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Local Electronic Structure and High Temperature Superconductivity.

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Abstract.
It is argued that a new mechanism and many-body theory of superconductivity are required for doped correlated insulators. Here we review the essential features of and the experimental support for such a theory, in which the physics is driven by the kinetic energy.

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I INTRODUCTION

High temperature superconductivity [1] is obtained by adding charge carriers into a highly-correlated antiferromagnetic insulating state. Despite the fact that there is a large "Fermi surface" containing all of the pre-existing holes and the doped holes, [2] it is impossible to understand the behavior of the system and, in particular, the origin of high temperature superconductivity unless the nature of the doped-insulating state is incorporated into the theory. In particular, the Fermi liquid theory of the normal state and the BCS theory of the superconducting state, which are so successful for conventional metals, were not designed for doped insulators, and they do not apply to the high temperature superconductors. (Section II.) Consequently it is necessary to develop a new mechanism and many-body theory of high temperature superconductivity.

In our view, the physics of the insulator and the doped insulator, including antiferromagnetism and superconductivity, is driven by a lowering of the zero-point kinetic energy. [3] This is well known for the antiferromagnetic state but, in addition, the motion of a single hole in an antiferromagnet is frustrated because it stirs up the spins and creates strings of ferromagnetic bonds. Consequently, a finite density of holes forms self-organized structures, designed to lower the zero-point kinetic energy. This is accomplished in three stages: a) the formation of charge inhomogeneity (stripes), b) the creation of local spin pairs, and c) the establishment of a phase-coherent high-temperature superconducting state. The zero-point kinetic

energy is lowered along a stripe in the first stage, and perpendicular to the stripe in the second and third stages.

Static or dynamical charge inhomogeneity, [4–8] or "topological doping" [9] is quite common for doped correlated insulators. In d dimensions, the charge forms one-dimensional arrays of $(d-1)$-dimensional structures that are also antiphase domain walls for the background spins. In $d = 1$ there is an array of charge solitons, [10] whereas, in $d = 2$, there are linear "rivers of charge" (stripes) threading through the antiferromagnetic background. [5–7] In $d = 3$ there are arrays of charged planes [7,8], as observed in the manganates. [11] These self-organized structures, which may be fluctuating or form ordered or glass phases, are a consequence of the tendency of the correlated antiferromagnet to expel the doped holes, and they lead to a lowering of the zero-point kinetic energy. The theoretical arguments that lead to this picture will be summarized in Sec. III.

It is clear that any new many-body theory must be based on the local electronic structure and there are strong indications of a link to high temperature superconductivity. First of all, in LSCO and YBCO the value of T_c is inversely proportional to the spacing between stripes in underdoped and optimally doped materials. [12,13] Secondly, μSR experiments [14,15] have found evidence for a phase in which superconductivity coexists with a cluster spin glass. In $YBa_2Cu_3O_{7-\delta}$, the spin freezing temperature goes to zero when the superconducting T_c is more than 50K. It is difficult to see how these two phases could coexist unless there is a glass of metallic stripes dividing the CuO_2 planes into randomly-coupled antiferromagnetic regions. A new mechanism and many-body theory of superconductivity, based on local charge inhomogeneity has been developed, [16–19] and there is substantial experimental support for the overall picture, as described in subsequent sections.

II BCS MANY-BODY THEORY

There are several reasons why the Fermi liquid theory of the normal state and the BCS theory of the superconducting state do not apply to the high temperature superconductors:

1) In BCS theory, the superfluid density n_s is given by all electrons in the Fermi sea, whereas, in the high temperature superconductors, n_s is proportional to the density of doped holes.

2) The outstanding success of BCS theory stems from the existence of sharp quasiparticles. However, an analysis of the temperature dependence of the resistivity shows that the quasiparticle concept does not apply to many synthetic metals, including the high temperature superconductors. [16,20] This idea is supported by angular resolved photoemission spectroscopy (ARPES) 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. [21,22]

3) If there are no quasiparticles, there is no Fermi surface in the usual sense of a discontinuity in the occupation number $n_{\vec{k}}$ at $T = 0$. This undermines the very

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foundation of the BCS mean-field theory, which is a Fermi surface instability.

4) In BCS theory, pairing and phase coherence take place at the same temperature T_c, and a good estimate of T_c is given by $\Delta_0/2$, where Δ_0 is the energy gap measured at zero temperature. However, this criterion does not give a good estimates of T_c for the high temperature superconductors, especially for underdoped materials: $\Delta_0/2T_c$ varies with doping and can be much greater than one. Rather, the value of T_c is determined by the onset of phase coherence [17,19] and is governed by the zero-temperature value of the "phase stiffness", $V_0 \equiv (\hbar c)^2 a/16\pi(e\lambda(0))^2$, which sets the energy scale for the spatial variation of the superconducting phase. Here $\lambda(T)$ is the penetration depth and a is a microscopic length scale that depends on the dimensionality of the material. [17]

5) 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 [22] shows that the major component of the gap function is proportional to $\cos k_x - \cos k_y$. It follows that, in real space, the gap function 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 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 a high transition temperature *in a natural way* by the usual Cooper pairing.

Clearly there is a need for a new mechanism and many-body theory to explain high temperature superconductivity.

III TOPOLOGICAL DOPING

It is well known that the motion of a single hole in an antiferromagnet is frustrated by the creation of strings of broken bonds. [23] This idea is supported by ARPES, which found that the bandwidth of a single hole is controlled by the exchange integral J, rather than the hopping amplitude t. [24]

When there is a finite density of holes, the system strives to relieve this frustration and lower its kinetic energy. If the holes were neutral the system would separate into a hole-free antiferromagnetic phase and a hole-rich (magnetically disordered or possibly ferromagnetic) phase, in which the holes are mobile and the cost in exchange energy is less than the gain in kinetic energy. [25–27] In practice the holes are charged, but macroscopic phase separation can take place whenever the dopants are mobile, as in oxygen-doped and photo-doped materials. We have reviewed the experimental evidence for this behavior elsewhere. [28,5] More recent experiments exploring oxygen doping in detail have been carried out by Wells *et al.*. [29]

When the dopants are immobile, charged holes can do no more than phase separate locally, by forming arrays of linear metallic stripes [5–7] which are "topological" in nature, since they are antiphase domain walls for the antiferromagnetic background spins. [9,30] This structure lowers the kinetic energy along the stripe but makes it more difficult, if anything, for a *single* hole to move perpendicular to the stripe direction. A hop transverse to a stripe takes the hole far above Fermi energy. [18] However, as we shall see, *pairs of holes* can move more easily transverse to a stripe, and they lower their kinetic energy first by forming spin pairs and, at a lower temperature, by making the system a high temperature superconductor.

It has been argued that charge stripes are energetically impossible because the driving energies are unable to overcome the Coulomb repulsion. [31] However, charge modulation is *inevitable* if the short-range interactions give a negative compressibility, κ, as they do between the spinodals of a system that, otherwise, would undergo phase separation. A general expression for the Debye screening length is $\lambda_D = \sqrt{\epsilon/4\pi e^2 n^2 \kappa}$, where ϵ is the dielectric constant, e is the charge and n is the density. When $\kappa < 0$, λ_D is imaginary, which indicates that the ground state is unstable to a density modulation. [32,33] Of course it requires a more detailed microscopic calculation to obtain the physical length scale.

The existence of charge and spin stripes in the $La_{2-x}Sr_xCuO_4$ family was established in an elegant series of experiments on $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$ by Tranquada and co-workers. [34] In a Landau theory of the phase transition, [30] the spin order parameter $\vec{S}_{\vec{q}}$ and the charge order parameter $\rho_{-\vec{Q}}$ first couple in third order $(\vec{S}_{\vec{q}} \cdot \vec{S}_{\vec{q}}\, \rho_{-\vec{Q}})$, so the ordering vectors must satisfy $\vec{Q} = 2\vec{q}$ or, in other words, the wavelength of the spin modulation is twice that of the charge modulation. This relation is found to be satisfied experimentally, [34] and it implies that the charge stripes also form antiphase domain walls in the magnetic order, which gives the precise meaning of the concept of topological doping. [9] The observation of essentially ordered stripes allowed a study of the evolution of the spin and charge order parameters, which not only provided input into the mechanism of stripe formation by showing that they are charge driven, but also established that *inelastic incommensurate magnetic* peaks observed previously [35] in $La_{2-x}Sr_xCuO_4$ were produced by fluctuating stripes. Recently, inelastic incommensurate magnetic peaks have been observed in underdoped $YBa_2Cu_3O_{7-\delta}$ by neutron scattering experiments, [36] thereby establishing that $YBa_2Cu_3O_{7-\delta}$ and the $La_{2-x}Sr_xCuO_4$ family have a common spin structure.

By now, the prediction of metallic stripes [5,6] has been confirmed in all families of materials in which extensive neutron scattering experiments have been performed (LSCO and YBCO). There is growing evidence of similar behavior in $Bi_2Sr_2CaCu_2O_{8+\delta}$: preliminary neutron scattering experiments show incommensurate magnetic peaks, and there is ARPES evidence [37] of spectral weight transfer associated with stripes. Also, a calculation of the effects of stripes in ARPES experiments [38] produced regions of degenerate states and a flat section of the "Fermi surface" near $(0, \pm\pi)$ and $(\pm\pi, 0)$, as observed experimentally. [39,40,21]

IV SPIN PAIRING

The existence of a cluster spin-glass state for a substantial range of doping in the high temperature superconductors [14,15] implies that the stripe dynamics is slow and that the motion of holes along the stripe is much faster than the fluctuation dynamics of the stripe itself. Thus an individual stripe may be regarded as a finite piece of one-dimensional electron gas (1DEG) located in an active environment of the 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

$$P^\dagger = \psi^\dagger_{1\uparrow}\psi^\dagger_{2\downarrow} - \psi^\dagger_{1\downarrow}\psi^\dagger_{2\uparrow}, \tag{1}$$

where $\psi^\dagger_{i,\sigma}$ creates a right-going ($i = 1$) or left-going ($i = 2$) fermion with spin σ. In one dimension, 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 [10]

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

where $\partial_x\theta_c \equiv \pi_c$. 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. Clearly, in one dimension, the temperature at which the spin gap forms is generically distinct from the phase ordering temperature because phase order is destroyed by quantum fluctuations, even at zero temperature. [10]

We emphasize that we are *not* dealing with a *simple* 1DEG, for which a spin gap occurs only if there is an attractive interaction in the the spin degrees of freedom. [10] The 1DEG on the stripe is in contact with an active (spin) environment, and we have shown that pair hopping between the 1DEG and the environment will generate a spin gap in both the stripe and the environment, even for purely repulsive interactions. [18] The same mechanism gives rise to spin gaps in spin ladders. Also, although the theory was worked out for an *infinite* 1DEG in an active environment, it is known from numerical calculations on finite-size systems that the conclusions are correct for any property that has a length scale small compared to the size of the system. Here, we use the theory only to establish the existence of a spin gap, which corresponds to a length scale of a few lattice spacings. Once a spin gap has been formed, the problem is reduced to the physics of the superconducting phase and its quantum conjugate (the number density), and high temperature superconductivity emerges when phase order is established. [16,17,19]

Experimentally the formation of an amplitude of the order parameter is indicated by a peak in $(T_1T)^{-1}$ (where T_1 is the spin-lattice relaxation rate), [41] and by

ARPES, [42] both of which are consistent with spin pairing. A drop in the specific heat [43] and a pseudogap in the c-axis optical conductivity, [44] both of which indicate that the charge is involved, occur at a higher temperature in underdoped materials, and are symptoms of the onset of stripe correlations. [18]

V PHASE COHERENCE

High temperature superconductivity is established when there is coherent motion of a pair from stripe to stripe. [18] This final step in the reduction of the zero-point kinetic energy is equivalent to establishing phase order, and it determines the value of T_c, especially in underdoped and optimally doped materials. [16,17,19]

It is sometimes argued that thermal phase fluctuations are excluded because the Coulomb interaction moves them up to the plasma frequency, ω_p, via the Anderson-Higgs mechanism. This argument, if correct, also would imply that critical phenomena near to T_c cannot display 3d-XY behavior. An explicit calculation shows why this objection is incorrect. The Fourier transform of the Lagrangian density in the long wavelength limit has the form [16,45]

$$\mathcal{L}(\vec{k},\omega) = \frac{1}{2}\vec{k}^2 a^2 [V_0(\omega) + V_1\omega^2\epsilon(\omega)]\theta^2(\vec{k},\omega) \tag{3}$$

where $\epsilon(\omega)$ is the dielectric function at $\vec{k} = 0$, $V_1 = \hbar^2 a/16\pi e^2$, and $V_0(0) \equiv V_0$ is the classical phase stiffness, defined above. At high frequency

$$\epsilon(\omega) = \epsilon_\infty - \frac{\omega_p^2}{\omega^2}. \tag{4}$$

Note that $V_0(\omega)$ vanishes at high frequency and, in general, it does not contribute to the plasma frequency. Then phase fluctuations occur at a frequency $\omega_p/\sqrt{\epsilon_\infty}$. At the same time, for $\omega = 0$, the Lagrangian has the form $\mathcal{L} = const.\vec{k}^2$, as required for classical phase fluctuations. In general, it is necessary to do a renormalization group calculation to obtain the zero-frequency limit, and we have shown that, for sufficiently good screening (large dielectric function), the behavior of the system is given by the classical (V_0) part of the Lagrangian. [16] The unusual form of the Lagrangian stems from the use of the dual phase-number representation, in which the V_0 term represents the kinetic energy (pair hopping) and the V_1 term is the potential energy (Coulomb interaction).

We have solved the following model of classical phase fluctions [17,19]:

$$H = -J_{\|} \sum_{<ij>_{\|}} \{\cos(\theta_{ij}) + \delta\cos(2\theta_{ij})\} - \sum_{<kl>_{\perp}} \left\{J_{\perp}^{kl}\cos(\theta_{kl})\right\}, \tag{5}$$

where the first sum is over nearest neighbor sites within each plane, and the second sum is over nearest neighboring planes. The values of the constants $J_{\|}$ and δ are taken to be isotropic within each plane and the same for every plane. The coupling

between planes, $J_{\perp}^{kl}$, is different for crystallographically distinct pairs of neighboring planes.

The results of this final stage of the calculation are in good agreement with experiment. For a reasonable range of parameter values (as constrained by the magnitudes of the penetration depths in different directions) the model gives a good estimate of T_c and its evolution with doping. It also explains [19] the temperature dependence of the superfluid density, obtained for a range of doping by microwave measurements. [46]

The phase diagram itself is consistent with this picture. The physics evolves in three stages. Above the superconducting transition temperature there are two crossovers, which are quite well separated in at least some underdoped materials. The upper crossover is indicated by the onset of short-range magnetic correlations and by the appearance of a pseudogap [44] in the c-axis optical conductivity (perpendicular to the CuO_2 planes) which might possibly indicate the establishment of a stripe glass phase. The lower crossover is where a spin gap or pseudogap (which is essentially the amplitude of the superconducting order parameter) is formed. Finally, superconducting phase order is established at T_c and, in fact, determines the value of T_c. [17,19]

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