Pairing and Phase Coherence in High Temperature Superconductors

V. J. Emery, a * S. A. Kivelson, and O. Zachar b †

a Dept. of Physics, Brookhaven National Laboratory, Upton, NY 11973
b Dept. of Physics, University of California at Los Angeles, Los Angeles, CA 90095

Mobile holes in an antiferromagnetic insulator form a slowly fluctuating array of quasi one-dimensional metallic stripes, which induce a spin gap or pseudogap in the intervening Mott-insulating regions. The mobile holes on an individual stripe acquire a spin gap via pair hopping between the stripe and its environment; i.e. via a magnetic analog of the usual superconducting proximity effect. This process is the analog of pairing in conventional superconductors. At non-vanishing stripe densities, Josephson coupling between stripes produces a dimensional crossover to a state with long-range superconducting phase coherence. In contrast to conventional superconductors, the superconducting state is characterised by a high density of (spin) pairs, but the phase stiffness, which is determined by the density and mobility of holes on the stripes, is very low.

1. Introduction

Superconductivity in metals requires pairing and long-range phase coherence [1]. In clean homogeneous conventional superconductors, pairing involves a relatively small fraction of the conduction electrons [2], but the superfluid density (which determines the phase stiffness) involves all of them. Here we argue that, in the high temperature superconductors [4], it is just the other way round: most of the holes are involved in pairing, but the superfluid density is proportional to the density of doped holes.

The poor phase stiffness of the high temperature superconductors is well known, and it implies that the transition temperature \( T_c \) is much less than the pairing temperature, \( \sim \Delta_0/2 \), where \( \Delta_0 \) is the energy gap at zero temperature. This separation of the energy scales has been demonstrated on phenomenological grounds [3]. In underdoped and optimally doped materials, \( T_c \) is determined by the onset of phase coherence, which occurs at a temperature of about \( \hbar^2 n_s(0)/4 m^* \). Here \( n_s(0) \), the two-dimensional superfluid density at zero temperature, determines the phase stiffness, and it is low because the high temperature superconductors are doped Mott insulators.

The need for a different approach to pairing is clear in view of the difficulty of achieving a high transition temperature via the conventional mechanisms. The problem is that a high pairing scale requires a strong attractive interaction which may favor other instabilities or, alternatively, produce a large mass renormalization which depresses the phase coherence temperature. Moreover, as the pairing energy increases, retardation becomes less effective, so it is all the more difficult to overcome the Coulomb repulsion. This problem is especially acute for the high temperature superconductors, which are doped Mott insulators with relatively poor screening. Angle resolved photoemission spectroscopy (ARPES) suggests that the energy gap has the form \( \cos k_x - \cos k_y \). This implies that, in real space, the gap function (and hence the pairing force) has a range of one lattice spacing, where the bare Coulomb interaction is very large.

In short, a theory of high temperature superconductivity must show how to obtain a large temperature scale for local superconductivity, without detriment to global phase coherence, despite poor screening of the Coulomb interaction. There are several phenomenological constraints on such a theory. First of all the order param-

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eter has charge $2e$. i.e., there is some kind of pairing. However ARPES experiments, which show that the chemical potential is near the center of the bare hole band, rule out real-space pairing, which anyway is implausible for a $d$-wave superconductor with a strong and poorly-screened Coulomb repulsion between electrons. More generally, the conventional view of superconductivity as a Fermi surface instability resulting from an attractive interaction between quasiparticles is inapplicable, since, according to analyses of resistivity \cite{6} and ARPES data \cite{8} there are no well-defined quasiparticles or Fermi surface in the normal state of high temperature superconductors.

2. Spin-gap Proximity effect

We have proposed \cite{9} that the high temperature superconductors satisfy these constraints in a unique manner. The mechanism of pairing is a form of internal magnetic proximity effect in which a spin gap is generated in Mott-insulating antiferromagnetic (AF) regions through spatial confinement by charge stripes, and communicated to the stripes by pair hopping. Many of the problems listed above are avoided because the order parameter relies on spin-pairing and does not require the existence of bound pairs of holes. The successive steps in the argument are as follows:

An AF insulator tends to expel holes \cite{10}. For neutral holes this leads to phase separation into hole-rich and hole-free regions \cite{10}, whereas, for charged holes, it gives rise to local charge inhomogeneity, typically in the form of topological doping \cite{12} in which metallic stripes are separated by insulating antiphase AF regions \cite{13}. There is much experimental evidence of ordered or fluctuating structures of this kind \cite{14,15,16}.

Topological doping \cite{12} is a general feature of doped Mott insulators, and it amounts to a strong (anti)correlation of spin and charge. However, within a metallic stripe or the intervening undoped regions there is a separation of spin and charge \cite{12}, as in the one-dimensional electron gas (1DEG). In the 1DEG, the boson representation of the operator $\psi_{1,\uparrow}\psi_{2,\downarrow} - \psi_{1,\downarrow}\psi_{2,\uparrow}$ (which annihilates pairs of fermions at opposite Fermi points, labelled by 1,2) may be written in the form $\exp(-i\theta_c)\cos\phi_s$, where $\theta_c$ and $\phi_s$ are associated with the charge and spin degrees of freedom respectively. This is an operator relation, and $\theta_c$, the superconducting phase field, is a property of the charge modes. On the other hand, pairing (or, equivalently a well-defined amplitude) corresponds to a finite expectation value of $\cos\phi_s$, which requires a spin gap \cite{17}.

A large spin gap (or pseudogap) arises naturally in a spatially-confined AF region, such as the medium between stripes. This behavior is well documented for clusters \cite{18}, frustrated spin chains \cite{19}, and spin ladders \cite{20}. In general, if there are $N$ spins in a unit cell, all spin excitations are gapped if $N$ is even, but one excitation is ungapped if $N$ is odd, i.e. there is a pseudogap. Such a spin gap does not conflict with the Coulomb interaction since the energetic cost of having localized holes in Cu 3d orbitals has been paid in the formation of the material.

The spin degrees of freedom of the 1DEG acquire a spin gap by pair hopping between the stripe and the AF environment \cite{16}. Because of the local separation of spin and charge, the spin-gap fixed point is stable even in the presence of strong Coulomb interactions, and there is no mass renormalization to depress the onset of phase coherence. Thus the phase stiffness of the mobile holes on the stripes is large enough to give a high superconducting transition temperature.

Both superconducting and charge density wave correlations develop on a given stripe. They compete at longer length scales, although they may coexist in certain regions of the phase diagram.

2.1. Symmetry of the order parameter:

If stripe order breaks the four-fold rotational symmetry of the crystal, the superconducting order will have strongly mixed extended-$s$ and $d_{x^2−y^2}$ symmetry. This will happen in a stripe-ordered phase, such as in La$_{1.6−x}$Nd$_{0.4}$Sr$_x$CuO$_4$, or in a possible “stripe nematic” phase, in which the stripe positional order is destroyed by quantum or thermal melting or quenched disorder, but the stripe orientational order is preserved. Such phases also would display large induced asymmetries in the electronic response in the $ab$-plane.

In tetragonal materials, the order parameter
must have a pure symmetry, but the way in which it emerges from the short-distance physics is very different from more conventional routes. If doping is not too high, $d_{x^2−y^2}$ order should give the long distance behavior because the extended-$s$ order parameter $(\cos k_x + \cos k_y)$ is small on the Fermi surface of the noninteracting system. Nevertheless, if the stripe fluctuations exhibit substantial orientational order at intermediate length scales, the interplay between the two types of superconducting order may be more subtle than in conventional, homogeneous materials.

2.2. Phase diagram

A feature of the stripe model is that, in lightly doped materials, the temperature scale, $T_{pair}$, at which pairing occurs on a single stripe is parametrically larger than the superconducting transition temperature, $T_c$, which is governed by the Josephson coupling between stripes. Moreover, both $T_{pair}$ and $T_c$ must be less than the temperature scale, $T_{AF}$, at which the local AF correlations are developed. The crossovers observed experimentally in underdoped high temperature superconductors have tentatively been identified $^{22}$ with these two phenomena.

3. Evidence for Spin Pairing

The idea that there is pairing in a large range of temperatures above $T_c$ is an immediate consequence of the fact that $T_c$ is significantly suppressed by phase fluctuations; i.e. that $T_c$ is close to the value obtained from the phase stiffness derived from the London penetration depth at zero temperature. Moreover the idea that “pairing” means a high density of singlets between stripes, rather than bound Cooper pairs provides a very natural explanation of the spin-gap behavior that has been widely observed in planar copper NMR measurements in underdoped cuprates $^{23}$. The interpretation of the spin gap as a superconducting gap has recently received considerable support from ARPES experiments $^{24}$ which find that the magnitude and wave vector dependence of the pseudogap above $T_c$ is similar to that of the gap seen well below $T_c$ in both underdoped and optimally doped materials. The temperature above which this gap structure disappears correlates well with the pairing scale deduced from NMR. The in-plane optical response, which shows a narrowing of the “Drude-like” peak, rather than a pseudogap structure $^{23}$, also is consistent with the idea of spin pairing.

3.1. Spectroscopic evidence

The most direct evidence for the proposed pairing mechanism would be the observation of an isolated spin-1, charge zero excitation, with an energy of order the superconducting gap, which could be identified as the low-energy excitation of a small undoped region $^{20}$. Neutron scattering experiments on optimally-doped YBa$_2$Cu$_3$O$_{7−δ}$ $^{27}$ have indeed found a spin triplet excitation, with wave vector $(π/a, π/a)$ and energy 40meV which first appears in the neighborhood of $T_c$. At lower doping $^{28}$, the energy of the mode decreases, and it first appears above $T_c$, although its intensity is enhanced below $T_c$. Recently, ARPES data in Bi$_2$Sr$_2$CaCu$_2$O$_{8+δ}$ have been interpreted as evidence for such a mode $^{29}$.

It is natural to interpret these experiments in terms of excitations of the pairs that give rise to high temperature superconductivity $^{27}$. However it is important to note that the observed cross section and Cu-Cu bilayer modulation of the triplet mode are very close to those of AF spin waves in the undoped antiferromagnet. (See e.g. Fig. 4 of ref. $^{27}$) This strongly suggests that the mode is associated with undoped regions of the material and not with mobile holes. The point is that the wave function of the mobile holes has a strong admixture of O(2p) orbitals and therefore a different magnetic form factor than in the undoped material, in which Cu(3d) orbitals predominate. Furthermore, in a conventional BCS picture, the intensity of the peak would be quite small because it is proportional to $N(0)\Delta_0$.

In our model $^{1}$, there is a composite order (involving the stripe and the AF regions), which does not break gauge invariance, but associates a superconducting phase factor $\exp(-iθ_c)$ with singlets in the AF regions. Thus, the triplet mode should appear below $T_{AF}$, and its intensity should begin to increase below $T_{pair}$ (where significant phase fluctuations begin), then grow substantially...
near $T_c$ (where long-range phase order is established). In optimally-doped $\mathrm{YBa}_2\mathrm{Cu}_3\mathrm{O}_{7-\delta}$, $T_{AF}$, $T_{pair}$ and $T_c$ are very close together, so it is reasonable that the mode is first observed close to $T_c$. The position and width of the peak reflect the wave function of the singlets; it occurs at $(\pi/a, \pi/a)$ because the singlets involve spins on opposite sublattices, and it corresponds to a singlet size of a few lattice spacings. A more detailed description of this behavior will be given in a future publication.

REFERENCES

1. J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. 106, 162 (1957).
2. The density of electrons involved in particle-hole mixing is $N(0)\Delta_0$, where $2N(0)$ is the density of states at the Fermi level.
3. V. J. Emery and S. A. Kivelson, Nature 374, 434-437 (1995).
4. J. G. Bednorz and K. A. Müller, Z. Phys. B 64, 189 (1986).
5. Z.-X. Shen et al., Phys. Rev. Lett. 70, 1553 (1993); H. Ding et al. Phys. Rev. B 54, R9678 (1996).
6. C. E. Gough et al., Nature 326, 855 (1987).
7. V. J. Emery and S. A. Kivelson, Phys. Rev. Lett. 74, 3253 (1995).
8. J. C. Campuzano et al, Phys. Rev. B 53, R14737 (1996).
9. V. J. Emery, S. A. Kivelson, and O. Zachar, Phys. Rev. B, submitted.
10. J. R. Schrieffer, S. C. Zhang, and X. G. Wen, Phys. Rev. Lett. 60, 944 (1988).
11. V. J. Emery, S. A. Kivelson, and H.-Q. Lin, Phys. Rev. Lett. 64, 475 (1990); C. S. Hellberg and E. Manousakis, preprint (cond-mat/9611194).
12. S. A. Kivelson and V. J. Emery, Synthetic Metals, 80, 151-158 (1996).
13. U. Löw, V. J. Emery, K. Fabricius, and S. A. Kivelson, Phys. Rev. Lett. 72, 1918 (1994); L. Chayes, V. J. Emery, S. A. Kivelson, Z. Nussinov, and J. Tarjus, Physica A225, 129 (1996).
14. Experimental evidence for stripes is given in J. M. Tranquada’s paper at this conference.
15. For other perspective on the origin and implications of stripes, see the papers of C. Castellani and J. Zaanen at this conference.
16. A. Luther and V. J. Emery, Phys. Rev. Lett. 33, 589 (1974).
17. V. J. Emery, Phys. Rev. B 14, 2989 (1976); G. T. Zimanyi, S. A. Kivelson, and A. Luther, Phys. Rev. Lett. 60, 2089 (1988); S. A. Kivelson and G. T. Zimanyi, Molec. Cryst. Liq. Cryst. 160, 457-481 (1988).
18. S. Tang and H. Q. Lin, Phys. Rev. B 38, 6863 (1988).
19. C. K. Majumdar and D. K. Ghosh, Math. Phys. 10, 1388 (1969).
20. For a review see E. Dagotto and T. M. Rice, Science, 271, 618 (1996).
21. D. A. Wollman et al., Phys. Rev. Lett. 71, 2134 (1993); A. G. Sun et al., Phys. Rev. B 50, 3266 (1994); D. A. Brawner et al., Phys. Rev. B 50, 6530 (1994); A. Mathai et al., Phys. Rev. Lett. 74, 4523 (1995).
22. B. Batlogg and V. J. Emery, Nature 382, 20 (1996).
23. W. W. Warren et al, Phys. Rev. Lett. 62, 1193 (1989); H. Yasuoka, T. Imai, and T. Shimizu, in Strong Correlation and Superconductivity, edited by H. Fukuyama, S. Maekawa, and A. P. Malozemoff, (Springer-Verlag, Berlin, 1989) p. 254.
24. A. G. Loeser et al., Science 273, 325 (1996); H. Ding et al., Nature 382, 51 (1996).
25. J. Orenstein et al., Phys. Rev. B 42, 6342 (1990); Z. Schlesinger et al., Phys. Rev. Lett. 65, 801 (1990); L. D. Rotter et al., Phys. Rev. Lett. 67, 2741 (1991); D. Basov et al., Phys. Rev. B 52, R13141 (1995).
26. V. J. Emery and S. A. Kivelson, Physica C 209, 597 (1993).
27. H. F. Fong et al., Phys. Rev. B 54, 6708 (1996), and references therein.
28. J. M. Tranquada et al., Phys. Rev. B 46, 556 (1992); P. Dai et al., Phys. Rev. Lett. 77, 5425 (1996); H. F. Fong et al., Phys. Rev. Lett. 78, 713 (1997).
29. Z. X. Shen and J. R. Schrieffer, unpublished; M. R. Norman et al., preprint (cond-mat/9702144).