Response of a $d_{x^2-y^2}$ superconductor to a Zeeman magnetic field

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We study the response of a two-dimensional $d_{x^2-y^2}$ superconductor to a magnetic field that couples only to the spins of the electrons. In contrast to the *s*-wave case, the $d_{x^2-y^2}$ state is modified even at small magnetic fields, with the gap nodes widening into normal, spin polarized, pockets. We discuss the promising prospects for observing this in the cuprate superconductors in fields parallel to the Cu-O planes. We also discuss the phase diagram, inclusive of a finite momentum pairing state with a linkage between the momentum of the pairs and the nodes of the relative wave function. [S0163-1829(98)04714-6]

Following the original work of Clogston and Chandrasekhar,¹ the modification of superconductivity by the Zeeman coupling between the spins of the electrons and an applied magnetic field has attracted intermittent attention.² Much of this has centered on the bound on the upper critical field H_{c2} provided by consideration of the Zeeman interaction alone ("Pauli limit") and on the nature of the phase boundary when this effect dominates. A more unusual aspect of this physics was uncovered by Fulde and Ferrell³ and by Larkin and Ovchinnikov⁴ in the possibility of a finite momentum pairing state at large magnetic fields, where the reference Fermi surface is spin split. Experimentally, the classic predictions on the nature of the s-wave phase boundary have been borne out by work on thin Al films,⁵ while recent work on unconventional superconductors has exhibited Pauli limited critical fields⁶ as well as the first evidence for a realization of the finite momentum pairing state.⁷ Very recently, the Zeeman suppression has also been discussed in experiments on mesoscopic samples.⁸

In this paper, motivated by the recent experimental identification of the pairing state in several of the cuprate superconductors, we discuss the Zeeman response of an ideal twodimensional $d_{x^2-y^2}$ superconductor. We believe that this is a useful exercise on three grounds. First, the cuprates are strongly two-dimensional systems and hence admit a geometry for measurements in a magnetic field, with the field parallel to the Cu-O planes, where the Zeeman response should dominate the orbital response at low temperatures. Second, we estimate that spin-orbit scattering, which attenuates the Zeeman response, is small enough in the cleanest samples to allow its neglect above fields as small as a few Tesla. Third and most interestingly, the existence of nodes in the gap function imply that (in contrast to the *s*-wave case) the superconducting state responds non-trivially at arbitrarily small values of the magnetic field. As is intuitively plausible, the response is paramagnetic with the destruction of superconductivity over parts of the Fermi surface where the Zeeman energy μB exceeds the local gap $\Delta(\mathbf{k})$, and a spin polarization of the resulting normal electrons. This leads to observable effects in all quantities that are sensitive to the density of states for quasiparticles.

In the following we will explicitly illustrate this by calculations on a weak coupling BCS model and present estimates that indicate that it is readily observable in the cuprates. For completeness, we also discuss the mean-field phase diagram of our model in the field-temperature plane, where we note the existence of finite momentum pairing with a linkage of the wave vector to the nodal structure of the gap function.

Choice of Hamiltonian. We study a two-dimensional (2D) electron system described by the Hamiltonian

$$H = \sum_{\mathbf{k},\sigma=\uparrow,\downarrow} \epsilon_{k} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} c_{\mathbf{k},\uparrow}^{\dagger} c_{-\mathbf{k},\downarrow}^{\dagger} c_{-\mathbf{k}',\downarrow} c_{\mathbf{k}',\uparrow}, \qquad (1)$$

where ϵ_k is the rotationally invariant kinetic energy measured from the Fermi energy ϵ_F , and for $|\epsilon_k|, |\epsilon'_k| < \epsilon_c \ll \epsilon_F$, the pairing potential *V* takes the form⁹

$$V_{\mathbf{k},\mathbf{k}'} = -2V_0 \cos(2\theta_k) \cos(2\theta_{k'}) + \mu^*, \qquad (2)$$

where $V_0 > 0$, μ^* is the renormalized *s*-wave repulsion and θ_k is the azimuthal angle of **k**; V=0 otherwise. At low temperatures the system is a superconductor with a gap function of the $d_{x^2-y^2}$ form $\Delta(\theta) = \Delta_0(T)\cos(2\theta)$, where Δ_0 satisfies

$$1 = \frac{N(0)V_0}{2\pi} \int_0^{2\pi} d\theta \int_0^{\epsilon_c} d\xi \frac{2\cos^2(2\theta)}{E(\xi,\theta)} \tanh\left(\frac{E(\xi,\theta)}{2k_BT}\right),$$
(3)

and $E(\xi,\theta) = \sqrt{\xi^2 + \Delta_0^2 \cos^2(2\theta)}$, N(0) is the single particle density of states for each spin species at the Fermi level. In the weak coupling limit $N(0)V_0 \ll 1$, assumed throughout this paper, this leads to a maximum gap $\Delta_{00} = \Delta_0(T=0) = 2.43\epsilon_c e^{-1/N(0)V_0}$, and a critical temperature $T_c = 0.467\Delta_{00}$. The quasiparticle spectrum is governed by the mean-field Hamiltonian

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$$H_{\rm MF} = \sum_{\bf k} E_{\bf k} (\alpha_{\bf k}^{\dagger} \alpha_{\bf k} + \beta_{\bf k}^{\dagger} \beta_{\bf k}), \qquad (4)$$

where $E_{\mathbf{k}} = \sqrt{\epsilon^2(k) + \Delta_0^2 \cos^2(2\theta_k)}$, and $\alpha_{\mathbf{k}}^{\dagger}(\beta_{\mathbf{k}}^{\dagger})$ are creation operators of up (down) spin quasiparticles.

We should note that the $d_{x^2-y^2}$ state that we are interested in, arises in (nearly) tetragonal lattice systems. Our choice of model here is intended to mimic this lattice physics with minimal and computationally favorable ingredients: we keep a rotationally invariant Fermi surface but introduce a pairing potential (2) that has the reduced symmetry of the lattice.

A uniform magnetic field (*B*) applied *parallel* to the 2D plane does not couple to the orbital motion of the electrons in the plane. It does, however, lift the spin degeneracy, and introduce the Zeeman term $H_Z = -\mu B \Sigma_{\mathbf{k}} (c_{\mathbf{k}\uparrow}^{\dagger} c_{\mathbf{k}\uparrow} - c_{\mathbf{k}\downarrow}^{\dagger} c_{\mathbf{k}\downarrow})$ into the Hamiltonian, where $\mu = g \mu_B/2$ is the magnetic moment of the electron, and \uparrow and \downarrow refer to spin direction along and opposite to the field direction, respectively. This modifies both the gap equation and the quasiparticle Hamiltonian to

$$1 = \frac{N(0)V_0}{2\pi} \int_0^{2\pi} d\theta \int_0^{\epsilon_c} d\xi \frac{\cos^2(2\theta)}{E(\xi,\theta)} \bigg[\tanh\bigg(\frac{E(\xi,\theta) + \mu B}{2k_B T}\bigg) + \tanh\bigg(\frac{E(\xi,\theta) - \mu B}{2k_B T}\bigg) \bigg];$$

$$H_{MF} = \sum_{\mathbf{k}} \left[(E_{\mathbf{k}} - \mu B) \alpha_{\mathbf{k}}^{\dagger} \alpha_{\mathbf{k}} + (E_{\mathbf{k}} + \mu B) \beta_{\mathbf{k}}^{\dagger} \beta_{\mathbf{k}}) \right].$$
(5)

Qualitatively, the Zeeman field lowers (increases) the energy of the spin up (down) quasiparticle states which in turn changes their occupation and affects the self-consistency condition for the gap function (which is now distinct from the true quasiparticle gap).

Weak-field response. We begin by considering weak magnetic fields and low temperatures: $\mu B, k_B T \ll \Delta_{00}$. An *s*-wave state is essentially unaffected in this limit. This is because the occupation numbers for quasiparticle states remain exponentially small at low *T* and *B*, due to the finite gap, even though the field shifts the quasiparticle bands linearly (at *T*=0 the gap function and the ground state are completely unaffected).

The situation, however, is qualitatively different in the case of the $d_{x^2-y^2}$ state studied here—in our case the gap vanishes at four nodal points on the Fermi surface—sufficiently close to these points there are always some spin up quasiparticle states whose energies become *negative* for arbitrarily small values of *B*. These states, which live in elliptical pockets, $E_k < \mu B$, near the Fermi surface (Fig. 1), develop a thermal occupation that is O(1) at *any* temperature. Translating back into electron operators, one sees that these pockets are in fact regions of the spin polarized normal state (fully polarized at T=0)—their inner and outer arcs are pieces of the spin split Fermi surface which come together when the angle dependent gap function exceeds the Zeeman energy. The loss of pairing in them and the area within k_BT , leads to an overall reduction of the gap function:



FIG. 1. Fermi surface pockets (shaded regions) produced by a Zeeman magnetic field. The electrons in the pockets are unpaired and spin polarized along the direction of the field. The dashed lines indicate the extent of the smearing of the Fermi surface by the superconducting order at zero field, and show that the lateral extrema of the "normal" pockets are bracketed by regions of paired electrons.

$$\Delta_{0}(T,B) = \Delta_{00} \left[1 - \left(\frac{k_{B}T}{\Delta_{00}}\right)^{3} F_{\Delta} \left(\frac{\mu B}{k_{B}T}\right) + O(\Delta_{00}^{-4}) \right], \quad (6)$$

where

$$F_{\Delta}(x) = \int_0^\infty t^2 \left[1 - \left(\tanh \frac{t+x}{2} + \tanh \frac{t-x}{2} \right) \middle/ 2 \right] dt.$$

Noting that $F_{\Delta}(0) \approx 3.61$ recovers the zero field answer, while for $x \ge 1$ $F_{\Delta}(x) \sim |x|^3/3$ whence,

$$\Delta_0(T=0,B) = \Delta_{00} \left[1 - \frac{1}{3} \left(\frac{\mu |B|}{\Delta_{00}} \right)^3 + O(B^4) \right].$$
(7)

Consequently, the reduction of the gap function at low fields and temperatures is quite modest, and the most important effect of the proliferation of quasiparticles in the ground state is the *finite* density of states (DOS) at the Fermi level, which qualitatively alters the low-energy physics of the system.¹¹ We now turn to the consequences for some physical quantities in this regime, where we may neglect the reduction of Δ_0 at leading order.

Specific heat. This takes the scaling form

$$C(T,B) = 2k_B N(0) \frac{(k_B T)^2}{\Delta_{00}} F_C \left(\frac{\mu B}{k_B T}\right), \qquad (8)$$

where

$$F_C(x) = \sum_{\sigma=\pm 1} \int_0^\infty t(t+\sigma x)^2 e^{t+\sigma x}/(e^{t+\sigma x}+1)^2 dt.$$

For fields in excess of the temperature, $x \ge 1$, $F_C(x) \sim (\pi^2/3) x$ whence $C = (2\pi^2/3) k_B^2 T N(0) \mu B / \Delta_{00}$ $= C_N \mu B / \Delta_{00}$, where C_N is the normal state specific heat; the linear *T* dependence at low *T* is a consequence of the finite DOS. For $\mu B \ll k_B T$, we recover the expected T^2 dependence upon using $F_C(0) = 9\zeta(3) \approx 10.8$.

Thermal conductivity. At low temperatures where impurity scattering may lead to a constant quasiparticle scattering rate,¹² the thermal conductivity κ_e should be proportional to *C*. Therefore κ_e should increase *linearly* with *T*, for $k_B T \ll \mu B$, while it increases with *T* quadratically in the absence of the field, as observed experimentally.¹³ This is to be contrasted with the recent experimental finding¹³ that a magnetic field applied *perpendicular* to the Cu-O plane of the cuprate superconductor *suppresses* the electronic thermal conductivity, presumably due to orbital effects.

Magnetization. *M* also takes a scaling form:

$$M(T,B) = 2\,\mu N(0) \,\frac{(k_B T)^2}{\Delta_{00}} F_M\!\left(\frac{\mu B}{k_B T}\right),\tag{9}$$

where

$$F_M(x) = \int_0^\infty t \left(\frac{1}{e^{t-x}+1} - \frac{1}{e^{t+x}+1} \right) dt.$$

The limits $F_M(x \ge 1) \sim x^2/2$, and $F_M(x \le 1) \sim (2 \ln 2)x$, imply $M \propto B^2$ when $\mu B \gg k_B T$, and $M \propto B$ when $\mu B \ll k_B T$.

Tunneling conductance. The T=0 tunneling conductance of a superconductor-insulator-metal junction at varying bias G(V) is, in principle, the most direct measurement of the single particle DOS of the superconductor. G goes to zero linearly with V for a $d_{x^2-y^2}$ superconductor in zero field. For $\mu B \gg k_B T$, the finite DOS leads to a finite conductance: $G(V=0) = G_n \mu B / \Delta_{00}$, where G_n is the tunneling conductance when the superconductor is in its normal state.¹⁴

Phase diagram. We now turn to the effects of strong magnetic fields. An *s*-wave superconductor undergoes a first order phase transition to the normal state when $\mu B = \Delta/\sqrt{2}$ (Δ is the *s*-wave gap) at T=0,¹ ignoring the finite momentum pairing instability (see below). This follows upon noting that the singlet *s*-wave state is insensitive to the Zeeman field, while the normal state lowers its energy in proportion to its Pauli susceptibility. The temperature-magnetic field phase diagram² exhibits a tricritical point where the first order line terminates, and the field tuned transition becomes continuous.

The $d_{x^2-y^2}$ superconductor *does* respond to the Zeeman field but far more weakly than the normal state. This leads to a phase diagram (Fig. 2) of the same topology as in the *s*-wave case. We find that at T=0 there is a first order transition to the normal state at $\mu B = 0.56\Delta_{00}$ (close to the value $0.5\Delta_{00}$ obtained without accounting for the paramagnetism of the $d_{x^2-y^2}$ state); at the transition the gap function has amplitude $0.92\Delta_{00}$. For $T < 0.56T_c$, the transition remains first order, and the normal (superconducting) state becomes local minimum of free energy at lower (higher) temperature, as represented by the dotted lines in Fig. 2; above $T=0.56T_c$ the transition becomes continuous.

Thus far we have only considered zero momentum pairing. At high fields one may suspect that it might be more favorable to try to pair across the spin-split Fermi surface of the partially polarized normal state; indeed it is known in the *s*-wave case^{3,4,10} that this happens at low temperatures. The pairing is then at a *finite* center of mass momentum for the Cooper pairs and the resulting transition from the high field normal state is continuous. At lower fields this Fulde-Ferrell-



Larkin-Ovchinnikov (FFLO) state gives way to the zero momentum pairing state by a first order transition.

In order to consider this possibility for the $d_{x^2-y^2}$ problem, we extend the pairing potential in Eq. (1) to allow pairing between electrons with total momentum **q**, for $q \ll \epsilon_c / v_F$, where v_F is the Fermi velocity:

$$\hat{V} = \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V_{\mathbf{k},\mathbf{k}'} c^{\dagger}_{\mathbf{k},\uparrow} c^{\dagger}_{-\mathbf{k}+\mathbf{q},\downarrow} c_{-\mathbf{k}'+\mathbf{q},\downarrow} c_{\mathbf{k}',\uparrow} .$$
(10)

As we will see later, the pairing momentum q is at most of order Δ_{00}/v_F , which is much less than ϵ_c/v_F . Therefore it is a reasonable approximation to neglect the dependence of the pairing matrix element $V_{\mathbf{k},\mathbf{k}'}$ on \mathbf{q} . The gap still takes the $d_{x^2-y^2}$ form and obeys

$$1 = \frac{N(0)V_0}{2\pi} \int_0^{2\pi} d\theta \int_0^{\epsilon_c} d\xi \frac{\cos^2(2\theta)}{E(\xi,\theta)} \times \left[\tanh\left(\frac{E(\xi,\theta) + z(\theta)}{2k_BT}\right) + \tanh\left(\frac{E(\xi,\theta) - z(\theta)}{2k_BT}\right) \right],$$
(11)

where $z(\theta) = \mu B + (v_F q/2)\cos(\theta - \theta_q)$, and θ_q is the polar angle of the pairing momentum **q**. In order to determine the (second order) phase boundary between the normal and FFLO states, one needs to find the solution of Eq. (11) with



 $\Delta = 0$ and the largest possible B. At T = 0, we find the initial pairing instability occurs at $q = 2\mu B/v_F$, $\theta_q = 0, \pi$ or $\pm \pi/2$ (i.e., for **q** along directions of *maximum* gap), and $\mu B \approx 1.06 \Delta_{00}$. At lower fields the system undergoes a first order transition to the q=0 state. As the condensation energy of the FFLO state is quite small (the state is gapless over much of the Fermi surface), an excellent estimate for this field is simply the value obtained earlier for the level crossing between the normal state and the q=0 state, which leads to the window $0.56\Delta_{00} \leq \mu B \leq 1.06\Delta_{00}$ for the stability of the FFLO state, which is considerably larger than the window $\Delta/\sqrt{2} \leq \mu B \leq \Delta$ for the 2D *s*-wave case.¹⁰ At finite temperatures, we find for $T/T_c < 0.06$, the direction of pairing momentum **q** remains the same as that of T=0; however, at $T/T_c > 0.06$ this changes discontinuously to $\theta_{q} = \pm \pi/4$ or $\pm 3\pi/4$, i.e., **q** now points in the directions of *minimum* gap. At finite T we again use the crossing point of the free energies of the normal and q=0 pairing states to estimate the boundary between the zero and finite momentum pairing states (Fig. 2), this window narrows and the magnitude of the pairing wave vector for the high field instability decreases and approaches zero at $T=0.56T_c$, where the high field phase boundary and the coexistence line between the q=0state and the normal state come together. In the FFLO phase, there is presumably a first order phase boundary across which the direction of the pairing momentum changes, which ends at the phase boundary separating the normal and FFLO states at $T/T_c \approx 0.06$. In the present work we have not attempted to study this phase boundary. For $T > 0.56T_c$, there is no region with $q \neq 0$ pairing and there is a continuous transition directly from the normal state to the q=0 state. This topology is also identical with that in the s-wave problem. We note that our results on the phase boundary separating the normal state and FFLO state agree with a previous study by Maki and Won,¹⁵ which are also confirmed in more recent work (Ref. 16); however in these works no estimate was given for the phase boundary separating the FFLO state and the usual zero momentum pairing BCS state.

Application to the cuprates. Our analysis has been purely two dimensional, and for such systems a magnetic field parallel to the plane would behave precisely as a Zeeman field. For layered systems the situation, analyzed in some detail by Klemm *et al.*,¹⁷ is more complicated for orbital effects become important near T_c where the interplanar coherence length is large. However, in the same approximation, there exists a lower temperature T^* , where the vortex cores fit between planes and the orbital H_{c2} diverges. Below T^* (estimated as $0.84T_c$ and $0.99T_c$ for YBCO and BSCCO, respectively18), assuming two dimensionality should be an excellent approximation and hence the Zeeman response should dominate. Another limitation of our analysis is the neglect of scalar impurity scattering which destroys the FFLO state in dirty superconductors, and of spin-orbit scattering which attenuates the pair-breaking effect of the Zeeman field. On these fronts, the news seems to be good: the state of the art YBCO and BSCCO samples are in the clean limit, and their residual resistivities translate into scattering times of order $\tau \sim 10^{-12}$ s, which lead via the Elliott estimate,¹⁹ to a spin-orbit scattering time $\tau_{\rm SO} \sim \tau/(\Delta g)^2$ $\sim 10^{-10}$ s $(\Delta g = g - 2 \approx 0.1).$ Consequently, $\tau_{\rm SO} > \hbar/(g\mu_B B)$ for fields above a Tesla and the neglect of spin-orbit scattering should not be too serious. A final caveat is the conventional BCS weak-coupling nature of our analysis, which is evidently problematic in the cuprates; because of the absence of a solution of the larger problems in the field, we are unable to say very much more on the issue.

Nevertheless, the qualitative physics uncovered by our model calculation, should be quite robust to any mechanism that yields a $d_{x^2-y^2}$ state in a single layer.²⁰ Experimentally, the low field effects discussed here should be readily observable, e.g., we estimate an enhanced specific heat of magnitude 0.1HT mJ/mol $-K^2$ ($k_BT < \mu B$) from the existing data on YBCO,²¹ while the high field phase transitions and the FFLO phase would appear only at fields of order 100 T, which are currently out of reach. Finally, while we have concentrated entirely on the parallel geometry, it is clear that a full account of the response at arbitrary orientations of the magnetic field will need to take account of the Zeeman physics discussed here.

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