Crossovers and Phase Coherence in Cuprate Superconductors

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High temperature superconductivity is a property of doped antiferromagnetic insulators. The electronic structure is inhomogeneous on short length and time scales, and, as the temperature decreases, it evolves via two crossovers, before long range superconducting order is achieved. Except for overdoped materials, pairing and phase coherence occur at different temperatures, and phase fluctuations determine both $T_c$ and the temperature dependence of the superfluid density for a wide range of doping. A mechanism for obtaining a high pairing scale in a short coherence length material with a strong poorly-screened Coulomb interaction is described.

I. INTRODUCTION

High temperature superconductivity is a property of 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, but $n/m^*$ vanishes as the dopant concentration tends to zero. (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.) The phase diagram, Fig. 1, shows that superconductivity occurs in a narrow range of doping close to the antiferromagnetic insulating state, and emerges gradually as the temperature is lowered, via two crossovers at which specific local electronic structure develops, and a phase transition where long-range phase order is established. Clearly, understanding the origin of high temperature superconductivity and the nature of the doped insulating state go hand in hand.

In our view, the driving force behind all of this behavior is the tendency of the antiferromagnet to expel the doped holes and so to form hole rich and hole free regions. For neutral holes this leads to a first-order phase transition (phase separation), but, for charged holes, the competition with the long-range part of the Coulomb interaction generates a dynamical local charge inhomogeneity, in which the mobile holes are typically confined in charged "stripes", which are antiphase domain walls for the spins in the intervening undoped regions. Locally, the electronic structure has a quasi one-dimensional character. There is extensive evidence, both direct and indirect, for this interpretation of the experiments.

Charge instabilities are a general consequence of the competition between phase separation and the long-range Coulomb interaction, and they are a common feature of oxides in general. However, the the mechanism of superconductivity and the nature of the superconducting state depend on the details of the underlying microscopic model. Here, we are interested in systems with purely repulsive interactions. Models with an effective short-range attraction are described by Di Castro.

II. CROSSOVERS

A crossover signifies a change in the short- or intermediate-distance behavior of a system as the temperature or some other thermodynamic quantity is varied. Unlike a phase transition, at which long range order is established, a crossover is not abrupt, and usually it appears at slightly different temperatures in different physical properties. The existence of two crossovers in the high temperature superconductors is evident in NMR experiments; the Knight shift begins to decrease at a tem-
temperature $T_1^*$, whereas $(T_1/T)^{-1}$ (where $T_1$ is the nuclear spin relaxation rate) does not start to decrease until a lower temperature $T_2^*$. In underdoped materials these two temperatures are well separated. For example, in HgBa$_2$Ca$_2$Cu$_3$O$_{6+\delta}$, $T_1^*$ is about 370K, whereas $T_2^*$ is about 230K. On the other hand, as shown in Fig. 1, the two crossovers merge just above $T_c$ in most optimally-doped materials. This is why it appeared at first that there was just one crossover at a “spin gap” temperature $T^*$. However, although a drop in $(T_1/T)^{-1}$ (which depends on the real part of the spin susceptibility $\chi$) indicates the opening of a spin gap (or pseudogap), a drop in the Knight shift (which depends on the real part of $\chi$) could indicate either the opening of a spin gap or the development of short-range antiferromagnetic correlations, or both. As $x \to 0$, $T_1^*$ approaches the temperature at which local antiferromagnetic correlations, not a spin gap, develop in the undoped systems [13]. At finite doping, other information is necessary to distinguish between the different possibilities.

In underdoped materials, the $c$-axis optical conductivity $\sigma_c(\omega)$ develops a pseudogap at a temperature that correlates well with the upper crossover $T_1^*$. [10] The spectral weight is transferred upwards to quite high frequencies, which indicates the development of short-range charge correlations and/or spin correlations. On the other hand, at a lower temperature $T_2^*$, the optical conductivity $\sigma_{ab}(\omega)$ in the $ab$-plane develops a pseudo-delta function or, in other words, a narrowing of the central “Drude-like” peak. [20] Essentially all of the spectral weight from a pseudogap region moves downwards, which indicates the development of superconducting correlations. Other experiments support this general picture. In particular, angle-resolved photoemission spectroscopy (ARPES) shows that the pseudogap in the normal state has essentially the same magnitude and momentum dependence as the gap in the superconducting state. [21]

### A. Lower Crossover: Phase Fluctuations

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 behavior, which may be deduced from the experiments, regardless of the underlying microscopic model, [24] is not unusual in the statistical mechanics of systems with a two-component order parameter, but it constitutes a major difference between high temperature superconductors and conventional superconductors, for which pairing and phase coherence are established at one and the same temperature.

The pairing scale is related to the size of the coherence length $\xi_0$ or equivalently the energy gap $\Delta_0$ at zero temperature, and, in the BCS mean field theory, $\Delta_0/2$ provides a good estimate of $T_c$. At the same time, the classical phase ordering temperature is determined by the “phase stiffness” $V_0$ which sets the energy scale for the spatial variation of the superconducting phase. The classical phase Hamiltonian is

$$H = V_0 \sum_{ij} \cos(\theta_i - \theta_j)$$

and, if $V_0$ is independent of $T$, the phase ordering temperature $T_\theta = AV_0$, where $A$ is a number of order unity. [22] At zero temperature, $V_0$ is given in terms of the superfluid density $n_s(T = 0)$ or, equivalently, the experimentally measured penetration depth $\lambda(T = 0)$:

$$V_0 = \frac{\hbar^2 n_s(0) a}{4 m^*} = \frac{(\hbar c)^2 a}{16 \pi (\epsilon(\lambda(0))^2}$$

where $a$ is a length scale that depends on the dimensionality of the material. An estimate for $T_c$ is given by the smaller of $\Delta_0/2$ and $T_\theta$.

The separation of the temperatures for pairing and phase coherence as the doping $x$ is decreased below its optimal value could, in principle, be accomplished either by decreasing $\xi_0$ (increasing $\Delta_0$) and elevating the pairing scale, or by decreasing $n_s(0)$ and depressing the phase coherence scale. Figure 1 clearly shows that the separation of scales is caused by the drop in the superfluid density (a property of a doped insulator) and not by a decrease in $\xi_0$ (a crossover to Bose-Einstein condensation).

For conventional materials, the value of $\Delta_0/2$ gives a very good estimate for $T_c$ whereas, for e.g. Pb, $T_\theta = AV_0$ is about 10K. [22] This is why BCS theory works so well. On the other hand, for underdoped high temperature superconductors, $\Delta_0/2$ is closer to $T_2^*$ than to $T_c$, [23] whereas $T_\theta$ is very close to $T_c$ itself, especially for underdoped materials. [22] In other words, because the high temperature superconductors are doped insulators, $n_s(0) \to 0$ as $x \to 0$, and phase ordering controls $T_c$. [24]

Phase fluctuations also give a good description of the temperature dependence of the superfluid density below $T_c$. It has been shown by University of British Columbia group [25] that, if the measured values of $\Delta^2(0)/\lambda^2(T)$ for YBa$_2$Ca$_2$Cu$_3$O$_{6-\delta}$ with $\delta$ equal to 0.01, 0.05, and 0.40, are plotted as functions of $T/T_c$, they all lie on the same curve. In other words, $T_c$ is the one and only energy scale involved in the temperature dependence of $\lambda(T)$ for overdoped, optimally doped, and underdoped samples of YBCO. Moreover, near $T_c$, all three samples display the critical behavior expected for classical phase fluctuations. Therefore, on empirical grounds, it is difficult to escape the conclusion that the entire temperature dependence of $\lambda(T)$ is governed by classical phase fluctuations. We have shown [25] that, in the superconducting state, phase fluctuations are indeed classical over a very wide temperature range because the low-frequency conductivity that exists in addition to the $\delta(\omega)$ peak of the superconducting condensate [26] is sufficient to screen the Coulomb interaction down to very low temperatures. Figure 2 shows the temperature dependence of $\Delta^2(0)/\lambda^2(T)$ for the three-dimensional version of the simple classical phase Hamiltonian given in Eq. (1), together with a comparison with the experimental data. [27] Of course, in YBCO, $V_0$ should be anisotropic within the CuO$_2$ planes and should be quite small in the direction perpendicular to the planes, so a more accurate model would have two additional dimensionless parameters that could be adjusted.
to fit the experiments. Nevertheless, it can be seen that the calculated and experimental curves are already very close, without any tuning of parameters.

The significance of phase fluctuations has been questioned by Geshkenbein et al. \cite{30} and by Millis et al. \cite{31} However, in estimating $T_C$, these papers incorrectly assumed that $V_0$ is the renormalized phase coupling, whereas it is, of course, the bare phase coupling that appears in Eq. (1). They made the unrealistic assumption that, in YBa$_2$Cu$_3$O$_{7-\delta}$ and YBa$_2$Cu$_3$O$_8$, there is a strong bare phase coupling between the bilayers, and made the incorrect assertion that bilayer coupling would double the estimate of $T_C$. Moreover they focussed solely on highly anisotropic materials with bilayers, and thereby failed to appreciate the overall picture which shows that $T_C$ is controlled by phase fluctuations in a wide variety of clean underdoped cuprate superconductors that do not suffer from these complications.

B. Upper Crossover: Local Inhomogeneity

The upward movement of spectral weight in $\sigma_c(\omega)$ at $T^*_1$ signifies the development of the charge and spin correlations associated with the formation of stripes. Locally, an individual stripe may be regarded as a one dimensional electron gas (1DEG) in an active environment and, for repulsive interactions, the dominant instability is to the formation of charge density waves (CDW). \cite{4} However the possibility that an array of stripes might form an ordered insulating CDW state at low temperatures is entirely eliminated if the zero-point energy of transverse stripe fluctuations is sufficiently large in comparison to the coupling between stripes. \cite{4} As a consequence, there exist novel, liquid-crystalline low-temperature phases – an electron smectic, with crystalline order in one direction, but liquid-like correlations in the other, and an electron nematic with orientational order but no long-range positional order. \cite{4} In the presence of symmetry breaking fields there is a crossover to the nematic region, rather than a phase transition.

The isotropic-to-nematic boundary has many of the characteristics of the upper crossover. At high temperatures the holes are more or less uniformly distributed, and randomly disrupt antiferromagnetic correlations. However, a self-organized stripe array, especially in a nematic phase, allows a mixture of local antiferromagnetic correlations and spin singlets to develop in the hole-free regions of the sample. \cite{4} Stripes tend to separate the spins into regions that are more or less disconnected from some of their neighbors, and there is much numerical and analytical evidence to show that some of the low-energy spin degrees of freedom acquire an energy gap in such a structure. \cite{4} This gap is a consequence of local physics, not impending long range antiferromagnetic order and, for this reason, it has the potential to be the source of superconducting pairing, as we shall see. Taking all of these effects together, the upper crossover is signified by a drop in the magnetic susceptibility as well as a spontaneous breakdown of fourfold rotational symmetry of the CuO$_2$ planes (wherever it exists).

As the concentration of holes increases, the separation between stripes eventually becomes comparable to their

![Superfluid density $\rho_s$](image-url)
width and all information concerning the Mott insulating state is lost. Here, the isotropic-to-nematic line ends at a zero temperature quantum critical point. Different versions of such a point, either 0+1 dimensional \[16,37\] or 2+1 dimensional \[19,37\] have been invoked to explain the unusual normal state properties of the high temperature superconductors.

### III. PAIRING MECHANISM

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 \[5\] 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 (\(\sim 0.5 \text{ eV}\), allowing for atomic polarization). It is not easy to find a source of an attraction that is strong enough to overcome such a Coulomb force at short distances and achieve high temperature superconductivity via the usual Cooper pairing.

#### A. Spin Gap Proximity Effect

The stripe structure provides a very natural way to overcome this problem. For a 1DEG, the singlet pair operator may be written

\[
\psi_{1\uparrow}^{\dagger} \psi_{2\downarrow}^{\dagger} + \psi_{2\uparrow}^{\dagger} \psi_{1\downarrow}^{\dagger} \sim e^{i\phi_c} \cos \phi_s
\]

Here \(\phi(x)\) is a Bose field and \(\pi(x)\) its conjugate momentum, \(\partial_x \theta \equiv \pi\) and the subscripts “c” and “s” indicate charge and spin fields respectively. This relation shows that the operator \(\cos \phi_s\) plays the role of the amplitude of the order parameter, whereas the operator \(\theta_c\) represents the superconducting phase. We have proved \[5\] that when pairs of holes hop on and off a stripe, they acquire a gap in their spin degrees of freedom because the undoped regions have a spin gap or pseudogap. As a result, \(\cos \phi_s\) acquires a finite expectation value, the amplitude of the superconducting order parameter becomes well-defined, and local quasi one-dimensional superconducting fluctuations become significant. This takes place at the lower crossover temperature \(T_2\), which is essentially a property of a single stripe and so is relatively insensitive to the value of \(x\), until it is cut off by \(T_1\) at larger dopant concentrations. Throughout the underdoped regime \(T_1\) is determined by pair hopping between stripes, and ultimately between the planes. This process is the microscopic version of the phase coupling in Eq. (1).

The order parameter also acquires its symmetry from the spin degrees of freedom. Nematic order breaks four-fold rotational symmetry and would lead to a mixed \(s\) and \(d\)-wave symmetry of the superconducting order parameter, even in an otherwise tetragonal material.

#### B. The Relation between Spin and Charge

The topological nature of the stripes \[1\] indicates a strong correlation of the spin and charge collective modes that is well supported by the neutron scattering experiments. \[2\] At the same time, on an intermediate length scale, there is a separation of spin and charge on an individual stripe, as in a 1DEG. \[3\] This dual relation between spin and charge is characteristic of a doped insulator in two dimensions, and it is of central importance for overcoming the Coulomb problem. The point is that A) pairing has its origin in insulating regions of the material, where the energetic cost of having localized holes in \(\text{Cu}\ 3d\) orbitals has been paid in the formation of the material, and B) on a stripe, the objects that form pairs are neutral fermions (spinons), which are not impeded by the Coulomb interaction. The validity of this picture is based on the well-established techniques developed in the theory of the 1DEG. \[4\]

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