Pairing on striped $t$-$t'$-$J$ lattices

Steven R. White
Department of Physics and Astronomy, University of California, Irvine, CA 92697-4575 USA

D. J. Scalapino
Department of Physics, University of California, Santa Barbara, CA 93106-9530 USA
(Dated: October 2, 2008)

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 anti-phase superconducting domain walls.

PACS numbers: 74.45.+c, 74.50.+r, 71.10.Pm

Experimental studies are providing new insight into the interplay of the charge, spin and $d$-wave pairing correlations in the underdoped cuprates. Scanning tunneling microscopy measurements on Cu$_{1.88}$Na$_{0.12}$CuO$_2$Cl$_2$ and Bi$_2$Sr$_2$Y$_{0.2}$Ca$_{0.8}$Cu$_2$O$_{8+8}$, 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 $\pi$-phase shifted antiferromagnetic regions. Moreover, when the temperature decreases below the spin ordering temperature, the planar $\rho_{ab}$ resistivity shows evidence of a Kosterlitz-Thouless[4] like behavior consistent with the development of 2D pairing correlations.[5] Remarkably, $\rho_{ab}$ 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$_x$CuO$_4$, superconductivity and static spin density waves coexist[7], and recent far-infrared measurements 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[8] for a range of dopings near $x = 1/8$. This is believed to be a striped state and Schafgans et al.[8] have 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 anti-phase domain walls in the $d$-wave order parameter, locked to the SDW stripes, are stabilized in the striped magnetic state.[3,11] 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, $\pi$-phase shifted antiiferromagnetism 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 $\pi$ phase shifts between the stripes, i.e. anti-phase 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 $\pi$-phase shifted $d$-wave pair field would provide a natural explanation for the observed suppression of the interlayer Josephson coupling.[3,11] A similar, low lying, modulated superconducting state was also found in VMC resonating valence bond (RVB) calculations.[16,17] Here, however, no incommensurate AF order was assumed.[18]

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

$$H = -t \sum_{\langle ij \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) - t' \sum_{\langle ij \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.)$$

$$+ J \sum_{\langle ij \rangle} \left( \vec{S}_i \cdot \vec{S}_j - \frac{n_i n_j}{4} \right).$$

(1)

Doubly occupied sites are excluded from the Hilbert space, $\vec{S}_i$ and $c_{i\sigma}$ 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.

Fig. 1II shows two $12 \times 8$ ladders (tubes) with cylindrical boundary conditions (CBCs). In Fig. 1IIa, a weak staggered magnetic field is applied to the open ends and the number of holes is fixed at 12, corresponding to a doping
across stripes, is intrinsic and the open ends and bound-
stripes and with antiferromagnetic order between
stripes. There are two reasons: first, it has been diffi-
cult to construct limited-size clusters allowing significant
particle number fluctuations on a stripe, and second, as
we show below, the model parameters which strongly fa-
vor 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

\[ \Delta_{ij} = \frac{1}{\sqrt{2}} (c_{ij}^+ c_{ji}^+ + c_{ji}^+ c_{ij}^+) \]  

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

\[ D_{ij} = \frac{1}{2} \left[ \Delta_{ij}^+ + \Delta_{ij} \right], \]

and we measure $D_{ij}$ on each link in the resulting (approx-
imate) 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 $\mu$. Up to $m = 6000$
states were kept per block during 23 sweeps in this cal-
culation. 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 cou-
ple 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 as-
associated with a stripe, we have studied a single stripe on
the $16 \times 5$ lattice with CBCs, shown in Fig. 2. In
this case boundary conditions were used to force the pres-
ence of a stripe similar to those shown in Fig. 1(b)-(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.
the induced pair field is shown in the middle figure of established. When the applied pair fields are in phase, $y$ on the outermost legs ($\text{doping of } 0$ an chemical potential fields applied to force two stripes. The center two legs have an applied 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, 0.25. (a) The hole density ($1 - n_i$) and spin density $\langle S^z_i \rangle$. (b) The measured pair field $\langle D_{ij} \rangle$. (c) The measured pair field at the $x = 12$, $y = 2 - 3$ rung versus the number of holes per unit length. The maximum value for $\langle D_{ij} \rangle$ in (c) is of order half of what one would find for a BCS ground state with $\Delta_0/t = 0.1$.

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 anti-phase 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 remains in phase across the stripes, as shown in Fig. 4(b). This implies that the energy to create an anti-phase domain wall is positive. To probe this, we have studied $12 \times 6$ ladders with open boundary conditions in both the $x$ and $y$ directions, and with magnetic and chemical potential fields applied to force two stripes. Fig. 4(b) 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. 2:** A cluster with a single forced stripe on a $16 \times 5$ ladder with CBCs, with the $x$ direction oriented vertically. For all dopings, on the $y = 5$ leg, a staggered field ($-1)^y h$ with $h = 0.05$ was applied, along with a chemical potential of 2.0. On the other 4 legs, a chemical potential $\mu$ 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 $x = 0.16$, 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, 0.25. (a) The hole density ($1 - n_i$) and spin density $\langle S^z_i \rangle$. (b) The measured pair field $\langle D_{ij} \rangle$. (c) The measured pair field at the $x = 12$, $y = 2 - 3$ rung versus the number of holes per unit length. The maximum value for $\langle D_{ij} \rangle$ in (c) is of order half of what one would find for a BCS ground state with $\Delta_0/t = 0.1$.

**Fig. 3:** The linear density versus $\mu$ for different values of the next nearest neighbor hopping $t'$ for $J = 0.5$ for the systems of Fig. 2.

**Fig. 4:** (a) Hole and spin densities for a $12 \times 6$ 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 ($-1)^y h$ 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 $x = 0.1981$, 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.

**Fig. 5** The right hand figure 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 anti-phase configurations are 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 anti-phase 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 anti-phase domain wall is of order 0.01t.

There are both similarities and differences between our DMRG results and those from VMC. 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 anti-phase $d$-wave domain wall is positive.

In comparing to experiments for the cuprates, the puzzle raised by our calculations, as well as the RMFT\textsuperscript{[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\textsuperscript{[13, 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.\textsuperscript{[21]} In this case, since the stripes alternate their orientation by $90^\circ$ 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.\textsuperscript{[22]}

We wish to thank J.E. Davis, S.A. Kivelson and J. Tranquada for insightful discussions. SRW acknowledges the support of the NSF under grant DMR-0605444.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig5.jpg}
\caption{Energy per site for the $12 \times 6$ 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.}
\end{figure}

\begin{thebibliography}{99}
\bibitem{1} Y. Kohsaka, C. Taylor, K. Fujita, A. Schmidt, C. Lupien, T. Hanaguri, M. Azuma, M. Takanö, H. Eisaki, H. Tak-\ldots agi, S. Uchida, J.C. Davis, Science \textbf{315}, 1380 (2007).
\bibitem{2} J.M. Tranquada et al., Nature \textbf{429}, 534 (2004).
\bibitem{3} P. Abbamonte et al., Nature \textbf{1}, 155 (2005).
\bibitem{4} J.M. Kosterlitz and D.J. Thouless, J. Phys. C \textbf{6}, 1181 (1973).
\bibitem{5} Q. Li, M. Hucker, G.D. Gu, A.M. Tsvelik and J.M. Tranquada, Phys. Rev. Lett. \textbf{99}, 67001 (2007).
\bibitem{6} B.I. Halperin and D.R. Nelson, J. Low Temp. Phys. \textbf{36}, 599 (1979).
\bibitem{7} B. Lake, H.M. Ronnow, N.B. Christensen, G. Aeppli, K. Lefmann, D.F. McMorrow, P. Vorderwisch, P. Smeibidl, N. Mangkorntong, T. Sasagawa, M. Nohara, H. Takagi, and T.E. Mason, Nature \textbf{415}, 299 (2002).
\bibitem{8} A.A. Schafgans, private communication.
\bibitem{9} E. Berg, E. Fradkin, E.-A. Kim, S.A. Kivelson, V. Oganesyan, J.M. Tranquada and S.C. Zhang, Phys. Rev. Lett. \textbf{99}, 127003 (2007).
\bibitem{10} A. Himeda, T. Kato and M. Ogata, Phys. Rev. Lett. \textbf{88}, 117001 (2002).
\bibitem{11} D. Poilblanc and T.M. Rice, Phys. Rev. B \textbf{39}, 9749 (1989); H.J. Schultz, Phys. Rev. Lett. \textbf{64}, 1445 (1990); J. Zaanen and O. Gunnarsson, Phys. Rev. B \textbf{40}, 7391 (1989).
\bibitem{12} K. Machida and M. Ichioka, J. Phys. Soc. Jpn. \textbf{68}, 4020 (1999).
\bibitem{13} S.R. White and D.J. Scalapino, $d_{x^2-y^2}$ Pair Domain Walls,\textsuperscript{[arXiv:cond-mat/9610104v1].}
\bibitem{14} S.R. White and D.J. Scalapino, Phys. Rev. Lett. \textbf{80}, 1272 (1998); Phys. Rev. B \textbf{60}, R753 (1999); Phys. Rev. Lett. \textbf{81}, 3227 (1998).\textsuperscript{[arXiv:cond-mat/9610104v1].}
\bibitem{15} Kai-Yu Yang, Wei-Qiang Chen, T.M. Rice, M. Sigrist and Fu-Chun Zhang,\textsuperscript{[arXiv:cond-mat/9610104v1].}
\bibitem{16} M. Raczkowski, M. Capello, D. Poilblanc, R. Fréard and A.M. Oleś, Phys. Rev. B \textbf{76}, 140505(R) (2007).
\bibitem{17} M. Capello, M. Raczkowski and D. Poilblanc, Phys. Rev. B \textbf{77}, 224502 (2008).
\bibitem{18} The experimental observation that the spin ordering temperature is coincident with the Josephson decoupling of the CuO$_2$ planes suggests that in fact the antiferromagnetic order plays an important role.
\bibitem{19} V.B. Zabolotnyy, A.A. Kordyuk, D.S. Inosov, D.V. Evtsushinsky, R. Schuster, B. Buechner, N. Wizent, G. Behr, Sungseng Pyon, H. Takagi, R. Follath and S.V. Borisenko,\textsuperscript{[arXiv:0809.2237v1].}
\bibitem{20} D. LeBoeuf et al., Nature \textbf{450}, 533 (2007).
\bibitem{21} A.J. Millis and M.R. Norman, Phys. Rev. B \textbf{76}, 220503 (2007).
\bibitem{22} A rough estimate of this suppression gives a factor of $(\Delta/t)^2$.
\end{thebibliography}