Unusual Superconducting State of Underdoped Cuprates

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There is increasing experimental evidence that the superconducting energy gap Δ_0 in the underdoped cuprates is independent of doping concentration x while the superfluid density is linear in x. We show that under these conditions thermal excitation of the quasiparticles is very effective in destroying the superconducting state, so that T_c is proportional to $x\Delta_0$ and part of the gap structure remains in the normal state. We then estimate H_{c2} and predict it to be proportional to x^2. We also discuss to what extent the assumptions that go into the quasiparticle description can be derived in the U(1) and SU(2) formulations of the *t-J* model. [S0031-9007(97)03242-0]

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While the anomalous properties of cuprate superconductors have been discussed from the very beginning, it has become clear in the past several years that it is in the underdoped region that the cuprates deviate most strongly from conventional materials, both in the normal and superconducting states. NMR [1], neutron [2], and c-axis optical conductivity [3] indicate the existence of a pseudogap in the normal state, and photoemission experiments [4,5] reveal that the pseudogap is of the same size and $\boldsymbol{k}$ dependence as the superconducting gap. Furthermore, as the doping concentrating x is reduced from optimal doping, the superconducting gap is constant or may be slightly increasing, while the transition temperature T_c is reduced. Thus a strong deviation from the BCS ratio between energy gap and T_c is to be expected. At the same time, London penetration depth and optical conductivity [6] show that the Drude weight in the normal state as well as the superfluid density in the superconducting state are proportional to x, and a linear relation between T_c and the superfluid density have been noted [7]. The small superfluid density has led a number of authors to suggest that phase fluctuation may be the determining factor of T_c and that the pseudogap may be interpreted as superconducting fluctuations [8,9]. A related interpretation in terms of Bose condensation of pairs has also been suggested [7,10]. A second school of thought starts with strongly correlated models such as the *t-J* model and interprets the pseudogap as the spin excitation gap in some resonating-valence-bond singlet state. In particular, this scenario is realized in a decomposition of the electron into a fermion which carries spin and a boson which represents a vacancy in order to enforce the constraint of no double occupation of the *t-J* model. At the mean field level, spin and charge are separated, and in the underdoped region of the mean field phase diagram the fermions are paired in some intermediate temperature range, and become a d-wave superconductor only below the Bose condensation temperature of the bosons [11,12]. Very recently, a modification of this mean field theory was proposed, which incorporates an SU(2) symmetry known to be important at half filling [13]. It was argued that the new SU(2) formulation allows a smoother connection to half filling and includes low lying fluctuations ignored in the original U(1) formulation. Features in the photoemission data are qualitatively explained by this approach, but so far discussions have been limited to the normal state.

In this Letter we examine the superconducting state of the underdoped cuprates. We begin with a phenomenological approach, based on the existence of well defined quasiparticles in the superconducting states. We show that the combination of a large energy gap and small superfluid density leads to unusual features. A key result is that the superconducting state is destroyed by the thermal excitation of just the low lying quasiparticles, leaving the large energy gap intact. We believe this is a more effective mechanism of destroying superconductivity than the phase fluctuation scenario. With very few assumptions we derive expressions for the temperature dependence of ρ_s and for T_c and H_{c2}. We then consider whether the quasiparticle approach can be derived from the microscopic treatments of the *t-J* model. We conclude that the U(1) formulation fails to obtain the correct temperature dependence of ρ_s, even if gauge fluctuations are included in the Gaussian approximation. We then indicate how the assumptions of the phenomenology can be derived from the SU(2) formulation, provided that quantum fluctuations of low lying excitations are taken into account.

We limit our discussion to clean superconductors and assume that the elementary excitations in the superconducting state are well defined quasiparticles with dispersion $E(\boldsymbol{k}) = [(\varepsilon_{\boldsymbol{k}} - \mu)^2 + \Delta_{\boldsymbol{k}}^2]^{1/2}$, where $\Delta_{\boldsymbol{k}} = \frac{1}{2}\Delta_0(\cos k_x a - \cos k_y a)$ is a d-wave gap with a maximum of Δ_0 at $(0,\pi)$. In a tight binding parametrization, $\varepsilon_{\boldsymbol{k}} = 2t_f(\cos k_x a + \cos k_y a)$. There are four nodal points. In the vicinity of the nodes near $(\frac{\pi}{2},\frac{\pi}{2})$, we have the anisotropic Dirac spectrum $E(k) = (v_f^2 k_1^2 + v_2^2 k_2^2)^{1/2}$, where $k_1 = (k_x + k_y - \pi/a)/\sqrt{2}$, $k_2 = (k_x - k_y)/\sqrt{2}$, $v_2 = \frac{1}{\sqrt{2}}\Delta_0 a$, and $v_f \approx 2\sqrt{2}\, t_f a$ for $\mu \approx 0$. We now make the key assumption that the presence of a vector potential shifts the quasiparticle spectrum according to

$$E(\boldsymbol{k},\boldsymbol{A}) = E(\boldsymbol{k}) + \frac{e}{c}\boldsymbol{v}_{\boldsymbol{k}} \cdot \boldsymbol{A}, \tag{1}$$

where $\boldsymbol{v}_{\boldsymbol{k}} = d\varepsilon_k/d\boldsymbol{k}$ is the normal state velocity. Equation (1) is correct to first order in $\boldsymbol{A}$ in the BCS theory. It has the consequence that the current carried by the quasiparticle is $-c dE/d\boldsymbol{A} = -e\boldsymbol{v}_k$, i.e., it is the same as the current in the normal state and is different from the group velocity $dE_k/d\boldsymbol{k}$. The difference arises from the fact that the superconducting quasiparticle is a superposition of particle and hole states. For high T_c superconductivity, we do not have the equivalence of BCS theory, so Eq. (1) must be regarded as an assumption, albeit a very reasonable one. This is particularly so near the node, where it is reasonable to believe that at the node the superconducting quasiparticle should be the same as the normal quasiparticle, so that its current should be given by $\boldsymbol{v}_{\boldsymbol{k}}$.

We next argue that the superfluid tensor defined by $\boldsymbol{j}_\mu = \frac{e}{c}\frac{\rho^s_{\mu\nu}}{m}A_\nu$ can be written as $\frac{1}{m}\rho^s_{\mu\nu} = \frac{1}{m}\rho^s(T = 0)\delta_{\mu\nu} - \frac{1}{m}\rho^n_{\mu\nu}$, where $\rho^s(T = 0)/m = x/a^2 m$ is directly measured by the weight of the Drude peak in the normal state and by λ_L^{-2}, where λ_L is the London penetration depth in the superconducting state. By taking $\lambda_L = 1600$ Å for $YBa_2Cu_3O_{6.95}$ ($YBCO_{6.95}$) and $x = 0.2$, we find $m = 2.1 m_e$. It is convenient to fit this mass to the bottom of a tight binding bandwidth with hopping integral t_h, and we have $t_h = (2ma^2)^{-1} = 0.122$ eV which happens to be very close to J. On the other hand, $\frac{1}{m}\rho^n_{\mu\nu}$ is given by the quasiparticle response to the $\boldsymbol{A}$ field. This we can calculate by writing the free energy in terms of noninteracting quasiparticles, i.e.,

$$F(\boldsymbol{A},T) = -kT\sum_{\boldsymbol{k},\sigma}\ln(1 + e^{-\beta E(\boldsymbol{k},\boldsymbol{A})}) \tag{2}$$

and differentiating twice with respect to $\boldsymbol{A}$. We note that the neglect of quasiparticle interaction is justified in the limit of small T and $\boldsymbol{A}$ because the density of states of quasiparticles vanishes linearly with energy, in contrast to the case of a Fermi liquid. As explained by Leggett [14], the Landau parameters enter in the form of mean field theory in Fermi liquid theory. The vanishing of the free quasiparticle response functions implies that the Landau parameters play no role in this limit. We therefore obtain

$$\frac{1}{m}\rho^n_{\mu\nu} = -2\sum_{\boldsymbol{k}}\frac{dE}{dA_\mu}\frac{dE}{dA_\nu}\frac{\partial f}{\partial E}. \tag{3}$$

Strictly speaking, there is an additional term of the form $2\sum_{\boldsymbol{k}}(\partial^2 E/\partial A_\mu \partial A_\nu) f(E)$. This term vanishes in BCS theory due to particle-hole symmetry and we shall assume that it is also negligible in the present case. Using Eq. (1), we replace dE/dA_μ by the normal state velocity $\boldsymbol{v}_\mu$ and $\rho_s(T)$ can be evaluated in a straightforward way

$$\frac{\rho^s}{m}(T) = \frac{x}{a^2 m} - \alpha T, \tag{4}$$

where $\alpha = [2\ln(2)/\pi]v_F/v_2 = [8\ln(2)/\pi]t_f/\Delta_0$. We see that for small x, the quasiparticle excitation is an effective way of destroying the superconducting state by driving ρ^s to zero. By extrapolating Eq. (4) to $\rho^s = 0$, we can estimate T_c as

$$kT_c \approx 1.13 x\Delta_0(t_h/t_f). \tag{5}$$

If we assume that Δ_0 is independent of x for underdoped cuprates, we see that T_c is proportional to x [or more precisely to $\rho_s(T = 0)/m$], thus providing an explanation of Uemura's plot [7]. We shall see that $t_h/t_f \approx 1.8$, so that while the value of T_c given by Eq. (5) is too large by a factor of 2, it is lower than the estimates based on phase fluctuation or Bose condensation, which typically gives $T_c \approx xt_h$. We emphasize that our mechanism is completely different from these other pictures, in that the quasiparticle spectrum and the energy gap Δ_0 comes into play. Obviously, Eq. (5) implies a strong deviation from the BCS ratio between T_c and Δ_0 for small x.

Another important implication is that superconductivity is destroyed when only a small fraction of the quasiparticles (with energy $\lesssim x\Delta_0$) are thermally excited. Thus the gap near $(0,\pi)$ must remain intact in the normal state, leaving a strip of thermal excitations which extend a distance proportional to x from the nodal points. This is qualitatively in agreement with the photoemission experiment. Of course our phenomenological picture does not provide a description of the normal state. It simply states that the normal state gap is an inescapable consequence of a finite Δ_0 and a vanishingly small superfluid density as $x \to 0$.

The fact that $d\rho_s/dT$ is independent of x and that both ρ_s and T_c are proportional to x means that a scaled plot of $\rho_s(T)/\rho_s(0)$ vs T/T_c should be independent of x for small T/T_c. In fact, such a scaled plot for $YBCO_{6.95}$ and $YBCO_{6.60}$ shows a remarkable universality over the entire temperature range [15]. We can use the data to extract the ratio v_F/v_2 using Eq. (4). Using the $YBCO_{6.95}$ data, we obtain a velocity anisotropy $v_F/v_2 = 6.8$, a slightly smaller ratio (by about 15%) as obtained from the $YBCO_{6.60}$ data. With our parametrization of the gap functions, we find $t_f/\Delta_0 = 1.7$. If we assume $\Delta_0 = 40$ meV, we find $t_f = 68$ meV, so that $t_h/t_f = 1.8$ as mentioned earlier. Our value of t_f implies a half-filled bandwidth $\sim 4t_f \approx 270$ meV which is consistent with the photoemission data. This gives $v_f = 1.18 \times 10^7$ cm/sec.

Equation (1) implies that in the presence of a magnetic field, the quasiparticle spectrum is shifted so that some of the quasiparticles are occupied in the ground state and a finite density of states is generated at the Fermi energy [16]. It was pointed out by Yip and Sauls [17] that this gives rise to a contribution for the supercurrent which is nonlinear in A. The quasiparticle contribution to the current is obtained by differentiating Eq. (2) with respect to $\boldsymbol{A}$. For $\boldsymbol{A}$ in the $\hat{x}$ or $\hat{y}$ direction and for $\boldsymbol{v}_f \cdot e\boldsymbol{A}/c \gg kT$, we find up to order A^2

$$\boldsymbol{j}(\boldsymbol{A},T) = -\left(\frac{e^2\rho^s(T)}{mc} - \frac{e^2}{\sqrt{2}\,2\pi c}\frac{v_f^2}{v_2}\left|\frac{e}{c}\boldsymbol{A}\right|\right)\boldsymbol{A}. \tag{6}$$

The second term is in agreement with Yip and Sauls [17] while the first term is given by Eq. (4).

We now use this picture to estimate the size of the vortex core and estimate H_{c2}. The idea is to identify the core size as the point where the critical current is reached. The critical current (i.e., the maximum of $\boldsymbol{j}$ as a function of $\boldsymbol{A}$) is estimated by setting $d\boldsymbol{j}/d\boldsymbol{A} = 0$ in Eq. (6). The field $\frac{e}{c}\boldsymbol{A}$ should be replaced by the gauge invariant local velocity $\frac{1}{2}$ $(\nabla\theta - \frac{2e}{c}\boldsymbol{A})$. Near the core $\nabla\theta$ dominates and we can replace $e\boldsymbol{A}/c$ by $(2R)^{-1}\hat{A}$. We obtain the following estimate for the core size when it is approached in the $\hat{x}$ or $\hat{y}$ direction,

$$R_1 = \frac{1}{\sqrt{2}\,2\pi}\,\frac{v_f^2}{v_2}\,\frac{m}{\rho^s}\,. \tag{7}$$

At $T = 0$ we can use our parametrization of $\Delta(\boldsymbol{k})$ to write it as $R_1 = x^{-1}(v_f/\pi\Delta_0)(t_f/\sqrt{2}\,t_h)$. Note that it is greater than the BCS coherence length $v_f/\pi\Delta_0$ by the factor x^{-1}. On the other hand, using the T_c estimate in Eq. (5), we can write

$$R_1 = v_F/(1.25\pi k T_c)\,, \tag{8}$$

which is quite close to the BCS coherence length written in terms of T_c instead of Δ_0. The two ways of writing the coherence length are of course equivalent in BCS theory, but very different for underdoped cuprates. A main conclusion of this Letter is that Eq. (8) is the proper expression for the coherence length.

When the core is approached from the (1,1) direction, similar considerations show that the core size is given by $\sqrt{2}\,R_1$. Thus the core takes on an approximately square shape. We estimate H_{c2} by assuming that the square vortex cores are closed packed, so that

$$H_{c2} = (hc/2e)/4R_1^2\,. \tag{9}$$

Because of the crudeness of the extrapolation process, we expect both the T_c and H_{c2} expressions to be overestimates. An estimate may be made by using Eq. (8) for R_1 and using the experimental T_c and we obtain for $YBCO_{6.6}$ $R_1 \approx 38$ Å and $H_{c2} \approx 56$ T which is close to the measured value of 50 T [18]. While the absolute value of H_{c2} is quite uncertain, the prediction that H_{c2} is proportional to x^2 [or more accurately to $\rho_s^2(T=0)$], as long as Δ_0 is constant for underdoped cuprates, should be amenable to experimental test. The ideal systems to test this correlation are underdoped YBCO or Hg cuprates, which fall on the Uemura plot [7] so that $\rho_s(T=0)$ is proportional to T_c and can be accurately determined. In principle the linear atomic-cell-orbital method is a good testing ground because x can be varied. Unfortunately, there are serious disorder effects for $x \leq 0.1$ and the nominally pure compound $x = 0.15$ is off the Uemura plot, for reasons which are not presently understood. Equation (1) breaks down in the presence of disorder, restricting our results to the clean limit.

At finite T the prediction that $H_{c2}(T) \sim \rho_s^2(T)$ which follows from Eqs. (7) and (9) is also interesting, in that we predict a linear decrease of H_{c2} with increasing T for low temperatures. In view of Eq. (8), the condition $\boldsymbol{v}_f \cdot e\boldsymbol{A}/c \approx v_f/2R_1 \gg kT$ which was used in the derivation of Eq. (6) is satisfied for $T < T_c$. Thus the scaling of H_{c2} with ρ_s^2 should be satisfied as long as T is not too close to T_c when critical fluctuations become important.

Next we comment on whether existing microscopic models can reproduce the assumptions of the quasiparticle description. In the U(1) formulation of the t-J model the normal state in the underdoped limit is described by d-wave pairing of fermions, so that there exists an energy gap Δ_0 which remains finite as $x \to 0$ in the normal state [11,12]. Superconductivity is driven by condensation of bosons and well defined quasiparticles are formed. The superconducting T_c occurs as an energy scale of $4\pi x t_h$ at the mean field level, and may be suppressed by gauge fluctuations [19]. In this theory the superfluid density is given by the Ioffe-Larkin rule [20], $\rho^s(T)^{-1} = \rho_f^{s-1} + \rho_b^{s-1}$. Since the energy gap appears in the fermion spectrum, we expect $\rho_f^s(T) = (1 - x) - T/\Delta_0$ while $\rho_b^s \approx x$ with a higher power in T correction. Then the U(1) theory predicts $\rho^s(T) = x - x^2T/\Delta_0$. While the $T = 0$ value is correctly given to be x, the temperature dependence is in strong disagreement with Eq. (3) and with experiment in that α is suppressed by x^2. The origin of this difficulty is that the fermion does not couple directly to $\boldsymbol{A}$, but to the U(1) gauge field $\boldsymbol{a}$ while the bosons couple to $\boldsymbol{A} + \boldsymbol{a}$. The external $\boldsymbol{A}$ produces a finite $\boldsymbol{a}$ but its magnitude is reduced by x. In the quasiparticle language, the shift of the spectrum in the presence of$\boldsymbol{A}$ is smaller than that given in Eq. (1) by x. It is difficult to escape from this conclusion in the U(1) theory, because gauge fluctuations are included at the Gaussian level which should be a good approximation in the superconducting state.

It was shown recently [13] that the U(1) formulation does not connect smoothly to the half-filled limit which is known to exhibit an SU(2) symmetry. For small x, there are indeed low lying gauge fluctuations with energy scale of order $x\Delta_0$ which are ignored in the U(1) formulation. A new SU(2) formulation was introduced, which allows these low energy fluctuations to be described in a natural way. The low energy effective theory contains a boson part and a fermion part: $L_{\text{eff}} = L_b + L_f$. (For details, see Ref. [13].) The boson part is given by

$$L_b = ib^\dagger(\partial_t - ieA_0 - ia_0\tau^3)b - \frac{1}{2m}\left|\left(\partial_i - i\frac{e}{c}A_i - ia_i\tau^3\right)b\right|^2 - \frac{D_1}{2m}(b^\dagger b)^2 - \mu b^\dagger b - D_2\frac{J}{2}(|b_1|^2 - |b_2|^2)^2, \tag{10}$$

where $b = (b_1 b_2)$, and $D_{1,2}$ are order one coefficients. The fermions are in a staggered flux phase and couple only to the a_μ gauge field. When $|b_1| = |b_2| \neq 0$, the system is in a superconducting state [which corresponds to the d-wave paired state in the U(1) formulation]. When $b_1 \neq 0$ and $b_2 = 0$, the system is in a metallic state [which corresponds to the staggered flux phase in the U(1) formulation]. Since $D_2 > 0$ the ground state is the superconducting state. The normal state at finite temperatures contains no boson condensation and is a state which fluctuates between d-wave pairing and the staggered flux phase of fermions. The fermion spectrum acquires a gap Δ_0 which is finite for small x.

We note that, in the superconducting state ($|b_1| = |b_2|$), a_μ and A_μ decouple under the mean field approximation. Therefore the low lying fermion quasiparticles do not couple to the external electromagnetic gauge field A_μ, and cannot reduce the superfluid density within mean field theory. However, unlike the U(1) case, quantum fluctuations of the gauge fields and the quantum fluctuations between the two bosons [both are omitted in the U(1) formulation] are important even at $T = 0$. Those quantum fluctuations induce a coupling between the fermion quasiparticles and the gauge potential $\boldsymbol{A}$. One such contribution is illustrated in Fig. 1. We find that the shift of the quasiparticle spectrum is of the form given by Eq. (1), except that the $\boldsymbol{v}_k \cdot \boldsymbol{A}$ is multiplied by a numerical constant of order unity. Thus the SU(2) theory incorporates the main ingredients underlying the present Letter, i.e., a finite gap Δ_0, a superfluid density proportional to x, and a quasiparticle spectrum given by Eq. (1). Details of this microscopic theory will be given elsewhere.

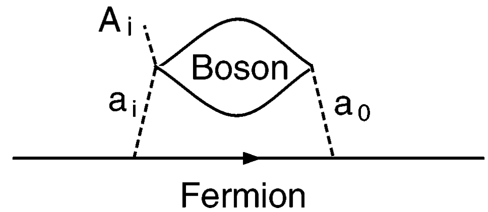

FIG. 1. Coupling between A_i and fermion quasiparticles.

We believe that our prediction that $H_{c2} \sim x^2$ is significant for two reasons. First, it is in contrast with models based on Bose condensation which should predict $H_{c2} \sim x$ since the coherence length in that case is the interparticle spacing $x^{-1/2}$. Second, $H_{c2} \sim x^2$ is a weak field in the sense that when compared with the hole density x, the number of Landau levels occupied is $x^{-1} \gg 1$ so that we are outside of the quantum Hall limit. Thus we expect the state for $H > H_{c2}$ to be a metallic state and the key question is what kind of metallic state it is. It is clear from the present discussion that for $x \ll 1$, the energy gap at $(0, \pi)$ survives inside the vortex core and therefore for $H > H_{c2}$. The magnetic field drives a region of gapless excitations in the Brillouin zone which extends a distance x from the nodal positions, qualitatively similar to the normal state above T_c. It seems to us that two possibilities remain. First the gapless excitations are well defined quasiparticles in the Landau sense. In this case, the Luttinger theorem requires that a breaking of translation symmetry must occur to produce the energy gap and the metallic state may be understood as some form of staggered flux phase. Alternatively, the gapless excitations are not Landau quasiparticles, but acquire residual width due to quantum fluctuations, making this state a genuine non-Fermi liquid state. This latter scenario is an exciting possibility which deserves further investigation.

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[1] See M. Takigawa *et al.*, Phys. Rev. B **43**, 247 (1991).
[2] J. Tranquada *et al.*, Phys. Rev. B **46**, 5561 (1992).
[3] C. C. Homes *et al.*, Phys. Rev. Lett. **71**, 1645 (1993).
[4] A. G. Loeser *et al.*, Science **273**, 325 (1996); J. Harris *et al.* (to be published).
[5] H. Ding *et al.*, Nature (London) **382**, 51 (1996).
[6] J. Orenstein *et al.*, Phys. Rev. B **42**, 6342 (1990).
[7] Y. Uemura *et al.*, Phys. Rev. Lett. **62**, 2317 (1989); **66**, 2665 (1991).
[8] V. Emery and S. Kivelson, Nature (London) **374**, 434 (1995).
[9] S. Doniach and M. Inui, Phys. Rev. B **41**, 6668 (1990).
[10] M. Randeria *et al.*, Phys. Rev. Lett. **69**, 2001 (1992).
[11] G. Kotliar and J. Liu, Phys. Rev. B **38**, 5142 (1988).
[12] H. Fukuyama, Prog. Theor. Phys. Suppl. **108**, 287 (1992).
[13] X. G. Wen and P. A. Lee, Phys. Rev. Lett. **76**, 50 (1996); P. A. Lee, N. Nagaosa, T. K. Ng, and X. G. Wen (to be published).
[14] A. J. Leggett, Rev. Mod. Phys. **47**, 331 (1975).
[15] D. A. Bonn *et al.*, Czech. J. Phys. **46**, S6, 3195 (1996); J. Phys. Chem. Solids **56**, 1941 (1995).
[16] G. Volovik, JETP Lett. **58**, 469 (1993).
[17] S. K. Yip and J. Sauls, Phys. Rev. Lett. **69**, 2264 (1992); D. Xu, S. K. Yip, and J. Sauls, Phys. Rev. B **51**, 16 233 (1995).
[18] G. S. Boebinger *et al.* (unpublished).
[19] P. Lee and N. Nagaosa, Phys. Rev. B **45**, 966 (1992).
[20] L. Ioffe and A. Larkin, Phys. Rev. B **39**, 8988 (1989).