Upper critical field H_{c2} in heavy-fermion superconductors

L. I. Burlachkov

L. D. Landau Institute of Theoretical Physics, Academy of Sciences of the USSR
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The anisotropy of the upper critical field near T_c in a cubic crystal and in the basal plane of a tetragonal crystal is calculated for the case in which the superconducting order parameter transforms under one of the degenerate representations of the rotation group. In the basal plane of a hexagonal lattice, there is no anisotropy of H_{c2} near T_c, regardless of the nature of the superconducting phase.

1. INTRODUCTION

The superconductivity which has recently been observed in systems with so-called heavy fermions [UBe_{13} (Ref. 1), UPt_3 (Ref. 2), $CeCu_2Si_2$ (Ref. 3), U_6Fe (Ref. 4), etc.] has several distinguishing features. The most important new fact is the power-law dependence of such properties as the electronic specific heat and the ultrasonic absorption coefficient which is observed experimentally in these substances at low temperatures. This power-law behavior is evidence that the energy gap vanishes at certain points or on entire lines on the Fermi surface. These results have inspired several guesses regarding the mechanism for and the type of the superconductivity. In particular, it has been suggested that the superconducting phases which are observed are of a triplet-pairing type and that their properties are analogous to the superconducting properties of the A phase of ^3He (Ref. 5). A list of the possible superconducting classes[6] indicates that the gap may vanish at certain points on the Fermi surface in the triplet case (more precisely, for an order parameter which is inversion-odd). In a singlet phase (with an even order parameter), there may be points and even lines on the Fermi surface on which the order parameter vanishes.

The properties of the superconducting phase which develops, e.g., its analogy with the A phase of ^3He, depend on the particular representation of the symmetry group of the crystal which this phase arises from, more precisely, which representation of this group corresponds to the transition temperature which determines the points of the instability of the normal metal with respect to a transition to a superconducting state. Because of the strong spin-orbit coupling (all these compounds contain heavy atoms) the spins are "frozen" in the lattice, greatly simplifying the analysis. Because of the center of inversion, the order parameter has a definite parity, giving us a natural generalization of a classification on the basis of the resultant spin of the pair (i.e., $S=0$ or $S=1$). The remaining transformations of the point rotation group give us, e.g., in the case of the cubic group (for the UBe_{13} crystal), five irreducible representations, of which two are one-dimensional, one is two-dimensional, and two are three-dimensional. Gor'kov[7] has pointed out that if one of the multidimensional representations is involved then the anisotropy of the upper critical field H_{c2} should be manifested even near T_c and even in the case of a cubic crystal. Gor'kov[7] considered one example (a simplified example) of this type of anisotropy of H_{c2} in the basal plane of a tetragonal crystal.

In the present paper we analyze in detail the possible anisotropy of H_{c2} for cubic, tetragonal, and hexagonal symmetries. Exact analytic expressions are derived for cases corresponding to tetragonal and hexagonal symmetries (more on this below). For the cubic group, we are obliged to resort to numerical calculations. Machida *et al*[8] have recently carried out a variational calculation for the field lying in the basal plane in the case of tetragonal and cubic groups. For tetragonal symmetry, we find an exact analytic expression in the present paper, while for cases not amenable to analytic solution we find more comprehensive and more accurate results of a direct numerical solution of the equations for the stability conditions.

We remind the reader that we are considering here only degenerate representations of the point rotation groups, since for one-dimensional representations there is no anisotropy of the field H_{c2} in the approximation of the Ginzburg-Landau functional, i.e., at $(T_c - T) \ll T_c$ (Ref. 9).

2. FORM OF THE GRADIENT TERMS IN THE GINZBURG-LANDAU FUNCTIONAL

We expand the order parameter in the basis functions of the corresponding irreducible representation:

$$\hat{\Delta}(\mathbf{p}) = \sum_i \eta_i \hat{\Phi}_i(\mathbf{p}),$$

where the transformation properties of the basis functions $\hat{\Phi}_i(\mathbf{p})$ under rotations of the lattice can, as usual, be transferred to the transformations of the coefficients η_i.

a) Tetragonal group

We consider the tetragonal group D_4 ($CeCu_2Si_2$ and U_6Fe are cases of this group). The group D_4 has a single degenerate representation: a two-dimensional representation whose basis functions transform as coordinate unit vectors under lattice rotations. The particular form of the basis functions is given in Ref. 6 for $S=0$ and $S=1$ for both tetragonal and other crystal symmetries. The free energy is invariant under the elements of D_4 (i.e., rotations of the lattice and also, as mentioned above, of the spins). Consequently, the general form of the second-order terms of the Ginzburg-Landau functional (including gradient terms) is

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$$F=\int\Big(-\alpha\eta_i^*\eta_i+\frac{1}{2m_1}\partial_i^*\eta_j^*\partial_i\eta_j+\frac{1}{4m_2}(\partial_i^*\eta_i^*\partial_j\eta_j+\partial_i^*\eta_j^*\partial_j\eta_i)+\frac{1}{2m_3}\partial_i^*\eta_i^*\partial_i\eta_i+\frac{1}{2m_4}\partial_z^*\eta_i^*\partial_z\eta_i\Big)\,dV, \qquad (1)$$

where $\partial_k = \nabla_k - 2ieA_k/c$ are gauge-invariant derivatives, $\alpha \propto (T_c - T)$, z is a fourfold axis, and i, j represent x, y.

In the gradient term of the free energy F, the tetragonal invariant $\partial_i^*\eta_i^*\partial_i\eta_i$ is important in addition to the invariants of cylindrical symmetry with respect to the z axis.

b) Cubic group

The cubic group O_h (e.g., UBe_{13}) has three degenerate representations: one two-dimensional representation, E, and two three-dimensional representations, F_1 and F_2 (here and below, the notation used for the representations of the point groups is that of Ref. 10).

For the two-dimensional representation E, the basis functions can be chosen to transform in accordance with

$$\Phi_1=z^2+\varepsilon x^2+\varepsilon^2y^2,\quad \Phi_2=\Phi_1^*,$$

where $\varepsilon = \exp(2\pi i/3)$. We introduce

$$\nabla_1=\mathbf{z}\partial_z+\varepsilon\mathbf{x}\partial_x+\varepsilon^2\mathbf{y}\partial_y,\qquad \nabla_2=\mathbf{z}\partial_z+\varepsilon^{-1}\mathbf{x}\partial_x+\varepsilon^{-2}\mathbf{y}\partial_y,$$

where $\mathbf{x}$, $\mathbf{y}$, $\mathbf{z}$ are unit vectors along the coordinate axes. The gauge invariants are then of the form

$$\frac{1}{2m_1}\nabla^*\eta_i^*\nabla\eta_i+\frac{1}{2m_2}(\nabla_1^*\eta_2^*\nabla_2\eta_1+\nabla_2^*\eta_1^*\nabla_1\eta_2). \qquad (2)$$

In the case of the three-dimensional representation F_1, the basis functions transform as unit vectors along the coordinates, and we find, by analogy with (1),

$$\frac{1}{2m_1}\partial_i^*\eta_j^*\partial_i\eta_j+\frac{1}{4m_2}(\partial_i^*\eta_i^*\partial_j\eta_j+\partial_i^*\eta_j^*\partial_j\eta_i)+\frac{1}{2m_3}\partial_i^*\eta_i^*\partial_i\eta_i,\quad i,j=x,y,z. \qquad (3)$$

Only the last version in (3) is purely cubic; the others are spherical.

The basis functions of the representation F_2 transform in accordance with

$$\Phi_x=e_{xyz}\mathbf{x},\ \Phi_y=e_{yzx}\mathbf{y},\ \Phi_z=e_{zxy}\mathbf{z}$$

(a repeated index does not imply a summation), where e_{klm} is the antisymmetric unit tensor. The gradient invariants obviously remain the same as in the case of the representation F_1.

c) Hexagonal group

The hexagonal group D_6 (e.g., UPt_3), has four one-dimensional and two two-dimensional representations, E_1 and E_2. For the coordinate representation E_1, the gradient part of the free energy is

$$\frac{1}{2m_1}\partial_i^*\eta_j^*\partial_i\eta_j+\frac{1}{4m_2}(\partial_i^*\eta_i^*\partial_j\eta_j+\partial_i^*\eta_j^*\partial_j\eta_i)+\frac{1}{2m_4}\partial_z^*\eta_i^*\partial_z\eta_i+\frac{1}{2m_3}[(\partial_x^*\eta_x^*\partial_x\eta_y+\text{c. c.})-(\partial_y^*\eta_y^*\partial_y\eta_x+\text{c. c.})+(\partial_x^*\eta_y^*\partial_y\eta_y+\text{c. c})-(\partial_y^*\eta_x^*\partial_x\eta_x+\text{c. c.})]; \qquad (4)$$

where z is a sixfold axis, and $i, j = x, y$.

In the case of representation E_2, the basis functions transform in accordance with $\Phi_1 = (x + iy)^2$, $\Phi_2 = (x - iy)^2$. Introducing $\nabla_1 = \mathbf{x}\partial_x + i\mathbf{y}\partial_y$, $\nabla_2 = \mathbf{x}\partial_x - i\mathbf{y}\partial_y$, we find invariants analogous to (2):

$$\frac{1}{2m_1}\nabla^*\eta_i^*\nabla\eta_i+\frac{1}{2m_2}(\nabla_1^*\eta_2^*\nabla_2\eta_1+\nabla_2^*\eta_1^*\nabla_1\eta_2)+\frac{1}{2m_3}\partial_z^*\eta_i^*\partial_z\eta_i. \qquad (5)$$

3. STUDY OF THE ANISOTROPY OF THE FIELD H_{c2}

Varying the free-energy functional with respect to η_i^*, we find an eigenvalue problem from which we can determine those values of the field H at which the medium becomes unstable with respect to the formation of a nucleating region of the superconducting phase.

We consider various orientations of the field with respect to the lattice in a cubic crystal and also in the basal planes of tetragonal and hexagonal crystals, i.e., cases in which BCS superconductors have a completely isotropic upper critical field H_{c2}.

a) Tetragonal group

Varying (1) with respect to η_x^* and η_y^*, we find

$$-\alpha\eta_x=[P_1(\partial_{xx}+\partial_{yy})+P_4\partial_{zz}+(P_2+P_3)\partial_{xx}]\eta_x+{}^1/_2P_2(\partial_{xy}+\partial_{yx})\eta_y,$$
$$-\alpha\eta_y={}^1/_2P_2(\partial_{xy}+\partial_{yx})\eta_x+[P_1(\partial_{xx}+\partial_{yy})+P_4\partial_{zz}+(P_2+P_3)\partial_{yy}]\eta_y, \qquad (6)$$

$$P_i=1/2m_i,\qquad \partial_{kl}=\partial_k\partial_l.$$

This problem was solved by a variational method in Ref. 8. A solution for the case $P_2 + P_3 = 0$ was given in Ref. 7. As it turns out, a general solution exists.

We assume that the field lies in the xy basal plane of a

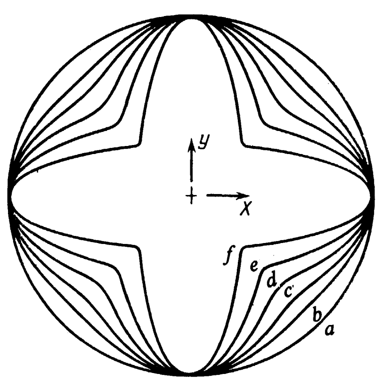

FIG. 1. The H_{c2} rosette in the basal plane of a tetragonal crystal. a—$P_1{:}P_2{:}P_3 = 1{:}1{:}0$; b—1:1:1/2; c—1:1:1; d—1:1:2; e—1:1:4; f—1:1:10.

tetragonal crystal: $H=(H\cos\varphi, H\sin\varphi, 0)$. We choose the vector potential in the form $A=(Hz\sin\varphi, -Hz\cos\varphi, 0)$, and we seek a solution in the following form [since the coordinates x and y enter (6) only through derivatives]:

$$\eta_x=f(z)\exp(ik_xx)\exp(ik_yy),$$
$$\eta_y=g(z)\exp(ik_xx)\exp(ik_yy).$$

The component of the vector $\mathbf{k}$ perpendicular to the field causes only a displacement of the nucleating region along z. With $\mathbf{k}=0$ we find from (6)

$$\begin{aligned}-\alpha\eta_x&=P_4\frac{\partial^2}{\partial z^2}\eta_x-[P_1+(P_2+P_3)\sin^2\varphi]\left(\frac{2e}{c}H\right)^2z^2\eta_x\\&\quad+2P_2\left(\frac{e}{c}H\right)^2z^2\sin 2\varphi\eta_y,\\-\alpha\eta_y&=2P_2\left(\frac{e}{c}H\right)^2z^2\eta_x\sin 2\varphi+P_4\frac{\partial^2}{\partial z^2}\eta_y\\&\quad-[P_1+(P_2+P_3)\cos^2\varphi]\left(\frac{2e}{c}H\right)^2z^2\eta_y.\end{aligned}\tag{7}$$

The differential operator in (7) can be reduced to diagonal form through the rotation $\eta_i=c_{ij}\eta_j'$, where

$$c_{ij}=\begin{vmatrix}\cos\beta & \sin\beta\\ -\sin\beta & \cos\beta\end{vmatrix},\quad \mathrm{tg}\,2\beta=\frac{P_2}{P_2+P_3}\mathrm{tg}\,2\varphi.$$

After some straightforward manipulations, we find the maximum value of H at which there is a solution which vanishes in the limit $|z|\to\infty$:

$$H_{max}=\alpha\frac{c}{2e}\left(P_4^{1/2}\left[P_1+\frac{P_2+P_3}{2}-\frac{1}{2}(P_2^2+(2P_2P_3+P_3^2)\cos^2 2\varphi)^{1/2}\right]^{1/2}\right)^{-1}.\tag{8}$$

In the case of a nonzero $\mathbf{k}$, we can no longer solve (6) analytically, but it has been shown by numerical methods (by the "matrix run-through" method) that a nonvanishing $\mathbf{k}$ lowers $H_{\max}$ from the value in (8). Accordingly, the dependence of H_{c2} on the direction in the xy plane of the tetragonal lattice is represented in (8). Figure 1 shows the H_{c2} "rosette" in the basal plane for various values of the ratios $P_1{:}P_2{:}P_3$ [the shape of the rosette does not depend on P_4, as can be seen from (8)].

b) Cubic group

For representation E we find, by analogy with (6),

$$\begin{aligned}-\alpha\xi_1&=\left[\left(P_1+\frac{1}{2}P_2\right)(\partial_{xx}+\partial_{yy}+\partial_{zz})-\frac{3}{2}P_2\partial_{zz}\right]\xi_1\\&\quad+\frac{\sqrt{3}}{2}P_2(\partial_{xx}-\partial_{yy})\xi_2,\\-\alpha\xi_2&=\frac{\sqrt{3}}{2}P_2(\partial_{xx}-\partial_{yy})\xi_1\\&\quad+\left[\left(P_1-\frac{1}{2}P_2\right)(\partial_{xx}+\partial_{yy}+\partial_{zz})+\frac{3}{2}P_2\partial_{zz}\right]\xi_2,\\\xi_1&=\frac{1}{2}(\eta_1+\eta_2),\quad \xi_2=\frac{i}{2}(\eta_1-\eta_2).\end{aligned}\tag{9}$$

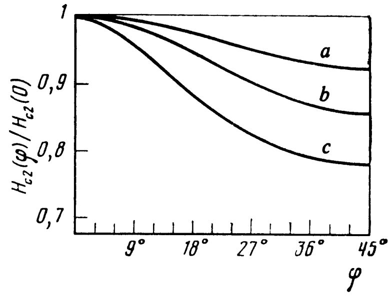

FIG. 2. H in the (100) plane; φ is the angle between H and the [100] axis. a—$P_1{:}P_2=11{:}3$; b—10:5; c—10:8.

If the field is parallel to the [110] axis of a cubic crystal, we find the following result, working as in the preceding case:

$$H_{c2}=\alpha\frac{c}{2e}\left([P_1-|P_2|]^{1/2}\left[P_1+\frac{1}{2}|P_2|\right]^{1/2}\right)^{-1}.$$

In particular, with $P=0$ the field H_{c2} is isotropic and equal to $\alpha c/2eP_1$.

The dependence of H_{c2} on the direction cannot be expressed analytically for an arbitrary orientation of the field, but it can be calculated to arbitrary accuracy by the matrix run-through method. Figures 2 and 3 show results calculated for the cases in which the field lies in the (100) and (110) planes, respectively, of a cubic lattice for various ratios $P_1{:}P_2$. The minimum value of H_{c2} is reached in the [111] direction, while the maximum value is reached in the [100] direction. The nature of the anisotropy depends on only $|P_2|$, so we need not study the case of negative P_2.

Figure 4 shows the case in which the order parameter transforms under one of the three-dimensional representations of the O_h group [the field is in the (100) plane]. The [100] directions may correspond to either a maximum or a minimum of H_{c2}, depending on the ratios $P_1{:}P_2{:}P_3$. If $P_3=0$, the field H_{c2} is isotropic [since the remaining invariants in (3) are spherical], equal to $(\alpha c/2e)(P_1^2-P_2^2/4)^{-1/2}$.

For all representations of the cubic group, as in the tetragonal case, H_{c2} is reached at a zero $\mathbf{k}$. The quantity $H_{c2}(\varphi)/H_{c2}(0)$ shown in the figures does not depend on T in the Ginzburg-Landau approximation.

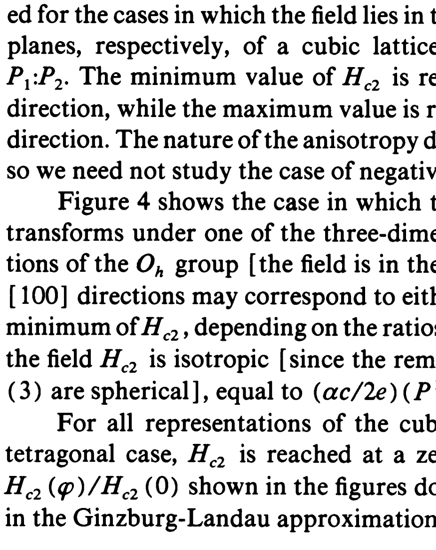

FIG. 3. H in the (110) plane; θ is the angle between H and the [100] plane. a, b, c—The same as in Fig. 2.

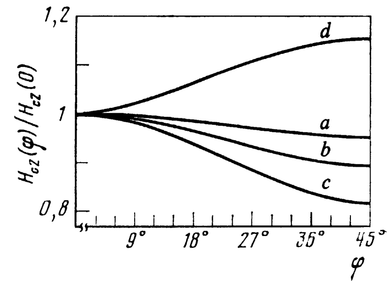

FIG. 4. H in the (100) plane. a—$P_1{:}P_2{:}P_3 = 10{:}3{:}2$; b—2:2;1; c—1:1:1; d—2:2:(− 1).

c) Hexagonal group

The representations of the D_6 group can be studied analytically. For E_1, for example, we find from (4)

$$\begin{aligned}-\alpha\eta_x &= P_4\frac{\partial^2}{\partial z^2}\eta_x - (P_1+P_2\cos^2\varphi+P_3\sin 2\varphi)\\ &\times\left(\frac{2e}{c}H\right)^2 z^2\eta_x + \left(\frac{1}{2}P_2\sin 2\varphi - P_3\cos 2\varphi\right)\left(\frac{2e}{c}H\right)^2 z^2\eta_y\\ -\alpha\eta_y &= \left(\frac{1}{2}P_2\sin 2\varphi - P_3\cos 2\varphi\right)\left(\frac{2e}{c}H\right)^2 z^2\eta_x\\ &+ P_4\frac{\partial^2}{\partial z^2}\eta_y - (P_1+P_2\sin^2\varphi - P_3\sin 2\varphi)\left(\frac{2e}{c}H\right)^2 z^2\eta_y.\end{aligned} \tag{10}$$

Transforming η_i by analogy with the tetragonal case, we find

$$H_{c2} = \alpha\frac{c}{2e}\left\{P_4^{1/2}\left[P_1 + \frac{1}{2}P_2 - \frac{1}{2}(P_2^2+4P_3^2)^{1/2}\right]^{1/2}\right\}^{-1}.$$

An analogous result is found for the representation E_2; i.e., H_{c2} is isotropic in the basal plane of a hexagonal crystal, regardless of the nature of the superconducting phase.

4. CONCLUSION

In summary, an anisotropy of the field H_{c2} can be observed in heavy-fermion superconductors even near T_c and even in the case of a cubic crystal or in the basal plane of a tetragonal crystal. The experimental observation of this effect would be of decisive importance for establishing the nontrivial nature of the superconducting phase. In the basal plane of a hexagonal structure, H_{c2} is isotropic near T_c, regardless of the nature of the phase, as we have shown above. Most superconducting classes[6] with a gap which vanishes at the Fermi surface belong to degenerate representations of the corresponding groups. Establishing the nature of the anisotropy of H_{c2} would be of assistance in determining the class of a given superconductor, although the anisotropy would be identical for the cases $S = 0$ and $S = 1$. A degeneracy may be lifted by internal stresses in a crystal.

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