IOPscience iopscience.iop.org

Home Search Collections Journals About Contact us My IOPscience

Broken symmetry in an unconventional superconductor: a model for the double transition in UPt_3

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1989 J. Phys.: Condens. Matter 1 8135

(http://iopscience.iop.org/0953-8984/1/43/014)

View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 171.66.16.96
The article was downloaded on 10/05/2010 at 20:42

Please note that terms and conditions apply.

J. Phys.: Condens. Matter **1** (1989) 8135–8145. Printed in the UK

Broken symmetry in an unconventional superconductor: a model for the double transition in UPt_3

D W Hess, T A Tokuyasu and J A Sauls
Department of Physics and Astronomy, Northwestern University, 2145 Sheridan Road, Evanston, Illinois 60208, USA

Received 15 March 1989, in final form 23 June 1989

Abstract. We present a model for the superconducting states of UPt_3 in which a two-dimensional order parameter couples to a field that breaks the hexagonal symmetry of the crystal. This symmetry-breaking field (SBF) splits the superconducting transition, leading to two superconducting phases in zero field. The high-temperature superconducting phase exhibits the broken hexagonal symmetry of the SBF, while the low-temperature phase spontaneously breaks time-reversal symmetry. We calculate the specific heat jumps at both transitions and compare with the recent measurements by Fisher *et al.* We find that sizeable strong-coupling corrections are needed to explain the magnitudes of the heat capacity jumps and the splitting of the transition. We show that a *kink* in the upper critical field occurs for fields in the basal plane. Comparison of the discontinuity in the slope of $H_{c2}(T)$ with the data of Taillefer *et al* (on a different UPt_3 crystal) is in qualitative agreement with the heat capacity data. We also predict a change in slope of $H_{c1}(T)$ at the temperature of the second peak in the heat capacity, for all field orientations. Observation of all three features in the same single crystal would provide convincing evidence for unconventional pairing in UPt_3 and would be a stringent test of the model presented here.

Recent specific heat measurements [1] show that the broad transition to the superconducting state in UPt_3 at $T_c \simeq 0.5$ K is actually two transitions separated by $\Delta T_c \simeq$ 60 mK. The authors argue that the splitting of the transition is an *intrinsic* property of UPt_3. In this article we present a Ginzburg–Landau (GL) theory of the superconducting states of UPt_3 based on the coupling of an *unconventional* order parameter to a small symmetry-breaking field (SBF) which lowers the symmetry of the normal metallic state.

It is known that the order parameter for systems exhibiting broken symmetry can be sensitive to weak perturbations that reduce the symmetry of the *normal* state. Superfluid ^{3}He is a good example. The dipolar interaction between ^{3}He nuclei is small, of order 10^{-7} K, compared with the superfluid transition temperature $T_c \simeq 10^{-3}$ K. Thus for most purposes the dipole energy can be neglected and the normal state of liquid ^{3}He can be considered to be separately invariant under rotations in either spin or coordinate space. The 3D Balian–Werthamer (BW) state—identified with the B phase of superfluid ^{3}He—is the ground state in weak-coupling BCS theory for an isotropic Fermi liquid with p-wave pairing and separate spin and orbital rotational symmetry of the normal phase. The weak dipole–dipole interaction in ^{3}He breaks *relative* spin and orbit rotational symmetry, and gives rise to the longitudinal NMR frequency in the B phase. What is less well known is that the dipolar interaction also gives rise to a splitting of the phase transition. The initial transition to the superfluid state corresponds to condensation into the 2D *planar* phase [2, 3]. At a slightly lower temperature a second transition takes place to a 3D superfluid state. Well below the second transition the order parameter is essentially that of the 3D BW state, albeit without the continuous degeneracy associated with relative rotations of the spin and orbital components of the order parameter. This splitting of the transition has not yet been observed in ^{3}He simply because the magnitude of the splitting is very small, $\Delta T_c \sim 0.1\ \mu$K [3]; however, there is little doubt that the splitting occurs.

An analogous effect explains the splitting of the phase transition in UPt_3; (i) a small symmetry-breaking term in the normal-state Hamiltonian leads to a small splitting of the superfluid transition for unconventional pairing, (ii) the dimensionality of the order parameter is lower at the first transition compared to the order parameter at the second transition, and (iii) the order parameter well below the second transition is essentially that of the unperturbed superfluid, except that the continuous rotational degeneracy that is present in the absence of the perturbation is eliminated. We also predict the existence of anomalies in the temperature dependence of the upper and lower critical field of UPt_3 which are a test of this theory.

UPt_3 is a hexagonal crystal with inversion symmetry; thus the full symmetry group of the normal state is $G = U(1) \times T \times D_{6h}$($U(1)$ is the gauge group, T is time-reversal, and D_{6h} is the point group). The transition to a conventional superconducting state breaks *only* gauge symmetry. An unconventional superconducting state breaks additional symmetries and is described by an order parameter that transforms according to a non-trivial irreducible representation of G. Any perturbation that reduces the dimensionality of the representation corresponding to the highest transition temperature can have an important effect on the superconducting transition.

We introduce a SBF which couples to the superconducting order parameter belonging to a nontrivial representation of the hexagonal symmetry group. Our results depend on symmetry arguments and general features of mean-field theory for a second-order phase transition and are not particularly sensitive to the origin of the SBF; however, two possibilities are obvious. Ozaki [4], Sigrist, Joynt and Rice [5] and Volovik [6] consider the coupling of the superconducting order parameter to lattice distortions. The latter authors show that the coupling to a lattice distortion can lead to a transition from one superconducting state to another in crystals with cubic, tetragonal or hexagonal symmetry, and calculate the specific heat jumps for the transitions. Secondly, recent neutron scattering measurements [7] indicate that UPt_3 has weak antiferromagnetic (AFM) order in the *ab* plane. The AFM order parameter (the SBF in this case) breaks the hexagonal symmetry and, if the pairing interaction is mediated by AFM spin fluctuations, leads to a different pairing interaction for the two different basis functions that span the 2D E_1 representation. (Joynt [8] mentions this possibility for UPt_3.) More precisely if the most attractive channel for pairing is the even-parity E_{1g} representation, the pairing interaction in the absence of the AFM order is of the form

$$V_{E_1}(\boldsymbol{k}_F, \boldsymbol{k}'_F) = V_{E_1}[\vartheta(\boldsymbol{k}_F)\vartheta(\boldsymbol{k}'_F) + \xi(\boldsymbol{k}_F)\xi(\boldsymbol{k}'_F)] \tag{1}$$

the effect of the SBF is then to lift the degeneracy of the two basis functions, thus lowering the symmetry from D_6 to D_2,

$$\begin{aligned} V(\boldsymbol{k}_F, \boldsymbol{k}'_F) &= V_\vartheta \vartheta(\boldsymbol{k}_F)\vartheta(\boldsymbol{k}'_F) + V_\xi \xi(\boldsymbol{k}_F)\xi(\boldsymbol{k}'_F) \\ &= V_{E_1}(\boldsymbol{k}_F, \boldsymbol{k}'_F) + V_\varepsilon[\vartheta(\boldsymbol{k}_F)\vartheta(\boldsymbol{k}'_F) - \xi(\boldsymbol{k}_F)\xi(\boldsymbol{k}'_F)] \end{aligned} \tag{2}$$

with $2V_\varepsilon = (V_\vartheta - V_\xi) \ll V_{E_1}$.†

We show that the coupling of a SBF to the order parameter in crystals with hexagonal symmetry has further experimentally verifiable consequences‡. The axial symmetry of $H_{c2}(T)$ in the basal plane is broken and a *kink* appears in $H_{c2}(T)$ at a temperature T_H, which depends on the strength of the SBF coupling and the stiffness coefficients appearing in the GL free energy. The splitting of the phase transition induced by the SBF leads to a strongly anisotropic superfluid density tensor in the *ab* plane, as well as a change in slope of the *lower critical field* $H_{c1}(T)$ at T_{c^*}, the temperature corresponding to the second specific-heat jump.

In addition to the splitting of the transition in zero field, a peak is observed in the ultrasound attenuation [13–15] as a function of field, suggesting that a phase transition takes place between superconducting states of different symmetry [16]. These observations are strong evidence that the superconducting states of UPt_3 are described by an unconventional order parameter. Group theoretical analysis [17] shows that the multidimensional order parameters in a hexagonal crystal contain two complex amplitudes which transform either like the E_1 or the E_2 representation§. Putikka and Joynt [9] proposed a spin-fluctuation model for the pairing interaction and argue that the order parameter of UPt_3 belongs to the E_{1g} representation. Norman [19] considers a similar model but concludes that the order parameter belongs to the 1D A_{1g} (even parity) or the 2D E_{1u} (odd parity) representation. We assume that the order parameter belongs to one of the E_1 representations. The gap function for the 2D states may then be written in terms of E_1 basis functions (see table 1 of [9]),

$$\Delta(\boldsymbol{k}_F) = i\sigma_y[\eta_x \vartheta(\boldsymbol{k}_F) + \eta_y \xi(\boldsymbol{k}_F)] \tag{3}$$

for an even-parity state, and

$$\Delta(\boldsymbol{k}_F) = i\sigma_y \boldsymbol{\sigma} \cdot [\eta_x \boldsymbol{\vartheta}(\boldsymbol{k}_F) + \eta_y \boldsymbol{\xi}(\boldsymbol{k}_F)] \tag{4}$$

for an odd-parity state in the limit of strong spin–orbit coupling. In either case the gap function is then parametrised by the two-component order parameter $\boldsymbol{\eta} = (\eta_x, \eta_y)$, which transforms as a vector in the *ab* plane (with complex components) under the operations of the hexagonal point group. The invariance of the free-energy functional under the rotation group D_{6h} requires that the homogeneous Ginzburg–Landau (GL) free-energy functional is of the form [17],

$$\Delta\Omega[\boldsymbol{\eta}] = \int d^3r\{\alpha(T)|\boldsymbol{\eta}|^2 + \beta_1|\boldsymbol{\eta}|^4 + \beta_2|\boldsymbol{\eta}\cdot\boldsymbol{\eta}|^2\} \tag{5}$$

where $\alpha = \alpha_0(T - T_{c0})$, $\alpha_0 > 0$, and T_{c0} is the transition temperature‖. Stability requires

† Of course the general form of the pairing interaction is an expansion in the full set of basis functions of the irreducible representations (see for example [9–11] where analogous expansions for cubic symmetry are introduced) of D_6,

$$V(\boldsymbol{k}_F, \boldsymbol{k}'_F) = \sum_{\mu}^{\text{irrep}} V_\mu \varphi_\mu(\boldsymbol{k}_F)\varphi_\mu(\boldsymbol{k}'_F).$$

Representations other than E_{1g} (in the absence of the SBF) are unimportant in the GL region (see for example [12] for a discussion of this point for p- and f-wave representations in an isotropic system). The exception is if two representations are nearly degenerate. In the absence of a weakly broken symmetry, and an associated small energy scale, there is no compelling reason to assume that two or more representations are nearly degenerate.

‡ Most of the results we obtain are also valid for tetragonal superconductors with an order parameter belonging to the 2D E_1 representation.

§ This assertion does not include the possibility of accidental degeneracy of order parameters belonging to different 1D representations. Such a case is discussed by Wölfle and Kumar [18].

‖ For a tetragonal crystal an additional invariant exists, namely $\beta_3(|\eta_x|^4 + |\eta_y|^4)$. For $\beta_2 > 0$ and $\beta_3 > -2+\beta_2$, the analysis presented below is the same provided one makes the replacement $\beta_1 \to \beta_1 + \frac{1}{2}\beta_3$ and $\beta_2 \to \beta_2 + \frac{1}{2}\beta_3$.

that $\beta_1 > 0$ and $\beta_1 + \beta_2 > 0$, thus the stable homogeneous equilibrium phase is determined by the sign of β_2. If $\beta_2 > 0$ the states $\boldsymbol{\eta} \sim (1, \pm i)$, which break time-reversal symmetry, are stable [17, 9]. These are the equilibrium phases in weak-coupling BCS theory for the E_1 representation, where $\beta_2 = \beta_1/2$, independent of the shape of the Fermi surface or form of basis functions [16]. However, if $\beta_2 < 0$ then an 'oriented' phase $\boldsymbol{\eta} \sim (0, 1)$ or $\boldsymbol{\eta} \sim (1, 0)$ is stable†.

The leading-order coupling of the superconducting order parameter to a SBF is given in terms of a symmetric tensor ε_{ij}. The coupling energy density has the form

$$\Delta\omega_{\mathrm{sbf}} = \boldsymbol{\eta}^* \cdot \underline{\underline{\boldsymbol{\varepsilon}}} \cdot \boldsymbol{\eta} \tag{6}$$

which is both gauge invariant and time-reversal invariant, but breaks rotational symmetry in the ab plane for fixed $\underline{\underline{\boldsymbol{\varepsilon}}}$‡. The tensor $\underline{\underline{\boldsymbol{\varepsilon}}}$ may be assumed traceless, since the trace of $\underline{\underline{\boldsymbol{\varepsilon}}}$ may be absorbed into the definition of T_c. Without loss of generality we can choose the tensor to be

$$\underline{\underline{\boldsymbol{\varepsilon}}} = \begin{pmatrix} \varepsilon & 0 \\ 0 & -\varepsilon \end{pmatrix}. \tag{7}$$

All other traceless, symmetric tensors correspond to a rotation in the ab plane with no change in the resulting thermodynamics of the phase transition. This coupling describes either a strain-field coupling to the order parameter or a direct coupling of the order parameter to the AFM staggered magnetisation, $\boldsymbol{N}$, of the form

$$\Delta\omega_{\mathrm{sbf}} \sim (\boldsymbol{\eta} \cdot \boldsymbol{N})(\boldsymbol{\eta} \cdot \boldsymbol{N})^*. \tag{8}$$

Symmetry-breaking fields which explicitly break time-reversal symmetry are also possible. For example, spin–exchange coupling of the triplet order parameter for the E_{1u} representation to an external magnetic field $\boldsymbol{H}$ or the spontaneous magnetisation, $\boldsymbol{M}$, is described by a contribution of the form

$$\Delta\omega_{\mathrm{sbf}} \sim \mathrm{Im}(\boldsymbol{\eta} \times \boldsymbol{\eta}^*) \cdot \boldsymbol{M}. \tag{9}$$

A term of this form gives rise to the A_1 phase of Cooper pairs with $S_z = -1$ in superfluid ^{3}He. However, we do not consider such a coupling here because the AFM order in UPt_3 is in the ab plane, in which case this coupling vanishes identically, and the effect of an external magnetic field $\boldsymbol{H}$ through such a coupling is dominated by the diamagnetic coupling of $\boldsymbol{\eta}$ to the field.

The symmetry-breaking term in (6) is combined with (5) to give

$$\Delta\Omega = \int \mathrm{d}^3r \{\alpha_+|\eta_y|^2 + \alpha_-|\eta_x|^2 + \beta_1|\boldsymbol{\eta}|^4 + \beta_2|\boldsymbol{\eta}\cdot\boldsymbol{\eta}|^2\} \tag{10}$$

where $\alpha_\pm = \alpha_0(T - T_{c\pm})$, $T_{c\pm} = T_{c0} \pm \varepsilon/\alpha_0$. We further assume that the coupling to the SBF is weak, $T_{c0} \gg \varepsilon/\alpha_0$. Immediately below T_{c+}, $\alpha_+ < 0$ and $\alpha_- > 0$ implying that the (0, 1) phase nucleates. At T_{c-} the sign of α_- changes, indicating that a second transition is possible. Below the temperature $T_{c^*} < T_{c+}$, a phase with finite η_x is stable, and for $T < T_{c^*}$ the order parameter continuously evolves toward one of the states $(1, \pm i)$. Note that time-reversal symmetry is again spontaneously broken, as in the solutions for $\varepsilon = 0$, but in this case only at the second transition T_{c^*}. Again there is a doubly degenerate

† The apparent degeneracy of these states is lifted in sixth order.

‡ Of course if $\boldsymbol{\eta}$ and ε_{ij} are simultaneously rotated the free energy must be invariant.

pair of order parameters. The second transition is the result of competition between the free energy of the SBF and the rotationally invariant quartic terms in the free energy; a finite value of η_x, with a relative phase $\pm i$ with respect to the η_y, diminishes the contribution from the term in the free energy with coefficient β_2 (positive). Clearly if $\beta_2 < 0$, then there is no advantage to a finite η_x component and (0, 1) is stable for all $T < T_{c+}$ in the GL regime.

The order parameter may be written in the form $(Ae^{i\zeta}, B)$, where ζ is the relative phase between the real amplitudes A and B. The free-energy density becomes

$$\Delta\Omega/V = \alpha_- A^2 + \alpha_+ B^2 + (\beta_1 + \beta_2)(A^2 + B^2)^2 - 4\beta_2 A^2 B^2 \sin^2(\zeta) \tag{11}$$

which for $\beta_2 > 0$ favours a relative phase of $\zeta = \pm\pi/2$. Furthermore, for $\alpha_+ < 0$ $(T < T_{c+})$ and $\alpha_- > 0$ $(T > T_{c-})$ the free energy is minimised by an order parameter with $A = 0$,

$$\boldsymbol{\eta} = \left(\frac{-\alpha_+(T)}{2(\beta_1 + \beta_2)}\right)^{1/2} (0, 1). \tag{12}$$

The heat-capacity jump at the transition T_{c+} is given by

$$\Delta C_+ = T_{c+} \frac{\alpha_0^2}{2(\beta_1 + \beta_2)}. \tag{13}$$

For $\alpha_- < 0$ the minimum-energy solution to the GL equations does not require $A = 0$. The instability of a second superconducting state is evident if we examine the coefficient of the quadratic term in A for $T < T_{c+}$,

$$\Delta\Omega/V = \tfrac{1}{2}\alpha_+ B^2 + [\alpha_-(T) + 2(\beta_1 - \beta_2)B^2(T)]\, A^2(T) + O(A^4). \tag{14}$$

With $B(T)$ given by (12) the instability to an ordered phase with finite $A(T)$ is determined by

$$\alpha_-(T_{c^*}) + 2(\beta_1 - \beta_2)B^2(T_{c^*}) = 0 \tag{15}$$

which gives the transition temperature

$$T_{c^*} = T_{c0}\left[1 - \frac{\beta_1}{\beta_2}\left(\frac{\varepsilon}{\alpha_0 T_{c0}}\right)\right]. \tag{16}$$

Note that the presence of the condensate with $B \neq 0$ suppresses (enhances) the transition temperature to the ordered state with broken time-reversal symmetry for $\beta_1/\beta_2 > 1$ $(\beta_1/\beta_2 < 1)$. The ratio of the two *physical* transition temperatures is then given in terms of two dimensionless ratios of the parameters of the GL functional,

$$\frac{T_{c^*}}{T_{c+}} = \left[1 - \frac{\beta_1}{\beta_2}\left(\frac{\varepsilon}{\alpha_0 T_{c0}}\right)\right]\left[1 + \left(\frac{\varepsilon}{\alpha_0 T_{c0}}\right)\right]^{-1} \simeq \left[1 - \left(1 + \frac{\beta_1}{\beta_2}\right)\left(\frac{\varepsilon}{\alpha_0 T_{c0}}\right)\right]. \tag{17}$$

The order parameter is easily calculated by minimising the GL functional with respect to both A and B,

$$A^2 = -\left\{\frac{\alpha_+ + \alpha_-}{8\beta_1} - \frac{\alpha_+ - \alpha_-}{8\beta_2}\right\} \qquad B^2 = -\left\{\frac{\alpha_+ + \alpha_-}{8\beta_1} + \frac{\alpha_+ - \alpha_-}{8\beta_2}\right\} \tag{18}$$

for $T < T_{c^*}$. The transition at T_{c^*} is second order; $A(T)$ vanishes continuously at T_{c^*},

$B(T)$ is continuous, but the slope of $B(T)$ is discontinuous at T_{c^*}. The discontinuity in the heat capacity—relative to the heat capacity in the normal state—is

$$\Delta C_* = T_{c^*}\, \alpha_0^2/2\beta_1 \tag{19}$$

thus, the ratio of the heat capacity jumps at the upper and lower transition is

$$\Delta C_*/\Delta C_+ = (T_{c^*}/T_{c+})(1 + \beta_2/\beta_1). \tag{20}$$

The measurements of [1], which show a splitting of the heat capacity in two single crystals of UPt_3, allow us to estimate the ratio β_2/β_1. From figure 1 of [1] we obtain $\beta_2/\beta_1 = 0.18$ for sample 1 and $\beta_2/\beta_1 = 0.12$ for sample 2. These values should be compared with the weak-coupling prediction of $\beta_2/\beta_1 = 0.5$, indicating sizeable strong-coupling corrections to the weak-coupling free energy†. Note, however, that unlike the case of liquid ^{3}He in which the strong-coupling corrections can stabilise a different superfluid phase than that predicted by the weak-coupling theory, the strong-coupling corrections inferred here do not imply an instability of the states with broken time-reversal symmetry. In fact it is important for the consistency of this theory that measurements imply $\beta_2/\beta_1 > 0$. The two transition temperatures, combined with the value of β_2/β_1, also determine the coupling to the SBF, $\varepsilon/\alpha_0 \simeq 9.1$ mK for sample 1 and $\varepsilon/\alpha_0 \simeq 6.5$ mK for sample 2.

The existence of a transition to a second superconducting state in zero field has observable consequences for the mixed state of UPt_3. In an applied magnetic field the order parameter is no longer uniform, so the free-energy analysis must include the contributions from gradients of the order parameter,

$$\Delta\Omega_{\text{grad}} = \int dx^3\{\kappa_i(D_i\eta_j)(D_i\eta_j)^* + \kappa_2(D_i\eta_i)(D_j + \eta_j)^* + \kappa_3(D_i\eta_j) \times (D_j\eta_i)^* + \kappa_4(D_z\eta_i)(D_z\eta_i)^*\} \tag{21}$$

where $D_i = \partial_i - i2eA_i/c$ and A is the vector potential‡. The transition into the mixed state at the upper critical field, H_{c2}, is determined by the linearised GL equations

$$\{\kappa_{123}D_x^2 + \kappa_1 D_y^2 + \kappa_4 D_z^2\}\eta_x + \{\kappa_2 D_x D_y + \kappa_3 D_y D_x\}\eta_y = \alpha_-\eta_x \tag{22}$$

$$\{\kappa_1 D_x^2 + \kappa_{123} D_y^2 + \kappa_4 D_z^2\}\eta_y + \{\kappa_3 D_x D_y + \kappa_2 D_y D_x\}\eta_x = \alpha_+\eta_y. \tag{23}$$

If the magnetic field is applied in the xy plane, we can choose a gauge in which A is in the $\hat{z}$ direction and the GL equations for the components of $\boldsymbol{\eta}$ which are parallel and perpendicular to $\boldsymbol{H}$ decouple and become Schrödinger-like equations for harmonic

† The strong-coupling corrections to the weak-coupling parameters are of order $\delta\beta_i = (\beta_i)_{\omega c}(T_c/E_n)|T_{qp}|^2$, where (T_c/E_n) is the ratio of the superconducting energy scale to the characteristic energy scale in the normal Fermi liquid, and $|T_{qp}|^2$ is the dimensionless scattering amplitude for normal-state quasiparticles, which is of order 1 or larger. Assuming $E_n \sim 5$ K, corresponding to the 'coherence temperature' in UPt_3, we expect sizeable strong-coupling corrections.

‡ In the case of tetragonal symmetry, there is an independent additional invariant, namely $\kappa_5(|D_x\eta_x|^2 + |D_y\eta_y|^2)$. The broken symmetry and kink features in the upper and lower critical field discussed below appear in the tetragonal case as well. The relevant expressions in this case may be obtained by the replacement $\kappa_{123} \rightarrow \kappa_{123} + \kappa_5$.

oscillators. The ground states of these harmonic oscillator equations determine H_{c2}. For fields $\boldsymbol{H}\|\hat{y}$ the upper critical field is determined by the maximum of

$$H_{c2} = \frac{\varphi_0}{2\pi}\begin{cases} \dfrac{-\alpha_+}{\sqrt{\kappa_{123}\kappa_4}} & \boldsymbol{\eta}\|\hat{y} \\ \dfrac{-\alpha_-}{\sqrt{\kappa_1\kappa_4}} & \boldsymbol{\eta}\|\hat{x} \end{cases} \tag{24}$$

while for $\boldsymbol{H}\|\hat{x}$

$$H_{c2} = \frac{\varphi_0}{2\pi}\begin{cases} \dfrac{-\alpha_+}{\sqrt{\kappa_1\kappa_4}} & \boldsymbol{\eta}\|\hat{y} \\ \dfrac{-\alpha_-}{\sqrt{\kappa_{123}\kappa_4}} & \boldsymbol{\eta}\|\hat{x}. \end{cases} \tag{25}$$

In the absence of any SBF, $\alpha_+ = \alpha_-$, and the order parameter *orients* with respect to the field so that the larger of the upper fields in (24) and (25) is always obtained; thus H_{c2} is isotropic near T_c [20]. The orientation of the order parameter is fixed by the SBF for T sufficiently close to T_{c+} (i.e. along the direction $\hat{y}$), in which case H_{c2} is given by the solutions with $\boldsymbol{\eta}\|\hat{y}$ in (24) and (25). The upper critical field varies from the solution $\boldsymbol{H}\|\hat{x}$ to that for $\boldsymbol{H}\|\hat{y}$ with the rotation of $\boldsymbol{H}$ in the ab plane, and is therefore *anisotropic*. At a lower temperature, a second transition occurs in a finite field for $\boldsymbol{H}\|\hat{y}$ ($\boldsymbol{H}\|\hat{x}$) and $\kappa_{23} > 0$ ($\kappa_{23} < 0$). If $\kappa_{23} < 0$ and $\boldsymbol{H}\|\hat{x}$ then the solution for T close to T_{c+} is $\boldsymbol{\eta}\|\hat{y}$ with the corresponding value of H_{c2} in (25). However, below a temperature $T_H < T_{c+}$ the solution is $\boldsymbol{\eta}\|\hat{x}$ with a corresponding change in H_{c2} from (25). Thus, the order parameter changes from $\boldsymbol{\eta}\|\hat{y}$ to $\boldsymbol{\eta}\|\hat{x}$ producing the kink in $H_{c2}(T)$ shown in figure 1. (Klemm *et al* [21] have previously predicted a kink in the upper critical field for the case of isotropic p-wave pairing with a uniaxial perturbation added to the pairing interaction.) The temperature of the transition from the (1, 0) phase to the (0, 1) phase along the H_{c2} curve is

$$T_H = (T_c - \sqrt{\kappa_1} - T_{c+}\sqrt{\kappa_{123}})/(\sqrt{\kappa_1} - \sqrt{\kappa_{123}}). \tag{26}$$

This behaviour contrasts with that for $\boldsymbol{H}\|\hat{y}$ where the solution with the lowest free energy is $\boldsymbol{\eta}\|\hat{y}$ and $H_{c2} = -\alpha_+/\sqrt{\kappa_{123}\kappa_4}$ for all $T < T_{c+}$; in this case no kink appears in $H_{c2}(T)$ (see figure 1). Note that a kink in $H_{c2}(T)$ will also occur if $\kappa_{23} > 0$; in this case the maximum discontinuity in the slope of $H_{c2}(T)$ occurs when the field is oriented along $\hat{y}$.

Taillefer *et al* [22] have recently observed a kink in $H_{c2}(T)$ for a field in the *ab* plane. From the slopes of $H_{c2}(T)$ above and below the transition point T_H we obtain two possible estimates of the stiffness coefficient, $\kappa_{23}/\kappa_1 = -0.62(1.6)$. The upper critical field data of Shivaram *et al* [23] also shows a kink and gives similar values for the stiffness coefficients. Moreover, from (26), we obtain an independent estimate that the SBF coupling $\varepsilon/\alpha_0 = 18$ mK, which is somewhat larger than those obtained from the analysis of the specific heat measurements (on different UPt_3 crystals) in zero field.

The lower critical field also shows a signature of the zero-field phase transition due to the SBF. The lower critical field is determined by the line tension (energy per unit length), ε_L, of a single vortex,

$$H_{c1} = 4\pi\varepsilon_L/\varphi_0 \tag{27}$$

where φ_0 is the flux quantum. For a type-II superconductor with a large field penetration length compared to the coherence length, as in UPt_3, the line tension of a vortex is

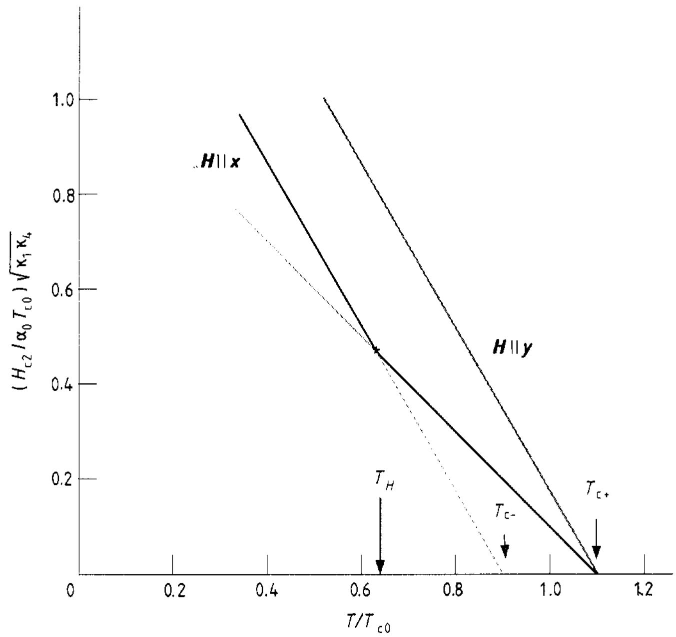

Figure 1. $H_{c2}(T)$ versus T/T_c for fields in the basal plane. The kink in $H_{c2}(T)$ is shown for $\kappa_{23} < 0$ and $\boldsymbol{H}\|\hat{\boldsymbol{x}}$. The order parameter changes from $\boldsymbol{\eta} \sim (0, 1)$ to $\boldsymbol{\eta} \sim (1, 0)$ at T_H. For $\boldsymbol{H}\|\hat{\boldsymbol{y}}$ the order parameter remains $\boldsymbol{\eta} \sim (0, 1)$ and there is no kink in $H_{c2}(T)$.

determined partly by the change in the order parameter inside the vortex core, but largely by the superfluid kinetic energy outside of the core. This kinetic energy is proportional to the superfluid density tensor, $\boldsymbol{\rho}_s$, and is easily calculated by solving London's equation for a single vortex,

$$\nabla \times [(\boldsymbol{\Lambda})^2 \cdot (\nabla \times \boldsymbol{h})] + \boldsymbol{h} = \varphi_0 \delta^{(2)}(\boldsymbol{x}_\perp)\hat{\boldsymbol{v}} \qquad (28)$$

where $\hat{\boldsymbol{v}}$ is the direction of the applied field and $\boldsymbol{x}_\perp$ are coordinates transverse to $\hat{\boldsymbol{v}}$. The anisotropic penetration length tensor, $\boldsymbol{\Lambda}$, is related to the superfluid density tensor by

$$(\boldsymbol{\Lambda})^2 = (m^2c^2/4\pi e^2)(\boldsymbol{\rho}_s)^{-1}.$$

For the zero-field order parameter, either above or below T_{c^*}, the superfluid density tensor is diagonal in the principal axes of the crystal: $(\boldsymbol{\rho}_s)_{ij} = 2(2m/h)^2(\tilde{\boldsymbol{\rho}}_s)_{ij}$, with

$$\tilde{\boldsymbol{\rho}}_s = (\kappa_{123}A(T)^2 + \kappa_1 B(T)^2)\hat{\boldsymbol{x}}\hat{\boldsymbol{x}} + (\kappa_1 A(T)^2 + \kappa_{123}B(T)^2)\hat{\boldsymbol{y}}\hat{\boldsymbol{y}}$$
$$+ \kappa_4(A(T)^2 + B(T)^2)\hat{\boldsymbol{z}}\hat{\boldsymbol{z}}. \qquad (29)$$

The anisotropy of the current in the xy plane is determined by the ratio $R = (\rho_{sxx}/\rho_{syy})$. As shown in figure 2, the anisotropy is large for $T_{c^*} < T < T_{c+}$, but $\underline{\underline{\boldsymbol{\rho}_s}}$ becomes nearly cylindrical for $T \ll T_{c^*}$, i.e. $R \simeq 1 - O(\varepsilon/\alpha_0 T_{c^*})$.

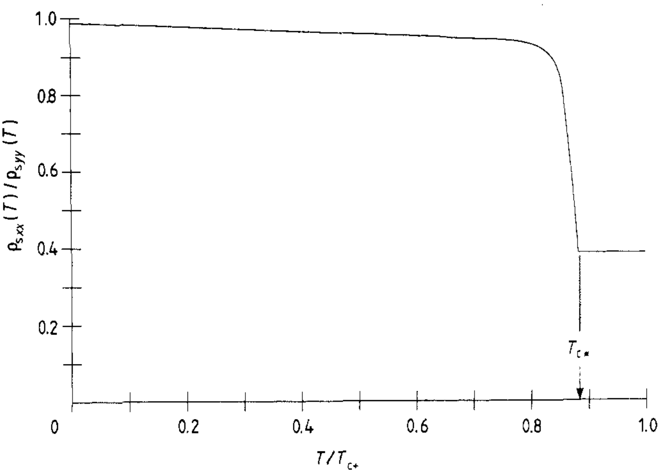

Figure 2. The ratio of the components of the superfluid density tensor, ρ_{sxx}/ρ_{syy}, as a function of temperature for $\kappa_{23}/\kappa_1 = -0.62(1.6)$ and $\beta_2/\beta_1 = 0.18$. At low temperature the superfluid density tensor is nearly isotropic in the basal plane.

For a vortex oriented along a principal axis, $\hat{x}_i$, the solution to London's equation for the field is

$$h = \frac{\varphi_0}{2\pi\lambda_j\lambda_k} K_0\left[\left(\frac{x_k^2}{\lambda_j^2} + \frac{x_j^2}{\lambda_k^2}\right)^{1/2}\right]\hat{x}_i \tag{30}$$

where (i, j, k) label the orthogonal principal axes. The line tension in the London limit is given by the kinetic energy and field energy outside of the vortex core,

$$\varepsilon_L = \frac{1}{8\pi}\int_{x_\perp > \xi} d^2x_\perp\{h^2 + (\nabla\times h)\cdot \underline{\underline{(\Lambda)}}^2 \cdot (\nabla\times h)\} \tag{31}$$

which gives for the lower critical field along a principal axis to logarithmic accuracy,

$$(H_{c1})_i = \frac{\varphi_0}{8\pi\lambda_j\lambda_k}\ln\left[\frac{1}{2}\left(\frac{\lambda_j^2}{\xi_j^2} + \frac{\lambda_l^2}{\xi_k^2}\right)\right]. \tag{32}$$

The temperature dependence of the lower critical field is determined by the penetration lengths transverse to the direction of the field, and since these functions reflect the dimensionality and anisotropy of the ground-state order parameter the lower critical field exhibits the phase transition induced by the SBF as shown in figure 3. The change in slope occurs at T_{c^*}, and for $h \| \hat{c}$ is given by

$$\frac{H'_{c1}(T_{c^*} - \delta)}{H'_{c1}(T_{c^*} + \delta)} = \left(1 + \frac{\beta_2}{\beta_1}\right)\frac{(\kappa_1 + \kappa_{123})^2}{4\kappa_1\kappa_{123}}. \tag{33}$$

For $\kappa_{23}/\kappa_1 = -0.62(1.6)$ determined from the fit to the kink in $H_{c2}(T)$, we find that the ratio $H'_{c1}(T_{c^*} - \delta)/H'_{c1}(T_{c^*} + \delta) \simeq 1.46$. It is interesting to note that stability constraints ($\beta_1/\beta_2 > 0$, $\kappa_1 > 0$ and $\kappa_{123} > 0$) on the bending and bulk coefficients of the free energy require that $H'_{c1}(T_{c^*} - \delta)/H'_{c1}(T_{c^*} + \delta) \geqslant 1$ through (33). Observation of this feature in the lower critical field, as well as the splitting of the heat-capacity jump and the kink in

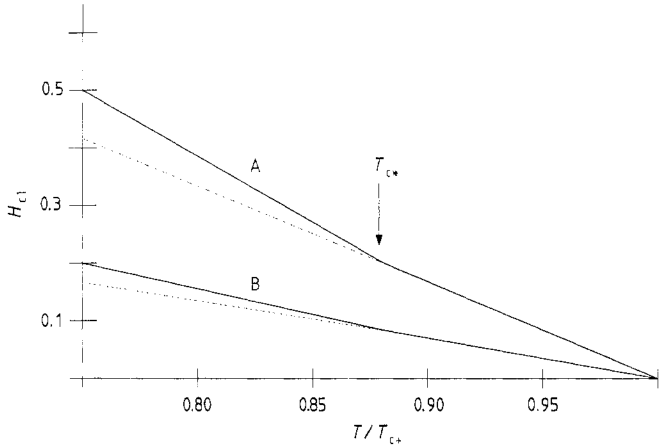

Figure 3. $H_{c1}(T)$ versus T/T_c in units of $(\varphi_0/8\pi\Lambda_x^2(T=0))$ for $\boldsymbol{H}\|\hat{c}$ with the parameters used in figure 2. The labelled curves correspond to the values $\kappa_{23} = 1.6$ (A) and $\kappa_{23} = -0.62$ (B). The broken lines are included to clearly show the kink that occurs at T_{c^*}.

$H_{c2}(T)$ for fields in the *ab* plane in the same single crystal would be a strong test of this model for unconventional pairing in UPt_3.

We have shown that the coupling of a two-dimensional unconventional order parameter to a field that breaks the basal plane symmetry of a hexagonal crystal splits the transition from the normal to superconducting state, producing an additional transition between unconventional superconducting phases of different symmetry. Besides the appearance of two jumps in the specific heat at T_{c+} and $T_{c^*} < T_{c+}$, there are further experimentally verifiable consequences. The rotational symmetry of the upper and lower critical fields is broken in the basal plane. The temperature-dependent upper critical fields for fields in the basal plane displays an abrupt change in slope, signalling a transition between two superconducting phases at finite field. The temperature of this transition is determined by the stiffness coefficients in the GL free energy. The lower critical field will also display a kink for all field orientations at the temperature of the zero-field transition. From comparison with recent specific heat measurements on UPt_3, we find $\beta_2/\beta_1 \simeq 0.15$, suggesting large strong coupling corrections. The size of the coupling to the SBF is found to be $\varepsilon/\alpha_0 \sim 7.8$ mK, which is somewhat smaller than $\varepsilon/\alpha_0 \sim 18$ mK obtained from an upper critical field measurement which also yield estimates for the bending coefficients in the free energy. From these estimates, we predict that for fields along the *c* direction, the ratio of the lower critical field slopes at $T = T_{c^*}$ is $\simeq 1.46$. While these results are encouraging, the observation of all these features on the *same* sample would provide a convincing case for unconventional superconductivity in UPt_3.

Acknowledgments

DWH acknowledges the hospitality of The Center for Materials Science at Los Alamos National Laboratory and JAS thanks the Institute for Theoretical Physics at Santa Barbara where part of this work was done. This research was supported in part by the National Science Foundation through the Northwestern University Materials Research

Center grant No DMR-85-20280, and through the Institute for Theoretical Physics grant No (PHY 82–17853), supplemented by funds from the National Aeronautics and Space Administration.

Note. Since this paper was submitted we received a preprint from Machida and Ozaki which obtains similar results to ours for the zero-field heat-capacity splitting; however, these authors do not consider the effects of the SBF on the critical fields. In addition, a preprint by B S Shivaram, J J Gannon Jr and D G Hinks reports measurements of a change in slope of $H_{c1}(T)$ and $H_{c2}(T)$ at slightly different temperatures but both of order 50–100 mK below the first superconducting transition, added support for an unconventional order parameter in UPt_3.

References

[1] Fisher R, Kim S, Woodfield B, Phillips N, Taillefer L, Hasselbach K, Floquet J, Giorgi A and Smith J 1988 *Preprint*
[2] Leggett A J 1975 *Rev. Mod. Phys.* **47** 331
[3] Fishman R S 1987 *Phys. Rev.* B **36** 79
[4] Ozaki M 1986 *Prog. Theor. Phys.* **76** 1008
[5] Sigrist M, Joynt R and Rice T 1987 *Phys. Rev.* B **36** 5186
[6] Volovik G 1988 *Sov. Phys.–JETP* **48** 41
[7] Aeppli G, Bucher E, Broholm C, Kjems J, Baumann J and Hufnagl J 1988 *Rev. Phys. Lett.* **60** 615
[8] Joynt R 1988 *Supercond. Sci. Technol.* **1** 210
[9] Putikka W and Joynt R 1988 *Phys. Rev.* **37** 2372
[10] Ueda K and Rice T 1985 *Phys. Rev.* B **31** 7114
[11] Klemm R and Scharnberg K 1985 *Physica* B **135** 53
[12] Sauls J A 1986 *Phys. Rev.* **34** 4861
[13] Qian Y, Xu M-F, Schenstrom A, Baum H-P, Ketterson J, Hinks D, Levy M and Sarma B 1987 *Solid State Commun.* **63** 599
[14] Müller V, Roth C, Maurer D, Schiedt E, Luders K, Bucher E and Bommel H 1987 *Phys. Rev. Lett.* **58**
[15] Schenstrom A, Xu M-F, Hong Y, Bein D, Levy M, Sarma B, Adenwalla S, Zhao Z, Tokuyasu T, Hess D, Ketterson J, Sauls J and Hinks D 1989 *Phys. Rev. Lett.* **62** 332
[16] Tokuyasu T, Hess D and Sauls J 1989 *Phys. Rev.* B at press
[17] Volovik G and Gor'kov L 1985 *Sov. Phys.–JETP* **61** 843
[18] Kumar P and Wölfle P 1987 *Phys. Rev. Lett.* **59** 1954
[19] Norman M 1989 *Preprint*
[20] Burlachkov L 1985 *Sov. Phys.–JETP* **62** 800
[21] Klemm R and Scharnberg K 1986 *J. Magn. Magn. Mater.* **54–57** 381
[22] Taillefer L, Piquemal F and Flouquet J 1988 *Physica* C **153–155** 451
[23] Shivaram B, Rosenbaum T and Hinks D 1986 *Phys. Rev. Lett.* **57** 1259