J$ model, to adequately model the charge transfer nature of the cuprates. With a finite $U$, the pair mobility is increased, favoring a pairing state [E. Jeckelmann, D.J. Scalapino, and S.R. White, Phys. Rev. B 58, 9492 (1998); S. Daul, D.J. Scalapino, and S.R. White, unpublished]. In addition, the effects of longer range coulomb interactions also will need to be included in more realistic models. Here our goal has been to understand the properties of the basic $t$-$J$ model.
Fig. 1. (a) Hole density and spin moments on a center section of a $16 \times 8$ $t - J$ lattice with $J/t = 0.35$ and an average hole density $x = 0.125$. The diameter of the circles is proportional to the hole density $1 - \langle n_i \rangle$ on the $i^{th}$ site and the length of the arrows is proportional to $\langle S^z_i \rangle$, according to the scales shown. The arrows are color coded to show different antiferromagnetic domains. This structure depends on the boundary conditions as discussed in the text. (b) For an $8 \times 8$ system with $x = 0.125$ whose hole density and spin pattern are almost identical to that shown in (a), the blue dots show the most probable configuration of all the holes and the strength of the exchange field $|\langle \vec{S}_i \cdot \vec{S}_j \rangle|$ between two sites is denoted by the thickness of the line connecting the sites. Anomalous antiferromagnetic correlations across holes are colored red. Only correlations where $\langle \vec{S}_i \cdot \vec{S}_j \rangle < 0$ are shown.
Fig. 2.  (a) Hole density and spin moments on a $13 \times 8$ lattice with cylindrical BCs, $J/t = 0.35$ and $\pi$-shifted staggered field $h$ on the open ends of magnitude 0.1. Here, there are 12 holes and the notation is similar to Fig. 1. (b) For a $7 \times 8$ system with four holes and one domain wall, the most probable configuration of all the holes and the strength of the exchange field surrounding them is shown, with the same notation as in Fig. 1(b). This site-centered domain wall’s hole density and spin patterns are nearly identical to those shown in (a). Anomalous antiferromagnetic correlations across holes are colored red.
Fig. 3.  (a) The two most probable hole configurations and associated local exchange field \( \langle \vec{S}_i \cdot \vec{S}_j \rangle \) correlations in the two-hole ground state of the system shown in Fig. 1(b). The scale and conventions are the same as in Fig. 1(b), but only the central \( 6 \times 6 \) region is shown. (b) Schematic illustration showing the one-electron hops from the diagonal configurations which lead to low energy configurations and contribute to a lowering of the kinetic energy.

Fig. 4.  Energy per hole for a domain wall on \( 16 \times 4 \) and \( 16 \times 6 \) lattices with \( J/t = 0.35 \) and the boundary conditions discussed in the text.
Fig. 5. Pair field correlations along a domain wall running the length of a $16 \times 4$ lattice with $J/t = 0.35$ and 8 holes.
Fig. 6. (a) Hole densities and spin moments on $12 \times 6$ systems with cylindrical boundary conditions. (b) $d$-wave pairing correlations for the same system with $t' = 0.1$, 0.2, and 0.3.