Upper Critical Field in p-Wave Superconductors with Broken Symmetry

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A uniaxially anisotropic p-wave interaction is shown to lead to either a polar or an axial state. We calculate the anisotropy of $H_{c2}(T)$ with the assumption that $E_F >> k_B T_c$. Weak-interaction anisotropy leads to a kink in $H_{c2,\perp}(T)$. Otherwise, our results are qualitatively similar to those for an anisotropic s-wave material. Our results indicate that the anisotropy of the $H_{c2}(T)$ data obtained for UPt_3 cannot be explained as intrinsic for a p-wave superconductor unless $E_F \cong k_B T_c$.

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Recently, there has been a great deal of interest in several materials known as "heavy fermion" superconductors. Various workers have interpreted the specific heat, ultrasonic attenuation, and $1/T_1$ data as evidence for p - wave, or triplet superconducting pairing.[1-3] More precisely, some data appear to be generally consistent with a polarlike state, in which the order parameter vanishes along a line on the Fermi surface. Other data appear to be more suggestive of an axial-like state [of which the Anderson-Brinkman-Morel (ABM) state of ^{3}He is the simplest example], in which the order parameter vanishes at isolated points on the Fermi surface. Some theoretical considerations[4,5] have supported a triplet spin state. More recently, group-theoretical arguments led to claims[6] that the most general forms for the possible triplet states do not permit a polar-type state. However, those workers apparently overlooked the consequences of an anisotropic pairing interaction. Any anisotropy forces the simplest p-wave state to be entirely of the favored symmetry: For a p-wave pairing interaction that favors one direction over the other two, a polar state has the highest T_c, and since its interaction with the axial (ABM) state is repulsive, it is the only allowable state for a sufficiently strong (~ 2 or greater) interaction anisotropy. Conversely, if the p-wave pairing interaction is weakest in one direction, an axial or ABM state is favored. Hence, the above experiment on UPt_3[2] is consistent with either singlet or triplet (p-wave) superconductivity in a hexagonal crystal.

Recently, the observed anisotropy of the upper critical field H_{c2} in UPt_3[7] was found to vary from unity at low temperatures to $\cong 1.7$ near T_c. This behavior is not expected for intrinsic s-wave superconductors, but has been interpreted as intrinsic for p-wave materials.[8] In this Letter, we investigate this claim in detail, and conclude that although the ultrasonic-attenuation result could possibly arise from intrinsic p-wave pairing with broken symmetry, the H_{c2} data appear to be difficult to interpret as intrinsic for any type of homogeneous superconductor, unless the Fermi energy $E_F \cong k_B T_c$. We believe it is more likely due to experimental difficulties.

Previously, we[9] calculated H_{c2} for clean p-wave superconductors with an isotropic effective mass and an interaction of the form $V\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}'$, and found that the polar state had the highest H_{c2}. No anisotropy of H_{c2} is obtained for that interaction, because the order parameter $\Delta(\hat{\mathbf{k}})$ is free to rotate relative to $\mathbf{H}$, and H_{c2} is optimized when the nodal plane of $\Delta(\hat{\mathbf{k}})$ is perpendicular to $\mathbf{H}$. Similarly the axes of the ABM state and the generalized ABM state [given by Eq. (45) in the first paper of Ref. 9, hereafter referred to as the SK state] are always parallel to $\mathbf{H}$. Consequently, $H_{c2}(T)$ for s- and p-wave superconductors with isotropic interactions are very similar.

Since the heavy-fermion superconductors to date appear to have f electrons near E_F, strong spin-orbit coupling is present, resulting in a number of possible states.[4,6] Basically, strong spin-orbit coupling requires that the axes of quantization of the spins be defined relative to the electron wave vectors. The appropriate quantization axes are therefore $\hat{\mathbf{e}}_\mu(\hat{\mathbf{k}}) = \hat{\mathbf{k}}$, $\hat{\boldsymbol{\theta}}_k$, and $\hat{\boldsymbol{\phi}}_k$. For p-wave ($l=1$) pairing, the pair states are therefore of the form $k|S_i(\hat{\mathbf{e}}_\mu)\rangle$, where the pair spin states $|S_i(\hat{\mathbf{e}}_\mu)\rangle$ are $(\downarrow_\mu\downarrow_\mu - \uparrow_\mu\uparrow_\mu)/\sqrt{2}$, $i(\uparrow_\mu\uparrow_\mu + \downarrow_\mu\downarrow_\mu)/\sqrt{2}$, and $(\uparrow_\mu\downarrow_\mu + \downarrow_\mu\uparrow_\mu)/\sqrt{2}$ for $i=1,2,3$, respectively. It is convenient to rewrite these pair spin states in terms of the Cartesian pair spin-state vector $(\mathbf{S})_j = \sum_i \mathbf{x}_i |S_i(\hat{\mathbf{x}}_j)\rangle$, where the $|S_i(\hat{\mathbf{x}}_j)\rangle$ are defined as above with the $\hat{\mathbf{e}}_\mu$ replaced by $\hat{\mathbf{x}}_j$. The resulting pair spin states are $\hat{\mathbf{k}}\cdot(\mathbf{S})_j$, $\hat{\boldsymbol{\theta}}_k\cdot(\mathbf{S})_j$, $\hat{\boldsymbol{\phi}}_k\cdot(\mathbf{S})_j$, $(S_z)_j$, and $\hat{\boldsymbol{\phi}}_k\times(\mathbf{S})_j\cdot\hat{\mathbf{z}}$. A number of the $|S_i(\hat{\mathbf{e}}_\mu)\rangle$ are degenerate. For example, in the z representation, $|S_1(\hat{\mathbf{k}})\rangle$ and $|S_3(\hat{\boldsymbol{\theta}}_k)\rangle$ are degenerate, but in the y representation, $|S_3(\hat{\boldsymbol{\theta}}_k)\rangle$ is degenerate with $|S_2(\hat{\mathbf{k}})\rangle$.

In the UPt_3, the crystal is hexagonal, and so the crystal field breaks the above symmetries.[4,6] A pairing interaction exhibiting this crystal symmetry and leading to p-wave states consistent with experiment[2,3] is of the form

$$V(\hat{\mathbf{k}},\hat{\mathbf{k}}') = 3\sum_i V_i \hat{\mathbf{k}}\cdot\hat{\mathbf{x}}_i \hat{\mathbf{k}}'\cdot\hat{\mathbf{x}}_i |S_i(\hat{\mathbf{x}}_j)\rangle\langle S_i'(\hat{\mathbf{x}}_j)|, \quad (1)$$

where the quantization axis $\hat{\mathbf{x}}_j$ is doubly degenerate as described above. The appropriate uniaxial anisotropy is obtained for $V_3 = V_c \neq V_1 = V_2 = V_{ab}$. The pair states resulting from such an interaction are of the form $\Delta(\mathbf{R},\hat{\mathbf{k}}) = \sum_i \Delta_i(\mathbf{R})\hat{\mathbf{k}}\cdot\hat{\mathbf{x}}_i|S_i(\hat{\mathbf{x}}_j)\rangle$. If all of the Δ_i were nonzero, the order parameter would not vanish anywhere on the Fermi surface.[6] However, for $V_c > V_{ab}$, only $\Delta_3 \neq 0$, resulting in a polar state for $H=0$! For $V_{ab} > V_c$, the zero-field state is an axial state of the simple ABM form. Note that this is true even for infinitesimal anisotropy in V_i.

One might worry about spin-paramagnetism effects if $\hat{\mathbf{x}}_3 = \hat{\mathbf{c}}$, especially with $V_c > V_{ab}$. In this case, the spin state for the c direction would be different from that for the a and b directions, which would be degenerate. As Anderson[4] pointed out, this a-b degeneracy leads to an $A1$ phase. In the c direction, the spin state in a given crystal-axis representation is nondegenerate, but as discussed above, the crystal representations are doubly degenerate: In momentum representation the spin quantization axis is a linear combination of $\hat{\mathbf{k}}$ and $\hat{\boldsymbol{\theta}}_k$. This implies that even if the state $|S_3(\hat{\mathbf{x}}_j)\rangle$ were to be favored, it would not be Pauli limited in the strong spin-orbit coupling limit! Similar arguments lead to the conclusion that in the strong spin-orbit coupling limit, there is no Pauli limiting for singlet superconductivity as well. Although this result may seem surprising to some, it corresponds exactly to the case of infinite spin-orbit scattering.

Hence, the only anisotropy due to the spins is that arising from the density of states and the resulting magnetization in a field. This anisotropy will always be very small for $\mu_B H/E_F \ll 1$. In UPt_3, the largest H_{c2} measured[7] is for $\mu_B H \cong 2k_B T_c$, so that the density of states anisotropy could only be relevant if $E_F \cong 1$ K. Although associating E_F with the temperature extracted from the specific heat[1] might lead to such a conclusion, the small normal-state magnetoresistance[7] and the characteristic energy from neutron scattering[10] lead to the conclusion that $E_F \gg 1$ K. These effects are thus more likely to occur in UBe_{13}, which has larger $\mu_B H/T_c$ and magnetoresistance values, as well as an anomalous $H_{c2}(T)$.[11] We shall neglect them in UPt_3 for simplicity's sake.

Our calculation of H_{c2} is standard: We assume weak coupling for a homogeneous clean type-II material. We would, of course, have nontrivial spin-orbit coupling effects near the surface of the material,[12] but these effects will not contribute to a bulk property such as H_{c2}. Although E_F may lie within a very narrow band, we neglect any temperature variation that might arise near T_c from band-structure or normal-state many-body effects. H_{c2} is therefore found by solving the linearized Gor'kov gap equation,[9,13]

$$\Delta(\mathbf{R},\hat{\mathbf{k}}) = 2\pi T\sum_{\omega_n}\int (d\Omega'/4\pi)N(0)V(\hat{\mathbf{k}},\hat{\mathbf{k}}')\int_0^\infty d\xi \exp(-2\xi|\omega_n|) \times\exp(-i\xi m v_F \operatorname{sgn}\omega_n \hat{\mathbf{k}}'\cdot\overleftrightarrow{\mathbf{M}}^{-1}\cdot\boldsymbol{\Pi})\Delta(\mathbf{R},\hat{\mathbf{k}}'), \quad (2)$$

where $N(0)$ is the density of states at the Fermi energy, $\boldsymbol{\Pi} = \nabla/i + 2e\mathbf{A}$, and $\overleftrightarrow{\mathbf{M}}^{-1}$ is the inverse effective mass tensor. We assume that $\overleftrightarrow{\mathbf{M}}^{-1}$ is diagonal; the effective masses in the c axis and a-b plane are m_c and m_{ab}, respectively, and $m = (m_{ab}^2 m_c)^{1/3}$. Equation (2) is identical to that used in Ref. 9, except for the interaction [Eq. (1)] and effective mass anisotropy. For $\mathbf{H}\parallel\hat{\mathbf{c}}$ or $\mathbf{H}\perp\hat{\mathbf{c}}$, the role of the effective mass anisotropy is simply to multiply the resulting H_{c2} by (m_c/m) and $(m_{ab}m_c/m^2)^{1/2}$, respectively.[14]

We first consider the case $V_c < V_{ab}$, implying $T_c^{ab} > T_c^c$. For $\mathbf{H}\perp\hat{\mathbf{c}}$, $H_{c2}(T)$ is given by the polar state of Ref. 9. For $\mathbf{H}\parallel\hat{\mathbf{c}}$, two possibilities arise. If $V_c/V_{ab} < 0.866$, the SK state always dominates over the polar state. For $V_c/V_{ab} > 0.866$, however, the polar state with transition temperature $T_c^c > 0.875\, T_c^{ab}$ has an $H_{c2}(0)$ which is higher than that for the SK state. There would be a first-order phase transition between the two states below the temperature T_0 at which their H_{c2}'s are equal, as well as a kink in the measured $H_{c2}(T)$ at T_0.

The more interesting situation arises when $V_c > V_{ab} > 0$, resulting in a zero-field polar state, appropriate for UPt_3. For $\mathbf{H}\parallel\hat{\mathbf{c}}$, we get the polar state $H_{c2}(T)$ of Ref. 9. However, for $\mathbf{H}\perp\hat{\mathbf{c}}$, a new $H_{c2}(T)$ arises. Although for $V_c \cong V_{ab}$, there is the possibility of a field-aligned polar state at low temperatures, this new "broken symmetry" polar state is the only possible one for sufficiently small V_{ab}.

In order to solve Eq. (2) for H_{c2}, we expand $\Delta(\mathbf{R},\hat{\mathbf{k}})$ in terms of the spherical harmonics $Y_{lm}(\hat{\mathbf{k}})$. For simplicity of notation, we choose $\mathbf{H}\parallel\hat{\mathbf{x}}_3$. Different orientations of $\mathbf{H}$ are equivalent to relabelings of the crystal axes. Thus, the expansion coefficient $\Delta_{10}(\mathbf{R})$ always describes the polar state. For $\mathbf{H}\perp\hat{\mathbf{c}}$ and sufficiently weak V_{ab}, we have to find a solution from the coupled equations for Δ_{11} and Δ_{1-1}. For the special case $V_{ab}=0$, these equations decouple, as $\Delta_{11} = -\Delta_{1-1}$, implying $\Delta(\mathbf{R},\hat{\mathbf{k}}) \propto \hat{\mathbf{k}}_1$; this state of completely broken symmetry (CBS) is a polar state with the magnetic field in its nodal plane. For $V_{ab} > 0$, the state with partial broken symmetry (PBS) is similar to the ABM and SK states [i.e., $\Delta(\mathbf{R},\hat{\mathbf{k}})$ is a linear combination of $\hat{\mathbf{k}}_1$ and $\hat{\mathbf{k}}_2$]; it merges into the SK state for $V_{ab}=V_c$.

Since the Abrikosov vortex lattice (in which Δ is the ground state of the harmonic oscillator) does not solve Eq. (2) for $\Delta_{1\pm1}(\mathbf{R})$, we expand in terms of the complete set of harmonic-oscillator eigenstates.[13] The expansion coefficients may be written as $x_n^{\pm}=\langle n|\Delta_{11}\rangle \pm \langle n|\Delta_{1-1}\rangle$, yielding the pair of equations

$$2\alpha_n^{\pm}x_n^{\pm} \pm b_{n-2}(x_{n-2}^{-}+x_{n-2}^{+}) - b_n(x_{n+2}^{-}-x_{n+2}^{+})=0, \quad (3)$$

where $\alpha_n^-=[V_cN(0)]^{-1}-a_n$, $\alpha_n^+=[V_{ab}N(0)]^{-1}-a_n\equiv\delta+\alpha_n^-$, and α_n^- and b_n are $1/V_cN(0)$ times $\alpha_n^{(1,2)}$ and β_n, given by Eqs. (35) and (36) of Ref. 9, respectively. These quantities α_n^- and b_n are functions of the reduced temperature $t=T/T_c$ and field $\bar{h}=(m_{ab}m_c/m^2)^{-1/2}h$, where $h=2eH/(2\pi T_c/v_F)^2$. Elimination of x_n^+ in favor of x_n^- yields

$$a_{n,n-2}x_{n-2}^{-}+a_{nn}x_n^{-}+a_{n,n+2}x_{n+2}^{-}=0, \quad (4)$$

where

$$a_{n,n-2}=-\delta b_{n-2}(1-c_n)/\alpha_{n-2}^{+}, \quad (5)$$

$$a_{n,n+2}=-\delta b_n(1-c_{n-2})/\alpha_{n+2}^{+}, \quad (6)$$

$$a_{nn}=2\alpha_n^-(1-c_n)(1-c_{n-2})-\delta(c_n+c_{n-2}-2c_nc_{n-2}), \quad (7)$$

and $c_n=b_n^2/\alpha_n^+\alpha_{n+2}^+$ for $n\geq0$; $c_{-2}=0$. The solution to Eq. (4) is in the form of a continued fraction,

$$a_{00}-\cfrac{a_{02}a_{20}}{a_{22}-\cfrac{a_{24}a_{42}}{a_{44}-\dots}}=0. \quad (8)$$

For $\delta\to0$, only a_{00} contributes, and we recover the SK state.

Near T_c, we expand to order H, obtaining $\alpha_n^-\to\ln(t)+(2n+1)\tilde{h}$ and $b_n\to-[(n+1)(n+2)]^{1/2}\tilde{h}$, where $\tilde{h}=7\zeta(3)\bar{h}/10$. Hence, to leading order in $T-T_c$, we obtain for $V_c>V_{ab}$ a polar state with H replaced by $\sqrt{3}H$. This factor of $\sqrt{3}$ was obtained previously[9] by expanding Eq. (2) to leading order in H. This expansion of Eq. (2) to order H can be done for arbitrary angle θ of $\mathbf{H}$ with respect to c, yielding an angular dependence of the slope of H_{c2} at T_c proportional to $[\cos^2\theta+(3m_{ab}/m_c)\sin^2\theta]^{-1/2}$. Away from T_c, or to higher order in H, one must employ the full continued-fraction equation.

The field as $t\to0$ can readily be found, with use of $\alpha_n^-\to\frac{1}{2}\ln(4\gamma h/e^{5/3})+d_n$, where

$$d_n=\tfrac{1}{2}\{\psi((n+1)/2)-\psi(\tfrac{1}{2})\}$$

and $\psi(z)$ is the digamma function; $b_n\to-(\frac{1}{2})[(n+2)/(n+1)]^{1/2}$. For $V_{ab}=0$, iteration of Eq. (8) yields

$$H_{c2,\perp}(0)/H_{c2,\parallel}(0)=0.466(m_{ab}/m_c)^{1/2}.$$

Thus, the anisotropy of the CBS state varies from $(3m_{ab}/m_c)^{1/2}$ at T_c to $2.14(m_{ab}/m_c)^{1/2}$ as $T\to0$.

In Fig. 1, we have plotted h_{c2} as a function of t for the polar state, the SK state, the ABM state, and the new CBS state. The ABM state has been included since for $V_{ab}=0$, the zeroth-order iteration of Eq. (8) reduces to it. The first-order iteration (i.e., adding a_{02}, a_{20}, and a_{22}) differs from the exact curve by less than 2%. The iteration thereafter converges very rapidly. We note that the CBS state has an $h_{c2}(t)$ curve which differs only slightly from that for a clean s-wave superconductor without Pauli limiting.

When $V_{ab}\neq0$, the slope of $H_{c2}(T)$ at T_c remains unchanged. However, as δ is increased, $H_{c2}(T)$ develops an upward curvature, until at $\delta=0$, the slope at T_c

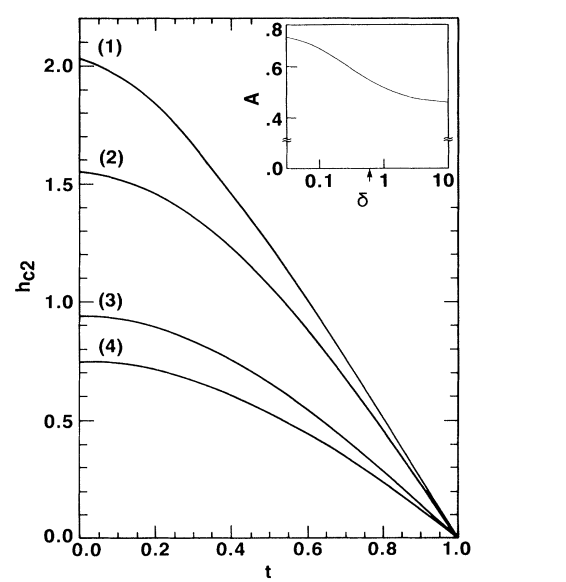

FIG. 1. Plots of $h_{c2}(t)$ with $m_c=m_{ab}$ for (1) the polar state, (2) the SK state, (3) the CBS state, and (4) the ABM state. Inset: anisotropy $A=h_{c2,\perp}(0)/h_{c2,\parallel}(0)$ as a function of $\delta=\ln(T_c^{ab}/T_c^c)$.

jumps discontinuously by the factor $\sqrt{3}$. This is precisely as for p-wave pairing in the layered compounds.[9] Iteration of Eq. (8) yields for arbitrary δ the resulting anisotropy of $H_{c2}(0)$ shown in the inset of Fig. 1 for the PBS state. Note that as $\delta \to 0$ and ∞, $H_{c2,\perp}$ reduces to that of the SK and CBS states, respectively. Between these two limits, the anisotropy of the PBS state is a monotonic function of δ. The arrow at $\delta = 0.617$ indicates the minimum interaction anisotropy required for the state at zero temperature to be the PBS state. This implies that for $V_{ab} > 0.540\, V_c$, there will be a kink in $H_{c2,\perp}(T)$ due to a transition from the PBS state to the polar state with $T_c = T_c^{ab}$. Below the kink temperature, the transition between these states will be first order.

To see if any of the above features can help to identify odd-l pairing, we have briefly examined a case of anisotropic even-l (singlet) pairing,

$$V(\hat{\mathbf{k}},\hat{\mathbf{k}}') = \{1 + \epsilon(\hat{\mathbf{k}}\cdot\hat{\mathbf{x}}_3)^2\} V \{1 + \epsilon(\hat{\mathbf{k}}'\cdot\hat{\mathbf{x}}_3)^2\}. \qquad (9)$$

The ratio of slopes of H_{c2} at T_c varies continuously from 1 to $\sqrt{5}$ times the mass anisotropy $(m_{ab}/m_c)^{1/2}$, as ϵ varies from zero to ∞. For separable interactions as above, there will not be a kink in $H_{c2,\perp}(T)$. However, it is easy to find a nonseparable interaction in which a kink would arise.[9]

Finally, we would like to discuss our results in view of the recent experiments[7] on UPt_3. Resistivity measurements[15] indicate that $m_{ab}/m_c \cong 2$. The anisotropy of H_{c2} at T_c appears to be somewhat greater than $\sqrt{2}$, but less than $\sqrt{6}$. It would be consistent with an anisotropic state arising from an even-parity interaction such as in Eq. (9). We note that for this effective mass anisotropy, there is no temperature at which an intrinsic p-wave superconductor would have an isotropic H_{c2}, so that the low-temperature part of the data of Chen *et al.*[7] is not expected for a homogeneous p-wave superconductor with $E_F \gg 1$ K. We anxiously await the results of ac susceptibility measurements on larger samples.

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