Critical field for surface superconductivity in UPt_3

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Phenomenological boundary conditions for the Ginzburg–Landau equations are derived in a model with a mixture of two different one-component order parameters for the heavy-fermion superconductor UPt_3. These boundary conditions are used to calculate the critical field for surface superconductivity, $H_{c3}(T)$. © *1995 American Institute of Physics.*

The splitting of the superconducting transition and the complex structure of the $H-P-T$ phase diagram in the compound[1] UPt_3 have yet to be explained. Several theoretical models have been proposed on the basis of a phenomenological theory which makes use of symmetry considerations.[2–4] These models can be put in two groups.

1. Models which work with two-component order parameters. It is pertinent to recall here that the superconducting order parameter corresponding to the ath irreducible representation of the point symmetry group G_0 of the crystal is of the form[2] (in the case of a strong spin–orbit coupling)

$$\hat{\Delta}(\mathbf{k},\mathbf{r})=\sum_j \eta_j(\mathbf{r})\hat{\Delta}_j^{(a)}(\mathbf{k}),$$

where $\hat{\Delta}_j^{(a)}$ are basis functions, 2×2 matrices in spin space. For the case of singlet pairing we would have $\Delta_{j,\alpha\beta}^{(a)}(\mathbf{k})=(i\hat{\sigma}_2)_{\alpha\beta}\psi_j^{(a)}(\mathbf{k})$, while for triplet pairing we would have $\Delta_{j,\alpha\beta}^{(a)}(\mathbf{k})=(i\hat{\sigma}_\mu\hat{\sigma}_2)_{\alpha\beta}d_j^{(a),\mu}(\mathbf{k})$. In our case we have $G_0=D_{6h}$, and one of the 2D representations E_1, E_2, split by the interaction with a field of lower symmetry, is selected as the representation[5] by which the order parameter is transformed. This field of lower symmetry might be, for example, an antiferromagnetic order in the UPt_3 crystal, which has orthorhombic symmetry (see Ref. 6, for example, for a review of these models and for references to the literature).

2. Models which assume that the superconducting state in UPt_3 is a superposition of two order parameters which differ in symmetry (i.e., which belong to different representations of the group D_{6h}), with slightly different transition temperatures. Here we consider the case of a mixture of two one-component order parameters ψ_1 and ψ_2. There can be combinations of either the type[7] $(\psi_1,\psi_2)\sim(A,B)$, where A and B are any of the representations $A_{1,2}$ and $B_{1,2}$ of the D_{6h} group[5] (hence another name for this model: the "AB model"), or the type[8] (A_1,A_2) and (B_1,B_2).

In the Ginzburg–Landau functional we must write all the terms allowed by the symmetry, both homogeneous and gradient terms, imposing the following requirements.

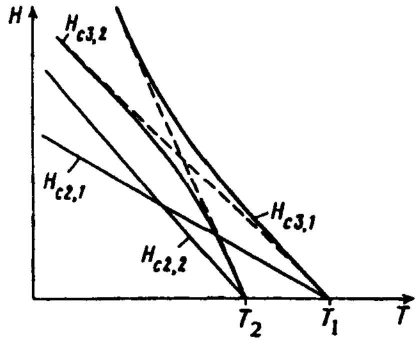

FIG. 1. Phase diagram for the AB model. Light lines—Upper critical fields $H_{c2,i}$; heavy lines—surface critical fields $H_{c3,i}$.

First, it is necessary to reproduce the experimental situation in which the lines of the upper critical field $H_{c2}(T)$ intersect for all directions of the external field (Fig. 1). Second, we consider only representations of the same spatial parity (this is not an absolute requirement; consequences of abandoning it are discussed in Ref. 9).

Within terms quadratic in ψ_1 and ψ_2, the Ginzburg–Landau functional thus becomes

$$F_0=F[\psi_1]+F[\psi_2], \tag{1}$$

where

$$F[\psi_i]=\alpha_i|\psi_i|^2+K_i|\mathbf{D}_\perp\psi_i|^2+K_i'|\mathbf{D}_z\psi_i|^2$$

(there is no summation over i); $\alpha_i=a\tau_i=a(T-T_i)$; $K_i, K_i'>0$; $T_{1,2}$ are the approximately equal transition temperatures ($T_1=T_0+\epsilon$, $T_2=T_0-\epsilon$, where $0<\epsilon\ll T_0$); and $\mathbf{D}=-i\nabla-(2\pi/\Phi_0)\mathbf{A}$ (Φ_0 is the flux quantum). An important point is that functional (1) has no terms which are cross terms in ψ_1, ψ_2, or their gradients (terms of this sort arise only in higher orders[8]). Consequently, the lines $H_{c2,i}(T)$ are independent, and under the conditions $K_1>K_2$, and $K_1K_1'>K_2K_2'$ they cross for all field directions[7].

To calculate the critical field for the surface superconductivity we need to know the boundary conditions on the Ginzburg–Landau equations. Within the framework of this phenomenological theory, surface effects (including boundary conditions) are incorporated by adding to the bulk functional F_0 some terms which are localized near the surface, which are permitted by the symmetry, and which are constructed from components of the order parameter and the normal vector $\mathbf{n}$ (Refs. 3 and 4). In addition to the quadratic terms which contains ψ_1 and ψ_2 separately, cross terms including $\psi_1^*\psi_2$ arise in our case: $n_Z(n_X^3-3n_Xn_Y^2)(\psi_1^*\psi_2+\text{c.c.})$ for (A_1,B_1) and (A_2,B_2); $n_Z(n_Y^3-3n_Yn_X^2)\times(\psi_1^*\psi_2+\text{c.c.})$ for (A_1,B_2) and (A_2,B_1) or $n_Z^2(n_Y^3-3n_Yn_X^2)(n_X^3-3n_Xn_Y^2)\times(\psi_1^*\psi_2+\text{c.c.})$ for (A_1,A_2) and (B_1,B_2)[(X,Y,Z) are the principal axes of the hexagonal lattice]. The surface energy density, for the (A_1B_1) pair, for example, is thus

$$F_{\text{surf}}=\{(g_1(n_X^2+n_Y^2)+g_2n_Z^2)|\psi_1|^2+(g_3(n_X^2+n_Y^2)+g_4n_Z^2$$
$$+g_5n_Z^2(n_X^3-3n_Xn_Y^2)^2)|\psi_2|^2+g_6n_Z(n_X^3-3n_Xn_Y^2)(\psi_1^*\psi_2+\text{c.c.})\delta(\mathbf{R}\cdot\mathbf{n}),$$

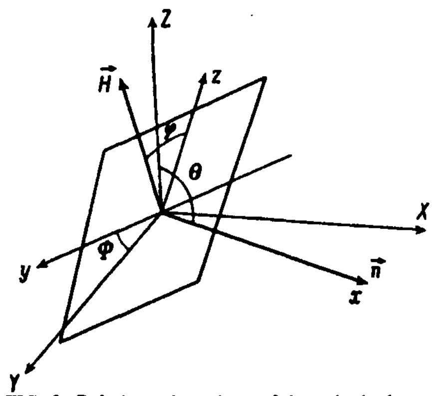

FIG. 2. Relative orientations of the principal axes of the crystal lattice, the plane of the surface of the superconductor, and the magnetic field.

where g_i are phenomenological coefficients.

We see that, although the bulk critical fields $H_{c2,i}(T)$ are independent for the different components of the order parameter, for all field orientations, this is not true for the corresponding surface fields, because of the coupling of the boundary conditions. The problem of finding $H_{c3,i}(T)$ becomes more complicated.

We supplement the coordinate system (X,Y,Z) by the system (x,y,z), which is tied to the plane of the surface of the sample (Fig. 2). The normal $\mathbf{n}$ has the components $n_X=\sin\theta\cos\Phi$, $n_Y=\sin\theta\sin\Phi$, and $n_Z=\cos\theta$. Boundary conditions at $x=0$ can be written

$$\frac{\partial\psi_1}{\partial x}=\beta_{11}\psi_1+\beta_{12}\psi_2, \quad \frac{\partial\psi_2}{\partial x}=\beta_{21}\psi_1+\beta_{22}\psi_2, \tag{2}$$

where the dependence of the real coefficients $\beta_{ij}=\beta_{ji}$ on the direction of $\mathbf{n}$ is determined by the form of the surface invariants.

We assume that the external magnetic field is in the yz plane: $H_x=0$, $H_y=H\sin\phi$, $H_z=H\cos\phi$. It is then convenient to use the gauge $A_x=0$, $A_y=H\,x\cos\phi$, $A_z=-H\,x\sin\phi$. In the coordinates (x,y,z), the Ginzburg–Landau equations take the same form for the two order parameters, so we will temporarily omit the index i. Furthermore, since y and z do not appear explicitly in the equations, we can immediately seek the order parameter in the form $\psi=\exp(ip_yy)\exp(ip_zz)f(x)$. We then find

$$a\tau f-K_{xx}\frac{d^2f}{dx^2}+K_{yy}(p_y-h_0x\cos\phi)^2f+K_{zz}(p_z+h_0x\sin\phi)^2f-2iK_{xz}p_z\frac{df}{dx}$$
$$-iK_{xz}h_0\sin\phi\left(f+2x\frac{df}{dx}\right)=0, \tag{3}$$

where

$$K_{xx}=K\sin^2\theta+K'\cos^2\theta, \quad K_{yy}=K,$$

$$K_{zz}=K\cos^2\theta+K'\sin^2\theta,\quad K_{xz}=(K-K')\cos\theta\sin\theta,$$

and $h_0=2\pi H/\Phi_0$.

To eliminate the last two terms in (3) and to put this equation in a simple form, we make the substitution (see also Ref. 10)

$$f(x)=\exp\left(-i\,\frac{K_{xz}}{2K_{xx}}\,h_0\sin\phi(x-x^*)^2\right)F(x),\quad h_0x^*\sin\phi=-p_z, \tag{4}$$

and we alter the scale along the z axis: $\tilde{p}_z=p_z\sqrt{K'/K_{xx}}$. As a result, we finally find

$$a\tau F-K_{xx}\frac{d^2F}{dx^2}+K\left(\left(p_y-\sqrt{\frac{K}{K_{xx}}}hx\cos\alpha\right)^2+\left(\tilde{p}_z+\sqrt{\frac{K}{K_{xx}}}hx\sin\alpha\right)^2\right)F=0, \tag{5}$$

where

$$h=\frac{2\pi\tilde{H}}{\Phi_0},\quad \tilde{H}=H\sqrt{\frac{K_{xx}}{K}}\sqrt{\cos^2\phi+\frac{K'}{K_{xx}}\sin^2\phi},\ \tan\alpha=\sqrt{\frac{K'}{K_{xx}}}\tan\phi, \tag{6}$$

Equation (5) is of precisely the same form as the equation for the isotropic case in a magnetic field $\tilde{\mathbf{H}}$ which has the components $\tilde{H}_x=0$, $\tilde{H}_y=\tilde{H}\sin\alpha$, $\tilde{H}_z=\tilde{H}\cos\alpha$. For this reason, it is convenient to separate the dependence of the order parameter on the directions along and perpendicular to $\tilde{\mathbf{H}}$ and to introduce the two parameters x_0 and k, which are related to p_y and p_z by

$$\sqrt{\frac{K}{K_{xx}}}\,hx_0=p_y\cos\alpha-\sqrt{\frac{K'}{K_{xx}}}\,p_z\sin\alpha,\quad q=p_y\sin\alpha+\sqrt{\frac{K'}{K_{xx}}}p_z\cos\alpha. \tag{7}$$

Equation (5) then becomes the simple equation of a harmonic oscillator. A solution of this equation which decays as $x\to+\infty$ is

$$F(x)=\exp\left(-\frac{Kh}{2K_{xx}}(x-x_0)^2\right)H_\nu\left(\sqrt{\frac{Kh}{K_{xx}}}(x-x_0)\right),$$

where $H_\nu(x)$ are the Hermite functions[11] with the index $\nu=-[1+(a\tau+Kq^2)/(Kh)]/2$.

Finally, partial solutions, which depend on $\mathbf{p}=(p_y,p_z)$, of the Ginzburg–Landau equations for the order parameters ψ_1 and ψ_2 take the form

$$\psi_{i,\mathbf{p}}=C_{i,\mathbf{p}}\,e^{ip_yy}\,e^{ip_zz}\exp\left(i\,\frac{K_{xz,i}}{2K_{xx,i}}\,h_0\sin\phi(x-x_i^*)^2\right)$$
$$\times\exp\left(-\frac{K_ih_i}{2K_{xx,i}}(x-x_{0,i})^2\right)H_{\nu_i}\left(\sqrt{\frac{K_ih_i}{K_{xx,i}}}(x-x_{0,i})\right), \tag{8}$$

where the $\mathbf{p}$ dependence of x_i^*, $x_{0,i}$, and ν_i is given by (4), (6), and (7). A direct check shows that this expression satisfies, as it should, the condition of a zero current across the boundary (along the x direction).

The general solution of the Ginzburg–Landau equations is of the form $\psi_i=\Sigma_{\mathbf{p}}\psi_{i,\mathbf{p}}$. Substituting it into boundary conditions (2), we verify that the components with different $\mathbf{p}$ are independent. Consequently, a condition under which the (infinite) system of equations for $C_i, \mathbf{p}$ can be solved reduces to the vanishing of a 2×2 determinant for any $\mathbf{p}$. Introducing the dimensionless parameter $r_i=\sqrt{K_i h_i/K_{xx,i}}x_{0,i}$, we find a transcendental equation which implicitly determines the dependence $h(\tau,\mathbf{p})$, i.e., $H(T,\mathbf{p})$:

$$\left(r_1-\sqrt{\frac{K_{xx,1}}{K_1h_1}}\beta_{11}+2\nu_1\frac{H_{\nu_1-1}(-r_1)}{H_{\nu_1}(-r_1)}\right)\times\left(r_2-\sqrt{\frac{K_{xx,2}}{K_2h_2}}\beta_{22}+2\nu_2\frac{H_{\nu_2-1}(-r_2)}{H_{\nu_2}(-r_2)}\right)$$

$$-\sqrt{\frac{K_{xx,1}K_{xx,2}}{K_1K_2h_1h_2}}\beta_{12}^2=0. \tag{9}$$

The critical field for the surface superconductivity which we are seeking is found by maximizing $H(T,\mathbf{p})$ with respect to the two parameters p_y and p_z. The form of the nucleus that appears is determined by Eq. (8).

Since Eq. (9) is quite complex, this program cannot be implemented analytically. Nevertheless, it can be solved numerically, for various values of β_{ij} and for various values of the parameters of functional (1). We wish to stress that Eq. (9) describes the behavior of only the "outer" $H_{c3}(T)$ line in Fig. 1. The linearized Ginzburg–Landau equations with a uniform magnetic field are obviously unsuitable for calculating the "inner" line.

We have a few qualitative comments regarding the behavior $H_{c3}(T)$. First, an obvious consequence of (6) is that a uniaxial anisotropy of the surface critical field should be observed in the yz plane, regardless of the orientation of the surface, as the magnetic field is rotated. An important property here, and one which is specific to a nontrivial superconductivity, is the substantial anisotropy of the parameters of the ellipse as the direction of the normal $\mathbf{n}$ is varied in the basal plane (i.e., as the angle Φ is varied). This anisotropy stems from the angular dependence of the parameters β_{ij}. For (A_1,B_1), for example, we have

$$\beta_{11}=g_1\sin^2\theta+g_2\cos^2\theta,\quad \beta_{22}=g_3\sin^2\theta+g_4\cos^2\theta+g_5\cos^2\theta\sin^6\theta\cos^2 3\Phi,$$

$$\beta_{12}=g_6\cos\theta\sin^3\theta\cos 3\Phi.$$

The solution of Eq. (9) must depend on the angle Φ. In this case the surface critical field will have a sixth-order anisotropy (see also Ref. 12). We wish to stress that, according to Ref. 13, the bulk critical fields H_{c2} in a hexagonal crystal do not depend on the direction in the basal plane. They cannot be used, therefore, to determine the symmetry of the order parameter.

With regard to the temperature dependence of the surface critical field, we note that it is convenient to begin with the very simple case $\beta_{12}=0$. The order parameters then become independent, and the lines of $H_{c3,i}(T)$, determined as in the one-component case,[12] cross (see the dashed lines in Fig. 1). If $\beta_{12}\neq 0$, this situation is obviously reminiscent of the quantum-mechanical problem of level crossing.[5] We would thus expect that the lines of the surface field would "repel each other" (Fig. 1). From the explicit expression for the surface cross terms we see that β_{12} vanishes for certain directions of the normal [in particular, for the (A_1,B_1) case, it vanishes for the directions $\theta=0$ and

$\pi/2$, or we have $\Phi=(2n+1)\pi/6$]. Consequently, for the various orientations of the surface of the sample we should observe, in addition to an anisotropy of slopes, a qualitative change in the picture due to the nature of the crossing of the $H_{c3,i}(T)$ lines. Furthermore, under the condition $h \gg \beta_{ij}^2$, all the terms in (9) which explicitly contain the magnetic field drop out, and the slopes of the straight lines $H_{c3,i}(T)$ are determined by the standard equations, i.e.,[14] $H_{c3}/H_{c2}=1.69$.

For the combination (B_1, B_2) under the conditions $\mathbf{H}, \mathbf{n} \perp \hat{\mathbf{c}}$, we find that the sixth-order anisotropy of the $H_{c3,i}(T)$ lines has opposite signs above and below the crossing point. This result agrees with the experimental results of Ref. 15.

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[1] L. Taillefer, J. Flouquet, and G. G. Lonzarich, Physica B **169**, 257 (1991).
[2] G. E. Volovik and L. P. Gor'kov, Zh. Éksp. Teor. Fiz. **88**, 1412 (1985) [Sov. Phys. JETP **61**, 843 (1984)].
[3] L. P. Gor'kov, Sov. Sci. Rev. A **9**, 1 (1987).
[4] M. Sigrist and K. Ueda, Rev. Mod. Phys. **63**, 239 (1991).
[5] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics: Non-Relativistic Theory* [in Russian] (Nauka, Moscow, 1989).
[6] J. A. Sauls, Adv. in Physics **43**, 113 (1994).
[7] A. Garg and D.-C. Chen, Phys. Rev. B **49**, 479 (1994).
[8] V. P. Mineev, Ann. Phys. (Paris) **19**, 367 (1994).
[9] V. P. Mineev and K. V. Samokhin, Zh. Éksp. Teor. Fiz. **105**, 747 (1994) [JETP **78**, 401 (1994)].
[10] D. K. Tilley, Proc. Phys. Soc. London **85**, 1977 (1965).
[11] A. F. Nikiforov and V. B. Uvarov, *Special Functions of Mathematical Physics* [in Russian] (Nauka, Moscow, 1984).
[12] K. V. Samokhin, Zh. Éksp. Teor. Fiz. **107**, 906 (1995) [JETP **80**, 515 (1995)].
[13] L. I. Burlachkov, Zh. Éksp. Teor. Fiz. **89**, 1382 (1985) [Sov. Phys. JETP **62**, 800 (1985)].
[14] D. Saint-James and P. G. De Gennes, Phys. Lett. **7**, 306 (1963).
[15] N. Keller, J. L. Tholence, A. Huxley, and J. Flouquet, Phys. Rev. Lett. **73**, 2364 (1993).

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