Microscopic Theory of High Temperature Superconductivity

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It is argued that the BCS many-body theory, which is outstandingly successful for conventional superconductors, does not apply to the high temperature superconductors and that a realistic theory must take account of the local electronic structure (stripes). The spin gap proximity effect is a mechanism by which the charge carriers on the stripes and the spins in the intervening regions acquire a spin gap at a relatively high temperature, with only strong repulsive interactions. Superconducting phase order is achieved at a lower temperature determined by the (relatively low) superfluid density of the doped insulator. This picture is consistent with the phenomenology of the high temperature superconductors. It is shown that, in momentum space, the spin gap first arises in the neighborhood of the points $(0, \pm \pi)$ and $(\pm \pi, 0)$ and then spreads along arcs of the Fermi surface. Some of the experimental consequences of this picture are discussed.

I. INTRODUCTION

The high temperature superconductors$^4$ are quasi-two dimensional doped insulators, obtained by chemically introducing charge carriers into a highly-correlated antiferromagnetic insulating state. There is a large “Fermi surface” containing all of the holes in the relevant Cu(3d) and O(2p) orbitals$^5$, but $n/m^*$ vanishes as the dopant concentration tends to zero.$^6$ (Here $m^*$ is the effective mass of a hole and $n$ is either the superfluid density or the density of mobile charges in the normal state.) Clearly, understanding the origin of high temperature superconductivity and the nature of the doped insulating state are intimately related.

The doped insulating state is well understood in one dimension: the added charges form extended objects, or solitons, which move through a background of spins that have distinct dynamics.$^7$ (This is the origin of the concept of the separation of spin and charge.) In two dimensions the doped-insulating state also is characterized by a one-dimensional array of extended objects, but they are slowly-fluctuating, metallic charge stripes that separate the spins into antiphase domains. These self-organized structures are driven by the tendency of the correlated antiferromagnet to expel the doped holes, and not by specific features of the environment of the CuO$_2$ planes.$^8$ The evolution of these ideas and the extensive evidence for this local electronic structure of the CuO$_2$ planes is described in a companion paper at this conference.$^9$

Rather general and phenomenological arguments indicate that the BCS many-body theory, which is so successful for conventional superconductors, must be revised for the high temperature superconductors. (Section II.) Once this is accepted, it is clear that any new many-body theory must be based on the local electronic structure of the doped insulator, especially structure on the scale of the superconducting coherence length. In Sec. III it will be shown that, locally, the stripe structure may be regarded as a quasi one-dimensional electron gas in an active environment provided by the antiphase spin domains. For a quasi one-dimensional system there are two routes to superconductivity — a low-$T_c$ route that is analogous to BCS theory and a potentially high-$T_c$ route in which a spin gap is formed at a relatively high temperature and is independent of the onset of phase coherence which takes place at a lower temperature that is governed by the superfluid density.$^{10}$ In a quasi-one-dimensional electron gas (1DEG), both routes require some sort of attractive interaction.$^1$ However, the active environment adds a new element to the picture by allowing the formation of a spin gap with purely repulsive interactions via the “spin-gap proximity effect.”$^{10}$ The driving force is a lowering of the zero-point kinetic energy of the mobile holes, and it constitutes our mechanism of high temperature superconductivity. In this way, the stripe picture allows us to derive the phenomenology of the high temperature superconductors.

The symmetry of the order parameter emerges once these ideas are re-expressed in momentum space. (Section IV.) It will be shown that $d$-wave symmetry gives the lowest energy if the range of the gap function in real space is one lattice spacing. However, second and third neighbor components of the gap function favor $s$-wave symmetry and, in certain circumstances, they could either mix with the $d$-wave component (breaking time-reversal symmetry or lattice-rotational symmetry) or even become dominant.

II. BCS MANY-BODY THEORY

It has been argued that the quasiparticle concept does not apply to many synthetic metals, including the high temperature superconductors.$^{11}$ This idea is supported by angular resolved photoemission spectroscopy (ARPES) on the high temperature superconductors, which shows no sign of a normal-state quasiparticle peak near the points $(0, \pm \pi)$ and $(\pm \pi, 0)$ where high temperature superconductivity originates.$^{12}$ If there are no quasiparticles, there is no Fermi surface in the
usual sense of a discontinuity in the occupation number \( n_x \) at zero temperature. This undermines the very foundation of the BCS mean-field theory, which is a Fermi surface instability that relies on the existence quasiparticles.

A major problem for any mechanism of high temperature superconductivity is how to achieve a high pairing scale in the presence of the repulsive Coulomb interaction, especially in a doped Mott insulator in which there is poor screening. In the high temperature superconductors, the coherence length is no more than a few lattice spacings, so neither retardation, nor a long-range attractive interaction is effective in overcoming the bare Coulomb repulsion. Nevertheless ARPES experiments \([13]\) show that the major component of the energy gap is \( \cos k_x - \cos k_y \). Since the Fourier transform of this quantity vanishes unless the distance is one lattice spacing, it follows that the gap (and hence, in BCS theory, the net pairing force) is a maximum for holes separated by one lattice spacing, where the bare Coulomb interaction is very large (~ 0.5 eV, allowing for atomic polarization). It is not easy to find a source of an attraction that is strong enough to overcome the Coulomb force at short distances and achieve high temperature superconductivity by the usual Cooper pairing in a natural way.

Thus, although the outstanding success of the BCS theory for conventional superconductors tempts us to use it for the high temperature superconductors, it is clear that we should resist the temptation and seek an alternative many-body theory. There is phenomenological support for this point of view. In the BCS mean-field theory, an estimate of \( T_c \) is given by \( T_c \sim \Delta_0/2 \), where \( \Delta_0 \) is the energy gap measured at zero temperature. This is a good approximation for conventional superconductors because the classical phase ordering temperature \( T_0 \) is very high. A rough upper bound on \( T_c \) is obtained by considering the disordering effects of only the classical phase fluctuations as \( T \sim T_0 = AV_0 \), where \( V_0 \) is the zero-temperature value of the “phase stiffness” (which sets the energy scale for the spatial variation of the superconducting phase) and \( A \) is a number of order unity. \([14]\) \( V_0 \) may be expressed in terms of the superfluid density \( n_s(T) \) or, equivalently, the experimentally-measured penetration depth \( \lambda(T) \) at \( T = 0 \):

\[
V_0 = \frac{\hbar^2 n_s(0)a}{4m^*} = \frac{(\hbar c)^2a}{16\pi(e\lambda(0))^2} \tag{1}
\]

where \( a \) is a length scale that depends on the dimensionality of the material. For a conventional superconductor such as Pb, \( T_0 \) is about \( 10^8 \)K, which implies that phase ordering occurs very close to the temperature at which pairing is established. \([14]\)

For the high temperature superconductors, especially underdoped materials, \( \Delta_0/2T_c > 1 \), and it varies with doping. The ratio \( \Delta_0/2T_c \) ranges from about 2 to 4 as a function of \( x \). On the other hand, \( T_0 \) provides a quite good estimate of \( T_c \) for the high temperature superconductors. \([14]\) an estimate that can be improved by making a plausible generalization of the classical phase Hamiltonian. \([14]\) This behavior is qualitatively consistent with the high-\( T_c \) route to superconductivity in the 1DEG, as discussed above.

This phenomenology led us to conclude \([14]\) that the spin gap observed in NMR and other experiments \([10]\) \( (e.g. \text{as a peak in } (T_1 T)^{-1} \text{ at a temperature } T_2^* \text{, where } T_1 \text{ is the nuclear spin relaxation time}) \) should be identified with a superconducting pseudogap and not with a pseudogap associated with impeding antiferromagnetic order at zero doping. This identification is now supported by ARPES experiments on underdoped materials, \([17]\) that find a pseudogap above \( T_c \) with the same shape and magnitude as the gap observed in the superconducting state. Also, in underdoped materials, the optical conductivity \( \sigma_{ab}(\omega) \) in the \( ab \)-plane develops a pseudo-delta function, or a narrowing of the central “Drude-like” coherent peak above \( T_c \). \([13]\) Essentially all of the spectral weight moves downwards, which indicates the development of superconducting correlations.

The existence of local superconducting correlations below \( T_2 \) indicates that the amplitude of the order parameter is well established but there is no long-range phase coherence. This situation could, in principle, be realized either by increasing \( \Delta_0 \) and elevating the pairing scale or by decreasing \( n_s(0) \) and depressing the phase coherence scale as the doping \( x \) is decreased below its optimal value. Experimentally, as \( x \) decreases, \( \Delta_0 \) varies very little (or even increases), whereas the superfluid density tends to zero as \( x \rightarrow 0 \). An increase in \( \Delta_0 \) would amount to a crossover to Bose-Einstein condensation, which also requires that the chemical potential descend into the band or that the doped holes form a separate band, both of which are contradicted by ARPES experiments. \([3]\) In other words, the separation of the temperature scales for pairing and phase coherence in underdoped high temperature superconductors is a consequence of the fact that the high temperature superconductors are doped insulators; it is not a crossover from BCS physics to Bose-Einstein condensation.

Another way of looking at the situation is to compare the superfluid density \( n_s(0) \) with the number of particles \( n_p \) involved in pairing. In BCS theory, at \( T = 0 \), \( n_p \) is of order \( \Delta_0/E_F \) (where \( E_F \) is the Fermi energy) and \( n_s(0) \) is given by all the particles in the Fermi sea; i.e. \( n_p > n_s(0) \). For Bose condensation \( n_p = n_s(0) \). We shall argue that, in the high temperature superconductors, \( n_p \gg n_s(0) \): most of the holes in the Fermi sea participate in the spin gap below \( T_2 \) but the superfluid density of the doped insulator is small. An intuitive although somewhat imprecise picture of the third possibility is provided by the hard-core dimer model \([19]\) in which all the holes participate in dimers, but the mobile charge density is proportional to \( x \).

### III. Spin Gap Proximity Effect

The existence of a charge-glass state \([1] \) in a substantial range of doping in the high temperature superconductors implies that the dynamics of holes along the stripe is much faster than the fluctuation dynamics of the stripe
itself. Thus, on a finite length scale (~50 Å), an individual stripe may be regarded as a one-dimensional electron gas (1DEG) in an active environment of undoped spin regions between the stripes. Then it is appropriate to start out with a discussion of an extended 1DEG in which the singlet pair operator $P^\dagger$ may be written

$$P^\dagger = \psi_{i1}^\dagger \psi_{i2}^\dagger - \psi_{i1}^\dagger \psi_{i2},$$

(2)

where $\psi_{i,\sigma}^\dagger$ creates a right-going ($i = 1$) or left-going ($i = 2$) fermion with spin $\sigma$. One route to superconductivity in the 1DEG is similar to the BCS many-body theory. At zero temperature in a gapless phase of the 1DEG, the correlation function $< P^\dagger(x, t) P(0, 0) >$ is a power law with an exponent $K_{-1} + K_s$, where $K_c$ and $K_s$ are the critical exponent parameters for the charge and spin degrees of freedom and specify the location of the system along lines of (quantum critical) fixed points.\[5\] For a non-interacting system, $K_c = K_s = 1$ so, if $K_{-1} + K_s < 2$, pairing correlations are enhanced and pair hopping between the different members of an array of 1DEG’s will lead to a BCS-like superconducting phase transition, in which pairing and phase coherence develop at essentially the same temperature. Typically this is a low-temperature route to superconductivity and, like BCS theory, it requires an attractive interaction between the charge carriers ($i.e.$ $K_c > 1$, $K_s = 1$).

However there is another route, that is much closer to the phenomenology of the high temperature superconductors. The fermion operators of a 1DEG may be expressed in terms of Bose fields and their conjugate momenta ($\phi_c(x), \pi_c(x)$) and ($\phi_s(x), \pi_s(x)$) corresponding to the charge and spin collective modes respectively. In particular, the pair operator $P^\dagger$ becomes\[3\]

$$P^\dagger \sim e^{i\sqrt{2\pi} \theta_c \cos (\sqrt{2\pi} \phi_s)},$$

(3)

where $\partial_t \theta_c \equiv \pi_c$. In other words, there is an operator relation in which the amplitude of the pairing operator depends on the spin fields only and the (superconducting) phase is a property of the charge degrees of freedom. Now, if the system acquires a spin gap, the amplitude $\cos (\sqrt{2\pi} \phi_s)$ acquires a finite expectation value, and superconductivity will appear when the charge degrees of freedom become phase coherent. Below the spin-gap temperature, the critical exponent of the pairing operator is given by $K_{-1}^{-1}$, which can more easily fall below 2 and generate superconductivity for an array, because there is no contribution from $K_s$.\[4\] More to the point the spin gap temperature can be quite high, even in a single 1DEG, and it is generically distinct from the phase ordering temperature.\[4\] Of course phase order can only be established in a quasi-one dimensional system because, in a simple 1DEG, it is destroyed by quantum fluctuations, even at zero temperature.

For an array of 1DEG’s, a spin gap occurs only if there is an attractive interaction in the spin degrees of freedom. However, this is no longer true if the array is in contact with an active (spin) environment, as in the stripe phases. We have shown that pair hopping between the 1DEG and the environment will convey a pre-existing spin gap from the environment to the 1DEG, or will generate a spin gap in both the stripe and the environment, even for purely repulsive interactions.\[10\] A simple intuitive picture of this process is as follows: The spin part of the singlet pair operator $P^\dagger$ on a stripe is $\pm (\downarrow \downarrow - \downarrow \uparrow) / \sqrt{2}$. On the other hand, locally, the spins in the environment have a Néel spin configuration ($\uparrow \downarrow \uparrow \downarrow \downarrow \downarrow$, $\ldots$). Then, by the exclusion principle, the amplitude for pair hopping between the stripe and the environment has a (spin) factor $1/\sqrt{2}$. However, pair hopping is enhanced by a factor $\sqrt{2}$, and the kinetic energy lowered if the spins in the environment also form singlets. Note that the sign of the singlet wave functions in the environment must be chosen to maximize the overall hopping amplitude of the pairs, as the phase $\theta_c$ varies along a stripe. This corresponds to the composite order parameter that appears in the quantum field theory treatment of the problem.\[14\] In principle, this process may not lead to a gap for all of the spins in the environment in the normal state. However, once pair hopping between the stripes becomes coherent, the remaining spins will acquire a gap via the spin gap proximity effect.\[10\]

This mechanism of high temperature superconductivity also avoids problem of the strong Coulomb interaction because it involves pairing of neutral fermions, or spinons, that are known to exist in the one-dimensional electron gas.\[5\] It allows a spin gap with a range of one lattice spacing in the environment and about two lattice spacings on a stripe.

Not only does this route to superconductivity correspond closely to the phenomenology of the high temperature superconductors but it also works for a short stripe. It is well known, e.g. from an analysis of numerical calculations, that, if the length scale associated with the spin gap is short compared to the length of a stripe, then the calculation for an infinite system is a good approximation for the finite system. Furthermore, once the spin degrees of freedom are frozen in this way, the remaining Hamiltonian corresponds to a phase-number model that we have used to analyse the effects of quantum phase fluctuations.\[14\] Superconductivity appears when the different stripes become phase coherent, and the superconducting coherence length is given by the spacing between stripes and not by the range of the pair wave function as in BCS theory. A consequence is that, in the superconducting state, the radius of a vortex core should have a very weak temperature dependence, and that the core should be an essentially undoped region with a spin gap. Both of these conclusions are supported by experiment.\[20, \ref{21}\]

IV. MOMENTUM SPACE

So far we have discussed the consequences of stripes in real space. But ARPES experiments show that the high temperature superconductors have a “Fermi surface” even though there are no well-defined quasiparticles. Therefore it is appropriate to ask how this physics is realized in momentum space. We have calculated the
spectral function of a simplified stripe model and have found a reasonable correspondence with the ARPES experiments. The spin and charge wave vectors transverse to vertical stripes span the “Fermi surface” in the neighborhood of the points (±π, 0) and give rise to regions of degenerate states. Horizontal stripes have the same effect in the neighborhood of (0, ±π). These are indeed the regions in which high temperature superconductivity originates. In practice, these regions are connected by arcs that are approximately 45° sections of a circle. Along these arcs, stripe wave vectors span the “Fermi surface” at isolated points at most. Therefore the arc must become aware of the stripes by many-body effects such as the scattering of a pair of particles with total momentum zero into the regions near the M points (±π, 0) and (0, ±π). This implies that the spin gap should spread over the arcs as the system is cooled below the spin-gap temperature, which is consistent with ARPES observations.

A. Symmetry of the order parameter

The momentum space picture also has consequences for the symmetry of the order parameter. The regions near to (±π, 0) and (0, ±π) communicate with each other via the arcs of the “Fermi surface”, and the relative phase of these regions must be chosen to maximize the amplitude of the order parameter along the arcs. As mentioned above, experimentally, the range of the gap function is nearest neighbor in real space for optimal doping, corresponding to the d-wave cos kx − cos ky or the extended s-wave cos kx + cos ky. Evidently the amplitude of the extended s-wave vanishes at the M points, so the d-wave order parameter has the greater condensation energy.

This view of the origin of the symmetry of the order parameter leads to a number of interesting consequences. First of all, the existence of a nearest-neighbor gap function along the arcs of the “Fermi surface” suggests that the arcs correspond to the regions between stripes. Second, for the second and third neighbor components of the gap function, the amplitudes of the d-wave components (sin kx sin ky and cos 2kx − cos 2ky) vanish at the M points but the amplitudes of the s-wave components (cos kx cos ky and cos 2kx + cos 2ky) are maximized. In certain circumstances, these s-wave components of the order parameter could either mix with the d-wave component (breaking time-reversal symmetry or lattice-rotational symmetry) or even become dominant. There is evidence from tunnelling spectroscopy that order parameter mixing is induced in surfaces of YBa2Cu3O7−δ. An s-wave order parameter or component of the order parameter might also appear in overdoped materials, where the stripe structure is breaking up: the increased meandering of the stripes will tend to mix the short-range gap function of the environment with the longer-range gap function on the stripes.

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