Anisotropy of the upper critical field in a hexagonal exotic superconductor

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An expression, valid for arbitrary orientations of the magnetic field and relatively accurate in a wide range of the Ginzburg–Landau free energy parameters is obtained for the upper critical field near T_c in a hexagonal exotic superconductor. It is shown that in the majority of cases the angular dependence of the upper critical field does not have extra nonmonotonicities in comparison with the usual anisotropic superconductors. For a weak breaking of the particle-hole symmetry near the Fermi surface and rather rigid constraints on the Ginzburg–Landau theory parameters, an extra minimum may arise in the angular dependence of H_{c2}. An extra maximum can arise only for sufficiently strong symmetry breaking.

1. The angular dependence of the upper critical field in usual anisotropic superconductors near T_c is, as is well known, an ellipsoid. The axes of this ellipsoid are given by the components of the anisotropic mass tensor, which enters into the expression for the Ginzburg–Landau free energy. The order parameter of such superconductors is a complex quantity Ψ. Symmetry breaking accompanying the superconducting phase transition occurs according to some one-dimensional representation of the initial symmetry group of the system. A more complicated form of the angular dependence of the upper critical field may arise in symmetry-degenerate superconductors, when the symmetry breaking corresponds to a multidimensional representation of the initial group.[1–3] Such exotic superconductors are characterized by a multicomponent complex order parameter with the number of complex components equal to the representation dimensionality (see Ref. 4 and also Refs. 5 and 6 and citations therein).

The simplest example of a specific anisotropy of H_{c2} is a tetragonal exotic superconductor in a magnetic field in the basal plane of the crystal (perpendicular to the high-symmetry axis).[1–3] Whereas for usual tetragonal superconductors the field H_{c2} is isotropic in the basal plane, in the case of exotic tetragonal superconductors H_{c2} can have an anisotropy of a rosette type. To first approximation, we mean here an envelope for two intersecting ellipses whose major axes are perpendicular to each other. Near the intersection points the curve is, of course, smoothed out. For ellipses with small eccentricity this smoothing takes place for a wide range of angles.[2]

Theoretical description of the special anisotropy of the upper critical field in superconductors with different crystal symmetry is an important problem, since experimental observation of such anisotropy could indicate an exotic character of superconductivity. In this respect, it is interesting to consider hexagonal superconductors, in particular, the heavy-fermion compound UPt_3. The possibility of exotic superconductivity in UPt_3 is now widely discussed (see, e.g., Ref. 5).

In this paper we obtain an approximate analytical expression for the upper critical field in a hexagonal exotic superconductor with strong spin-orbit coupling. This expression is valid for arbitrary orientations of magnetic field and is sufficiently accurate in a rather wide range of allowed values of the Ginzburg–Landau free-energy parameters. For fields perpendicular or parallel to the hexagonal axis our result agrees with the exact solutions found for these particular cases.[2,7,8] The expression found below for the angular dependence of H_{c2} is an important generalization of the corresponding result of Ref. 9 to a wider range of allowed values of the parameters and agrees with the former in its applicability range.

The angular dependence of the upper critical field is related to the ratios of the coefficients in the gradient terms of the Ginzburg–Landau free energy. These ratios depend, in particular, on the degree of the particle–hole symmetry breaking near the Fermi surface. If such a symmetry holds to sufficient accuracy, the angular dependence of H_{c2} in the plane containing the hexagonal axis has the form of a distorted ellipse. The distortion of the ellipse appears to be relatively small. For most allowed values of the Ginzburg–Landau free energy parameters, the angular dependence of H_{c2} does not have extra nonmonotonicities in comparison with the usual dependence. There is, however, a relatively narrow range of parameters in which weakly manifested anisotropy of the upper critical field, of rosette type, with relatively low-magnitude extra nonmonotonicities is realized. These nonmonotonicities could become more noticeable under stronger breaking of the particle-hole symmetry near the Fermi surface. Then the angular dependence of H_{c2}, as a whole, can differ more noticeably from an ellipse in a wide range of angles. This is the qualitative difference of the anisotropy of the upper critical field in a hexagonal exotic superconductor from that in a usual hexagonal superconductor.

2. In a hexagonal exotic superconductor with strong spin-orbit coupling the order parameter has two components (η_1, η_2). The corresponding Ginzburg–Landau functional, accurate to second-order invariants, can be written in the form (see Refs. 4 and 5)

$$F=\int dV[-a\eta_i\eta_i^*+K_1p_i^*\eta_j^*p_i\eta_j+K_2p_i^*\eta_i^*p_j\eta_j+K_3p_i^*\eta_j^*p_j\eta_i+K_4p_z^*\eta_i^*p_z\eta_i]. \quad (1)$$

Here $a=\alpha(T_c-T)$, $p=-i\nabla-(2e/c)\mathbf{A}$, and the z axis is parallel to the hexagonal axis of the crystal. The indices i and j take on the values 1 and 2, which, for the operator $\mathbf{p}$, correspond to the x- and y-components.

If the sum of the gradient terms in (1) is positive-definite we get the following restrictions on the coefficients K_n ($n=1$–4):

$$K_1+K_2+K_3>|K_2|,\ K_1>|K_3|,\ K_4>0. \quad (2)$$

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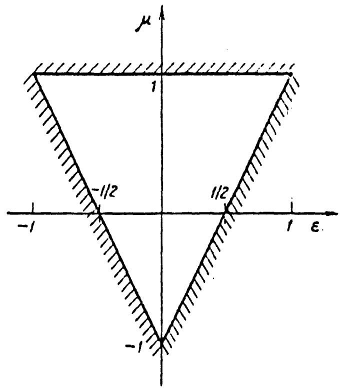

FIG. 1. The range of allowed values of the parameters ε and μ.

Consider the two dimensionless parameters

$$\varepsilon=\frac{K_2+K_3}{2K_1+K_2+K_3},\quad \mu=\frac{K_2-K_3}{2K_1+K_2+K_3}. \qquad (3)$$

From (2) we find that $1\pm\varepsilon>|\mu\pm\varepsilon|$. The obtained range of allowed values of ε and μ is shown in Fig. 1. It is essential that the inequalities $|\varepsilon|<1$ and $|\mu|<1$ always hold, i.e., the parameters ε and μ can, in fact, always be considered as rather small. Solving the problem of the upper critical field anisotropy, we will use perturbation theory in the parameters ε and μ up to second order inclusive.

The expression (1) for the free energy can be rewritten in the form

$$F=\int dV[-a\eta_i\eta_i^*+\eta_i^*(\hat H_{ij}^{(0)}+\hat V_{ij})\eta_j]. \qquad (4)$$

Here the matrix differential operator $\hat H_{ij}=\hat H_{ij}^{(0)}+\hat V_{ij}$ is split into two parts in such a way that the perturbation theory in $\hat V_{ij}$ is just the perturbation theory in ε and μ. The zeroth order operator $\hat H_{ij}^{(0)}=\hat H^{(0)}\delta_{ij}$ has the same form as in the case of a usual hexagonal superconductor:

$$\hat H^{(0)}=-\frac{1}{2}(2K_1+K_2+K_3)(p_x^2+p_y^2)-K_4p_z^2. \qquad (5)$$

Owing to the cylindrical symmetry of the upper critical field, the magnetic field $\mathbf{B}$ can be considered lying in the xz plane of Cartesian coordinates in Eq. (1). For the field $\mathbf{B}=B(\sin\theta, 0, \cos\theta)$ we choose the vector potential in the form

$$A_y=B(x\cos\theta-z\sin\theta).$$

If we change integration variables in Eq. (4),

$$x'=\frac{1}{K_4^{1/2}D(\theta)}[\zeta x\sin\theta+z\cos\theta],$$

$$y'=\left(\frac{\zeta}{K_4}\right)^{1/2}y,\quad z'=\left(\frac{\zeta}{K_4}\right)^{1/2}\frac{1}{D(\theta)}(-x\cos\theta+z\sin\theta). \qquad (6)$$

where

$$D^2(\theta)=\cos^2\theta+\zeta\sin^2\theta,\quad \zeta=\frac{2K_4}{2K_1+K_2+K_3}. \qquad (7)$$

The zeroth order operator $\hat H^{(0)}$ takes the form of the usual Hamiltonian of a nonrelativistic charged particle with isotropic mass in magnetic field along the x' axis. In comparison with the multiplicity of the Landau-level degeneracy, the eigenvalues $E_n^{(0)}$ of the operator $H_{ij}^{(0)}$ have additional double degeneracy. To each level $E_n^{(0)}$ there correspond two independent combinations of solutions of the form $\eta_{1,n}=(\eta_n^{(0)},0)$ and $\eta_{2,n}=(0,\eta_n^{(0)})$, where $\eta_n^{(0)}$ is the wave function of a charged particle in the nth Landau level. Generally speaking, the perturbation $\hat V_{ij}$ lifts the mentioned double degeneracy.

The effect of the parameters ε and μ on the lifting of the given level degeneracy is, however, different. To first order in ε and μ of perturbation theory for degenerate levels, the degeneracy is lifted completely, i.e., for all field orientations. At the same time, for $|\mu|\ll\varepsilon^2$ in first-order perturbation theory in ε the degeneracy lifting is not complete, since the levels still cross each other, if the field is along the hexagonal axis (i.e., $\theta=0$). The remaining level crossing for $\theta=0$ is lifted only in second-order perturbation theory in the parameter ε. Thus, the ratio of the parameters ε and μ plays here an important role.

If $|\varepsilon|\sim|\mu|$, the main features of the angular dependence of the upper critical field can be described already in the framework of first-order perturbation theory for degenerate levels. If $|\mu|\lesssim\varepsilon^2$ then, to describe the behavior of H_{c2} in the vicinity of the angle $\theta=0$, it is necessary to allow for the lifting of the level crossing for $\theta=0$ in second-order perturbation theory.

The fact that the parameter μ is nonzero is due, as is well-known, to the breaking of the particle-hole symmetry near the Fermi surface.[4] Since this asymmetry is usually rather small, the realization of the relation $|\mu|\lesssim\varepsilon^2$ seems not only possible, but also highly probable. However, the relation $\varepsilon\sim\mu$, incidentally, is likewise not excluded, at least for small values of ε. Because of this, we allow below for the lifting of the level degeneracy for any ratio of ε and μ, i.e., both in first- and second-order perturbation theory (in the parameters ε and μ) for degenerate levels.

In the general case, joint treatment, on equal basis, of terms of first and second order of smallness in the framework of perturbation theory for degenerate levels results in highly complicated formulas. But the problem can be considerably simplified because unperturbed wave functions are the wave functions of an oscillator and the structure of the perturbation-matrix elements is simple. Furthermore, to find the upper critical field it is necessary to consider only the ground Landau level for zero momentum of motion along the magnetic field. As a result, we arrive at the following expression for the upper critical field:

$$H_{c2}(\theta)=\frac{ac\zeta}{2|e|K_4D(\theta)}\left\{1-\frac{\varepsilon^2}{D^2(\theta)}\left(\cos^2\theta+\frac{\zeta^2\sin^4\theta}{8D^2(\theta)}\right)-\frac{1}{2D(\theta)}\left[\frac{\varepsilon^2\zeta^2}{D^2(\theta)}\sin^4\theta+\left(\varepsilon^2\left(1+\frac{\cos^2\theta}{D^2(\theta)}\right)-2\mu\right)^2\cos^2\theta\right]^{1/2}\right\}^{-1}. \qquad (8)$$

As the angular dependence (8) of H_{c2} (θ) is symmetrical with respect to the changes $\theta\to-\theta, \pi\pm\theta$, it is sufficient to consider the variation of the angle θ in the interval $(0, \pi/2)$. It is easy to make sure that for the angles $\theta=\pi/2, 0$ Eq. (8) has the values, which agree, to an accuracy of ε^2 and μ^2 inclusive, with the exact solutions found in Refs. 2, 7, and 8 for the given field orientations. For example, it follows from (8) that for $\theta=0$ the upper critical field depends on the sign of the difference $(\varepsilon^2-\mu)$. For orientations $\theta=0, \pi/2$ the angular dependence (8) of $H_{c2}(\theta)$ always has extrema. The analysis of Eq. (8) shows that for most allowed values of the parameters K_1 and K_4 there are no extra extrema (and, consequently, nonmonotonicities) in the angular dependence of the upper critical field. However for fairly rigid constraints on the ratio of the parameters K_1 and K_4 the function $H_{c2}(\theta)$ has one extra extremum in the interval $(0, \pi/2)$. This extremum is a minimum if

$$\varepsilon-\varepsilon^2-(2\varepsilon^2-\mu-\mu\varepsilon)\,\mathrm{sgn}(\varepsilon^2-\mu)<\frac{K_4}{K_1}-1$$
$$<\varepsilon+|\varepsilon|(1+\varepsilon)-\frac{(\varepsilon^2-2\mu)^2}{2|\varepsilon|}, \qquad (9)$$

and a maximum if both inequalities in (9) are reversed. In other cases the extra extremum is absent.

Parametric regions of existence of an extra extremum are conveniently shown in the plane with coordinates $\mu/|\varepsilon|$ and $(\zeta-1)/|\varepsilon|$, leaving only the first-order terms in ε and μ in inequalities such as Eq. (9) (see Fig. 2). In region I the upper critical field has an extra minimum and in regions II and III an extra maximum.

The relative magnitude and position of the extra extremum of the function $H_{c2}(\theta)$ depends considerably on the ratio of the parameters μ and ε. If the particle-hole asymmetry near the Fermi surface is not very large and $|\mu|\sim\varepsilon^2$ or smaller, the inverse inequalities (9) cannot hold. Therefore for $|\mu|\lesssim\varepsilon^2$ the function $H_{c2}(\theta)$ can have only an extra minimum if inequalities (9) hold in the range $\sin^2\theta_{\min}\sim|\varepsilon^2-\mu|/|\varepsilon|$. The relative depth of this minimum

$$[H_{c2}(0)-H_{c2}(\theta_{\min})]/H_{c2}(0)\sim|\varepsilon^2-\mu| \qquad (10)$$

has the second order of smallness in ε and is also characterized by a numerical factor smaller than or of order unity. Thus, the effect is not large in magnitude and special in character. Its origin is easy to understand, if we take it into account that to zeroth order in ε and μ the angular dependence of $H_{c2}^{(0)}$ is an ellipse with the ratio $(K_4/K_1)^{1/2}$ of the z and x axes. If $|\mu|\leqslant\varepsilon^2$, the angular dependence (8) in the intervals $\theta>\theta_{\min}$ and $\theta<\theta_{\min}$ also has the form of ellipses whose axes have a different ratio, and differing also from $(K_4/K_1)^{1/2}$ to the terms of order ε, μ and ε^2 (for $\theta>\theta_{\min}$ a fragment of one ellipse is realized, and for $\theta<\theta_{\min}$ a fragment of the other). If the initial ellipse had a small eccentricity (i.e., the parameter $(K_4/K_1)-1$ is sufficiently small), the axis changes due to the allowance for the terms of order ε, μ and ε^2 could result in the smaller axis changing into the larger one (e.g., in the range $\theta<\theta_{\min}$). The extra minimum in the $H_{c2}(\theta)$ dependence arises just in this case, when the difference between the large and small axes of the initial ellipse is relatively small [see Eq. (9)] and when the large axes of two ellipses, which are realized in the ranges $\theta>\theta_{\min}$ and $\theta<\theta_{\min}$, are perpendicular to each other. Since $\sin\theta_{\min}\lesssim|\varepsilon|^{1/2}$, we have for small values of $|\varepsilon|^{1/2}$, irrespective of the presence or absence of the extra minimum, a small deformation, in a relatively narrow interval $\theta<\theta_{\min}$, of the ellipse realized in a wide interval of angles $\theta>\theta_{\min}$.[9] In Fig. 3 we have plotted the function $H_{c2}(\theta)$ for $|\mu|\ll\varepsilon^2$, $\varepsilon=0.33$ and three values of the parameter $K_4/K_1=0.85$; 1.37; and 1.85. The second value satisfies the inequalities (9) and, correspondingly, the second curve in Fig. 3 has a small extra minimum. In Fig. 4 similar curves are plotted for $\varepsilon=0.33$, $\mu=-0.1$ ($|\mu|\approx\varepsilon^2$), and $K_4/K_1=0.75$; 1.05; and 1.58.

In the case $|\mu|\sim\varepsilon$, when the particle-hole symmetry near the Fermi surface is sufficiently broken, the extra extremum position is, generally speaking, no longer related to the

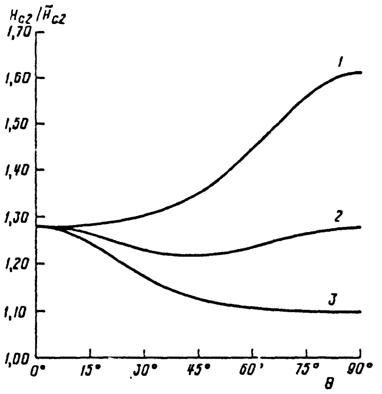

FIG. 3. The angular dependence of the upper critical field $H_{c2}(\theta)$ in the units of $\tilde{H}_{c2}=ac\zeta/(2|\varepsilon|K_4)$ for $\varepsilon=0.33$, $\mu=0$ and $K_4/K_1=0.85$; 1.37; and 1.85 (curves *1*, *2*, and *3*, respectively).

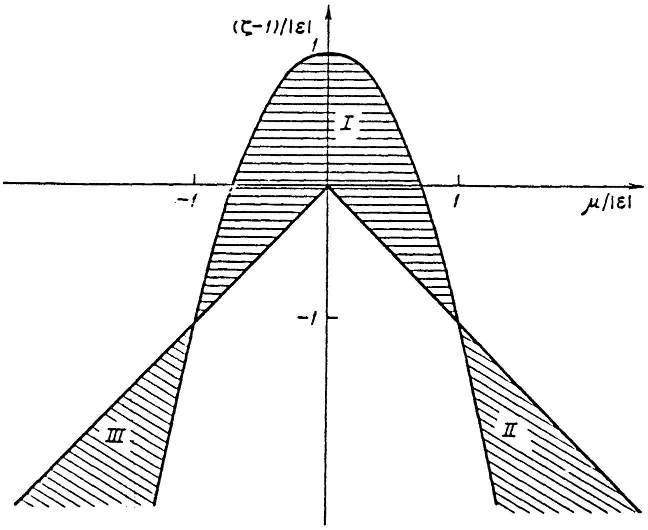

FIG. 2. The range of existence of extra extrema in the angular dependence of the upper critical field.

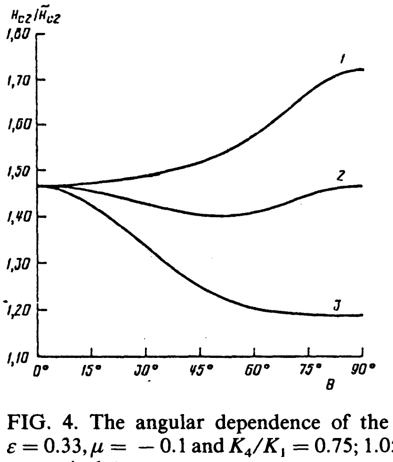

FIG. 4. The angular dependence of the upper critical field H_{c2} for $\varepsilon=0.33$, $\mu=-0.1$ and $K_4/K_1=0.75$; 1.05; and 1.58 (curves *1*, *2*, and *3*, respectively).

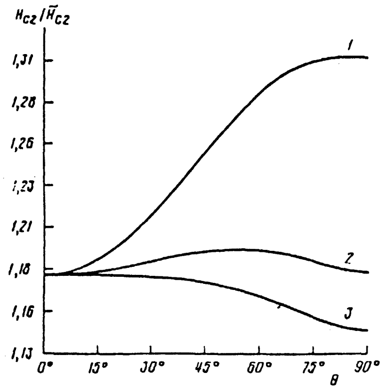

FIG. 5. The angular dependence of H_{c2} for $\varepsilon = 0.1$, $\mu = 0.15$ and $K_4/K_1 = 0.72$; 0.89; and 0.94 (curves *1*, *2*, and *3*, respectively).

small parameter and can be anywhere in the interval $(0, \pi/2)$, depending on the specific values of ε, μ and K_4/K_1. For $|\mu| < |\varepsilon|$ the function $H_{c2}(\theta)$ has an extra minimum in region I of Fig. 2, and for $|\mu| > |\varepsilon|$ a maximum in regions II and III. The relative magnitude of the extra extremum is of order $|\varepsilon|$ for $|\mu| \sim |\varepsilon| \sim |\zeta - 1|$. In the limit $|\zeta - 1| \gg |\mu| \gg |\varepsilon|$ its relative magnitude is $\mu^2/|\zeta - 1|$. In Fig. 5 we have plotted the angular dependence of the upper critical field for $\varepsilon = 0.1$, $\mu = 0.15$ ($|\mu| > |\varepsilon|$), and three different values of the parameter $K_4/K_1 = 0.72$; 0.89; and 0.94. The second value is in the region II of Fig. 2 and the relevant curve has an additional maximum in the interval $(0, \pi/2)$.

3. The method used above to calculate the angular dependence of the upper critical field is in many respects similar to the one previously used in Ref. 9 for the calculation of the anisotropy of the upper critical field and fluctuation diamagnetism in a rhombohedral exotic superconductor. In the particular case when the rhombohedral distortion of a crystal is absent, we have also obtained in Ref. 9 the expression for the anisotropy of H_{c2} in a hexagonal exotic superconductor. From the very beginning we have used the inequality $|\mu| \ll \varepsilon^2$ that restricts the applicability range of the result, and used perturbation theory in K_2/K_1. Expression (8), which is valid in fact for any ratio of the parameters ε and μ, is an important generalization of the result of Ref. 9. Our choice of the parameters ε and μ for the construction of perturbation theory seems to be adequate in the case of hexagonal exotic superconductors. In the particular case $|\mu| \ll \varepsilon^2$ expression (8) agrees with the corresponding result (22) of Ref. 9 to the needed accuracy, if the relation between the parameters ε, ζ and K_2/K_1 for $K_2 = K_3$ is allowed for (in Ref. 9 we have introduced the notation $P_1 = K_1$, $P_2 = K_4$, $P_3 = K_2 = K_3$ and $\alpha = \theta$). Discussing the anisotropy of the upper critical field in a hexagonal exotic superconductor, we have noted in Ref. 9 the absence of extra nonmonotonicities in the behavior of $H_{c2}(\theta)$. Such nonmonotonicities are really absent for most allowed values of the parameters K_4 and K_1. At the same time, as shown above, in a relatively narrow range of parameters (9) for $|\mu| \ll \varepsilon^2$, there is an extra minimum missed in Ref. 9, the magnitude of which has the second order of smallness. This remark does not alter the results of Ref. 9, only refines them.

The range of the parameters ε and μ in which the perturbation theory suggested above is applicable depends on the angle θ. This is seen already from simplest estimates based on the smallness (in comparison with unity) of the total contribution of the terms in ε and μ in the braces in Eq. (8). Thus, for $\theta = 0$ and $\varepsilon^2 < \mu$ we arrive at the inequality $|\mu| \ll 1$, and for $\varepsilon^2 > \mu$ we get $|2\varepsilon^2 - \mu| \ll 1$. At the same time, in the case $\theta = \pi/2$ we have $|\varepsilon| \ll 1$. On the other hand, since always $|\varepsilon| < 1$ and $|\mu| < 1$ (see Fig. 1), expression (8) can be regarded as approximately describing the anisotropy of the upper critical field almost in the whole range of allowed values of ε and μ. The real quantitative criterion of applicability of expression (8) for $H_{c2}(\theta)$ is its deviation from the exact solution. The use of the above exact solutions obtained for $\theta = 0$ and $\pi/2$ (see Refs. 2, 7 and 8) allows to find out that at least for these orientations the relative error of Eq. (8) is almost always very small. In fact, the exact expression for $H_{c2}(\theta = 0)$ for $\varepsilon^2 < \mu$ completely coincides with (8) for $\theta = 0$. If $\mu < \varepsilon^2$, the relative error $\Delta H_{c2}/H_{c2}$ of Eq. (8) for $\theta = 0$ is small in the whole range of the allowed values of ε and μ and reaches a maximum value of 10.1% for $\mu = 0$ and $|\varepsilon| = 0.5$. Note that the exact solution $H_{c2}(\theta = 0)$ for $\varepsilon^2 > \mu$ can be presented in the form of a power series in the parameters ε and μ, if $|2\varepsilon^2 - \mu + \mu^2/4| < 1$, when the function $(1 + 2\varepsilon^2 - \mu + \mu^2/4)^{1/2}$ can be expanded in such a series. For example, for $|\mu| \ll \varepsilon^2$ we find that $|\varepsilon| < 0.7$. Outside the given interval of ε and μ the perturbation theory used above is inapplicable for $\theta = 0$ and $\varepsilon^2 > \mu$. Equation (8) can be used under these conditions as an approximation.

For $\theta = \pi/2$ the exact solution $H_{c2}(\theta = \pi/2)$ and Eq. (8) do not depend on μ. The relative error of (8) grows with $|\varepsilon|$ and equals 0.25, 1.6, 7, 14, and 29.5% for $|\varepsilon| = 0.3$, 0.5, 0.7, 0.8, and 0.9, respectively. Thus, only in a narrow vicinity of two upper angles of the triangle in Fig. 1 is the relative error of Eq. (8) for $\theta = \pi/2$ large. Since this happens only near the boundary of the range of allowed parameter values and for $0.8 \leqslant \mu < 1$, which corresponds to a very strong particle-hole symmetry breaking, the above vicinities are of no interest. For the angles within the interval $(0, \pi/2)$ the relative error of Eq. (8) in the whole range of the allowed values of ε and μ is unknown. An exception is the values $|\varepsilon| \ll 1$ and $|\mu| \ll 1$, when the usual perturbation theory estimates in ε and μ are applicable. Nevertheless, the good accuracy of Eq. (8) for $\theta = 0$ and $\pi/2$ allows us to hope that it is quite satisfactory for all values of the angle θ and most allowed values of ε and μ.

In connection with the substantial effect of antiferromagnetism on the properties of the superconducting state in UPt_3 (see, e.g., Refs. 5 and 10–12), the question arises of the applicability range of Eq. (8) in the presence of antiferromagnetic ordering. As is well-known, antiferromagnetic ordering gives rise to splitting of the superconducting transition and to a change in the slope (a kink) of the temperature dependence of the upper critical field. According to Ref. 12, in the temperature range below the kink temperature, $T < T_k$, the antiferromagnetism, in effect, affects only the temperature T_c. Furthermore, experimental data indicate that in UPt_3

$$T_c - T_k \ll T_c$$

and the temperature dependence $H_{c2}(T)$ near T_k and somewhat below can be approximately considered linear.[13] Therefore for $T \leqslant T_k$, in a certain temperature range, the Ginzburg–Landau theory is still applicable. This leads to applicability of Eq. (8) for the angular dependence of the upper critical field in this temperature range.

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