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The surface energy and H_{c1} for a superconductor with a tricritical point

I A Fomin† and B Lyons

Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, Physikhochhaus, Postfach 6980, D-7500 Karlsruhe, Federal Republic of Germany

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Abstract. The energy of a plain boundary between a superconducting and normal region for a superconductor with a tricritical point is found as a function of the parameters entering the Ginzburg–Landau expansion of the free energy of such a superconductor. We define the regions of these parameters over which this energy is positive and negative. The structure of a quantized vortex is defined in the limit of large values of the parameter of Ginzburg and Landau, and the characteristic features of a temperature dependence of H_{c1} are discussed in comparison to those of usual superconductors.

1. Introduction

In recent years, much attention has been given to the investigation of superconducting materials which demonstrate anomalous properties and cannot properly be described by the conventional BCS theory. This calls for possible modifications to the theory, which could account for the observed anomalies. Even with a scalar order parameter in the Ginzburg–Landau theory, there are still new possibilities which have, as of yet, not been previously investigated. It was recently suggested by one of the authors [1], in connection with the anomalies observed in heavy-fermion superconductors, and in particular UPt_3, that in certain situations superconductivity could be exemplified as a first-order phase transition. Such a situation arises, naturally, if one allows for a negative coefficient in front of the quartic term in the Ginzburg–Landau expansion of the free energy, F_s. It is henceforth necessary to include the next-higher-order term into the expansion of the free energy, and under the usual assumptions, one arrives at the following expression for the density of the free energy:

$$F_s = F_n + a|\psi|^2 + b/2|v|^4 + d/3|v|^6 \tag{1}$$

where ψ is an order parameter which is assumed to be a scalar complex function. The change in sign of the coefficient b influences both the thermodynamic and magnetic properties of such a superconductor. The point at which b changes sign is known as a tricritical point (this will be referred as a TCP in what follows). In the vicinity of this point, the dependence of b on temperature and pressure (or density) has to be taken into account and this coefficient cannot be treated as a parameter of a given material any longer. Incorporation of a sixth-order term in expansion (1) brings about the ensuing change in the Ginzburg–Landau equations:

$$(1/4m)(-i\hbar\nabla - (2e/c)\boldsymbol{A})^2\psi - \partial F_s/\partial\psi^* = 0 \tag{2}$$

$$\text{curl curl } \boldsymbol{A} = (4\pi/c)\left[(ie\hbar/2m)(\psi^*\nabla\psi - \psi\nabla\psi^*) + (2e^2/mc)|\psi|^2\boldsymbol{A}\right]. \tag{3}$$

† Permanent address: L D Landau Institute for Theoretical Physics, Kosygin Street, GSP-117940 Moscow, Russia.

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The effect of this change can already be seen from a dimensional analysis of these equations. There are, as usual, two characteristic lengths in the problem as seen in [2]—a penetration depth δ and a correlation length ξ; they are expressed in terms of the coefficients a, b, d and the universal constants e, $\hbar$, m, c as in [1]:

$$\delta^2 = mc^2/8\pi e^2\psi_0^2 \qquad \xi^2 = -\hbar^2/4m(2a + b\psi_0^2)$$

where $\psi_0^2 = (\sqrt{b^2 - 4ad} - b)/2d$ is the equilibrium value of the order parameter. The ratio of these two lengths is referred to as the parameter of Ginzburg and Landau, denoted by κ:

$$\kappa^2 = (\delta/\xi)^2 = (1/2\pi)(mc/e\hbar)^2\sqrt{b^2 - 4ad} = (1/2b_0)\sqrt{b^2 - 4ad}$$

where the notation $b_0 = \pi(e\hbar/md)^2$ is introduced. The characteristic field is

$$H_0 = (\hbar c/2e)/\xi\delta.$$

Using δ and H_0 as the units, one can introduce dimensionless quantities; $\psi' = \psi/\psi_0$, $\tau' = \tau/\delta$, $B' = B/H_0$, $A' = A/H_0\delta$, $F_s' = (8\pi/H_0^2)F_s$. In these units, the coefficients entering expression (1) can be expressed in terms of one dimensionless parameter

$$\theta = b/\sqrt{b^2 - 4ad}.$$

Then, the dimensionless density of the free energy takes on the following form:

$$F_s' - F_n' = [(1+\theta)/2]|\psi'|^2 + (\theta/1)|\psi'|^4 + [(1-\theta)/6]|\psi|^6 \tag{4}$$

In dimensionless units, equations (2) and (3) have the form

$$\left(-(i/\kappa)\nabla' - A'\right)^2\psi' - [(1+\theta)/2]\psi + \theta\psi|\psi|^2 + [(1-\theta)/2]\psi|\psi|^4 = 0 \tag{5}$$

$$\text{curl curl } A' = (i/2\kappa)\left(\psi'^*\nabla\psi' - \psi'\nabla\psi'^*\right) - |\psi'|^2 A'. \tag{6}$$

In comparison to the usual case in [2], an additional dimensionless parameter θ enters into these equations. A superconducting phase can exist as thermodynamically stable for θ varying within the interval between $-2 < \theta < 1$. When $\theta = 1$, or equivalently, $a = 0$ in equation (1), one has a second-order phase transition line. When θ is close to unity, the sixth-order term in expansion (4) is small and the properties of a superconductor are defined by the first two terms, as in the usual case. The other boundary of the interval, i.e. $\theta = -2$, is a line of the first-order transitions ($3b^2 = 16$d). The dependence of ξ, δ and H_0 on temperature in the vicinity of a first-order transition line is different to the behaviour manifested by these quantities near a second-order transition line. Neither ξ nor δ diverge when $\theta < -2$; ξ diverges on approaching the boundary of overheating of a superconducting phase, which corresponds to $\theta \to -\infty$ (or $b^2 - 4ad$ in the usual units). When $\theta = -2$, the superconducting phase can exist only as a metastable phase. The characteristic field, H_0, does not coincide with the thermodynamic critical field, H_{cm}, and it remains finite upon a first-order transition; H_0 turns to zero as θ tends to the negative infinity.

Within the domain of stability of a superconducting phase, one can signify two more characteristic regions:

(1) the vicinity of $\theta = 0$ (or $b = 0$) where the properties of a superconductor are defined by an interplay between the first and the third term on the RHS of (4); and

(2) the vicinity of $\theta = -1$ (or $a = 0$, $b < 0$); where only the second and third terms on the RHS of (4) are of importance. The line $\theta = -1$ has the meaning of a limit of overcooling of the normal phase.

It should be pointed out also that of the parameters κ and θ can neither be considered as inherent constants of a particular material; they can vary with temperature even within the Ginzburg–Landau region.

The formal differences with respect to the usual case, which have been summarized above, give rise to changes in the physical properties of the superconductor in the vicinity of a TCP, or when b is negative. Some of these properties are anomalous with respect to the standard point of view. Such anomalies can be used to identify possible superconductors with a TCP. A general discussion of the thermodynamic and magnetic properties of superconductors with a TCP was given in [1]. A more systematic theoretical investigation into the nature of superconductors with a TCP would be of considerable benefit in the endeavour to find and validate superconductors with a TCP. In section 2, we find the surface energy, i.e. the energy of a phase boundary between a normal and a superconducting region of a superconductor with a TCP. In section 3, the characteristic features of the H_{c1} line for superconductors with a TCP are considered in comparison with those of a usual superconductor.

2. The surface energy

To find the energy of a phase boundary between a normal and superconducting region, we follow the usual scheme [2]. We orient the x axis perpendicular to the boundary. The magnetic field, $\boldsymbol{B}(x)$, is assumed to be parallel to the z axis. The vector potential can be chosen in the form $A_x = A_z = 0$, $A_y = A(x)$, and the order parameter can be assumed to be a real function. With these simplifications, equations (5) and (6) become equations in one dimension:

$$(1/\kappa^2)\mathrm{d}^2\psi/\mathrm{d}x^2 - A^2\psi + [(1+\theta)/2]\psi - \theta\psi^3 - [(1-\theta)/2]\psi^5 = 0 \qquad (7)$$

$$\mathrm{d}^2 A/\mathrm{d}x^2 - \psi^2 A = 0. \qquad (8)$$

The boundary conditions for this problem are

$$\psi \to 1 \qquad \mathrm{d}\psi/\mathrm{d}x \to 0 \qquad \mathrm{d}A/\mathrm{d}x \to 0 \qquad \text{at } x \to +\infty$$
$$\text{(in the superconducting region)} \qquad (9)$$

$$\psi \to 0 \qquad \mathrm{d}\psi/\mathrm{d}x \to 0 \qquad \mathrm{d}A/\mathrm{d}x \to \sqrt{(2+\theta)/6} \qquad \text{at } x \to -\infty$$
$$\text{(in the normal region).} \qquad (10)$$

The condition on $\mathrm{d}A/\mathrm{d}x$ in the normal region is due to the normalization of the field which is used here. As was shown earlier [1], the thermodynamic magnetic field H_{cm} is related to H_0 via $H_{cm}^2 = H_0^2(2+\theta)/6$. The system of equations (7) and (8) have a first integral

$$(1/\kappa^2)(\mathrm{d}\psi/\mathrm{d}x)^2 + (\mathrm{d}A/\mathrm{d}x)^2 - A^2\psi^2 + [(1+\theta)/2]\psi^2 - (\theta/2)\psi^4 - [(1-\theta)/6]\psi^6$$
$$= E = \text{constant.} \qquad (11)$$

For the boundary conditions (10), $E = (2+\theta)/6$. When a proper solution of equations (7) and (8) is found, the corresponding surface energy can be calculated with the aid of

$$\sigma_{\mathrm{n}} = \delta\frac{H_0^2}{4\pi}\int_{-\infty}^{+\infty}\left[\left(\frac{\mathrm{d}A}{\mathrm{d}x} - \sqrt{\frac{2+\theta}{6}}\right)\frac{\mathrm{d}A}{\mathrm{d}x} + \frac{1}{\kappa^2}\left(\frac{\mathrm{d}\psi}{\mathrm{d}x}\right)^2\right]\mathrm{d}x. \qquad (12)$$

Eventually, σ_{nr} is defined as a function of κ^2 and θ. At a given field, κ^2 and θ are constrained by the condition for the existence of two phases in equilibrium $H = H_{cm}(\kappa, \theta)$ or, as was shown earlier [1]

$$\kappa^6(1-\theta)^2(2+\theta) = (H/H_{\mathrm{d}})^2 \qquad (13)$$

where $H_d = \sqrt{(8/\pi/d)b_0^3/d^2}$ is a generic characteristic field of a material.

To begin with, let us find the surface energy for a zero magnetic field. In this case, two phases coexist at $\theta = -2$ and the integral (12) takes the form

$$\left(1/\kappa^2\right)(\mathrm{d}\psi/\mathrm{d}x)^2 - \tfrac{1}{2}\psi^2\left(1-\psi^2\right)^2 = 0. \qquad (14)$$

This equation is easily solved. The solution satisfying boundary conditions (9) and (10) is

$$\psi^2 = \tfrac{1}{2}\left[1 + \tanh\left((\kappa/\sqrt{2})x\right)\right] \qquad (15)$$

or, in the original units

$$\psi^2 = \tfrac{1}{2}\psi_0^2\left[1 + \tanh\left(x/\xi\sqrt{2}\right)\right] \qquad (16)$$

with $\psi_0^2 = -\frac{3}{4}b/d$ and $\xi = (\hbar/|b|)\sqrt{2d/3m}$. When solution (15), together with the condition that $B = \mathrm{d}A/\mathrm{d}x = 0$ is substituted into equation (12), we obtain

$$\sigma_{\mathrm{ns}}^{(0)} = H_0^2\xi/16\pi\sqrt{2} = (\hbar a/4)\sqrt{3/dm}. \qquad (17)$$

This energy is always positive. On the other hand, one knows that in the vicinity of $\theta = 1$, σ_{ns} is negative for $\kappa > 1/\sqrt{2}$. Regions of positive and negative σ_{ns} are separated in the θ, κ plane by a line $\kappa = \kappa_\sigma(\theta)$, on which the condition

$$\sigma_{\mathrm{ns}}(\theta, \kappa) = 0 \qquad (18)$$

is met. One point on this line is known [2], which is $\theta = 1$, $\kappa = 1\sqrt{2}$. Since, at $\theta = -2$, for all κ, σ_{ns} is positive we conclude that $\kappa_\sigma(\theta)$ tends to infinity as $\theta \to -2$. To find a leading term on the asymptotics of $\kappa_\sigma(\theta)$ at $\theta \to -2$, let us substitute expression (12) into equation (18) and rewrite it in the following form:

$$\frac{1}{\kappa^2}\int_{-\infty}^{+\infty}\left(\frac{\mathrm{d}\psi}{\mathrm{d}x}\right)^2\mathrm{d}x = \int_{-\infty}^{+\infty}\left(\sqrt{\frac{2+\theta}{6}} - \frac{\mathrm{d}A}{\mathrm{d}x}\right)\frac{\mathrm{d}A}{\mathrm{d}x}\mathrm{d}x. \qquad (19)$$

The integral on the LHS remains infinite at $\theta = -2$, and, in order to evaluate it in a leading order in $\theta + 2$, one can use (15). A straightforward integration gives the result $\kappa/4\sqrt{2}$. The evaluation of the RHS of equation (19) is effected by implementation of the fact that $\kappa \gg 1$ when θ is in the neighbourhood of -2; this, in turn, means that the characteristic range over which the magnetic field changes is much greater than the corresponding range of ψ. The main contribution to the integral comes from a region in which ψ, with good accuracy, is equal to the equilibrium value. We can assume that in (8), ψ changes at $x = 0$ discontinuously from 0 to 1. The solution to (8), satisfying the boundary conditions at both infinities, is then

$$\frac{\mathrm{d}A'}{\mathrm{d}x} = \begin{cases}\sqrt{(2+\theta)/6}\,\mathrm{e}^{-x} & x > 0 \\ \sqrt{(2+\theta)/6} & x < 0\end{cases}. \qquad (20)$$

Together with this and the equation for $\mathrm{d}A'/\mathrm{d}x$, the integral on the RHS of (19) is equal to $(2+\theta)/12$. Finally, we obtain for (19)

$$1/4\sqrt{2}\kappa = (2+\theta)/12$$

or

$$\chi_\sigma(\theta) = 3/\sqrt{2}(2+\theta). \qquad (21)$$

It turns out that equation (21), being a leading term in the expansion of $\chi_\sigma(\theta)$ on $2 + \theta$ at $\theta \to -2$ gives the correct result for $\theta = 1$ as well. One can expect that it will give

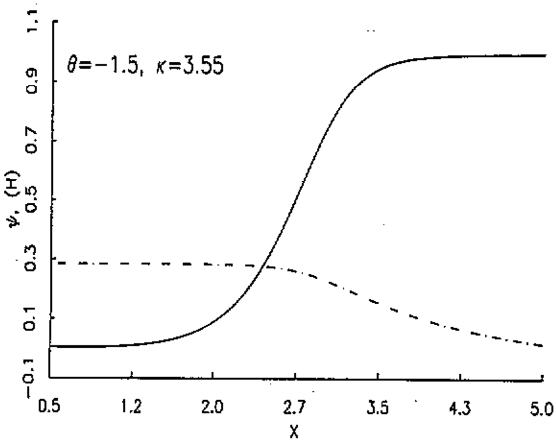

Figure 1. Variation of the order parameters ψ (full curve) and magnetic field H (dotted curve) in the domain wall for $\theta = -1.5$, $\kappa = 3.55$. The surface energy is zero for the values of θ and κ. All quantities are given in reduced units.

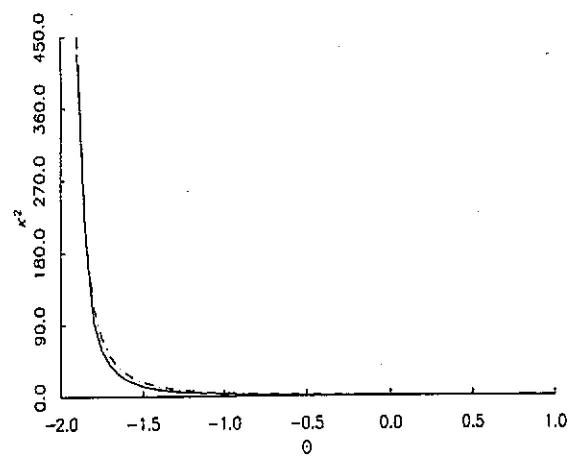

Figure 2. The full curve is a curve $\kappa_\sigma(\theta)$ on which $\sigma_{ns} = 0$, obtained by numerical solution of the problem. Below the line $\sigma_{ns} > 0$, whereas, above $\sigma_{ns} < 0$. The broken curve is the dependence $\kappa(\theta)$, given by asymptotic equation (21).

a reasonable result in the intermediate region. For a more exact evaluation of $\chi_\sigma(\theta)$ the problem was solved numerically. Some of the results of this analysis are represented in figures 1 and 2. Equation (21) turned out to be a good approximation for all θ. To resolve the difference between numerical and asymptotic results we had to plot, as depicted in figure 3, both curves in the θ and $1/\chi$ coordinates.

The curve of coexistence, (13) starts at $\theta = -2$ in a region of positive σ_{ns}, but, when the magnetic field increases, it goes into a region of larger θ and at a certain field, H_σ, it crosses the curve $H_\sigma(\theta)$ and σ_{ns} on the coexistence curves changes its sign. For heavy-fermion materials, which could be candidates for application of this analysis, typical values of κ are large ($\kappa \simeq$ 10–100), this means that in order to evaluate H_σ we can apply the asymptotic equation (21). Combining this equation with equation (13), one can obtain, in the limit $\kappa \gg 1$ the result

$$H_\sigma = H_0/2^{3/4}\sqrt{\kappa} \tag{22}$$

or, directly in terms of the coefficients b and d:

$$H_\sigma = \left(3\sqrt{\pi}/d\right)b_0^{1/4}(|b|/2)^{5/4}. \tag{23}$$

One can see from equation (22) that, for large κ, the interval of fields for which σ_{ns} is

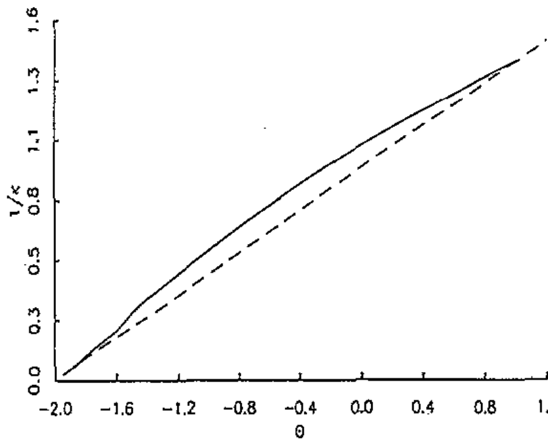

Figure 3. Comparison of the numerical solution for $\kappa_\sigma(\theta)$ with the asymptotic equation (21). In the coordinates θ, $1/\kappa$ asymptotic dependence (21) is represented by the straight line.

positive, is small in comparison to the characteristic field H_0. This reflects the tendency to approach the properties of a type-II superconductor with increasing κ.

3. Flux lines and H_{c1}

To specify the domain of existence of the Meissner phase, one needs to know the lower critical field H_{c1}, i.e. the field at which creation of quantized vortices becomes energetically advantageous. This field is defined by the energy F'_v of such a vortex per unit length [2]

$$H_{c1} = (\kappa/4\pi)F'_v. \tag{24}$$

In order to evaluate this energy, one has to find a proper solution of the Ginzburg–Landau equation. In contrast to the problem considered in the previous section, the order parameter is, in this case, an essentially complex function: $\psi = f e^{i\chi}$, and its phase changes by $2\pi n$ (n is an integer number) on any contour circumfering a vortex line. Following the usual procedure [2, 3], we discuss only one-quantum cylindrically symmetric vortex.

The equations of Ginzburg and Landau in that case can be written, as in [3]

$$(1/\kappa^2\rho)(d/d\rho)(\rho\, df/d\rho)^2 - (1/f^3)(dB/d\rho)^2 + [(1+\theta)/2]f - \theta f^2 - [(1-\theta)/2]f^5 - 9 \tag{25}$$

$$(1/\rho)(d/dp)\big[(\rho/f^2)(dB/d\rho)\big] = B. \tag{26}$$

The boundary conditions on the vortex are

$$f \to 1 \qquad B \to 0 \qquad dB/d\rho \to 0 \qquad \text{as } \rho \to \infty \tag{27}$$

$$f \to 0 \qquad \big(1/f^2\big)dB/d\rho \to -1/\kappa\rho \qquad \text{as } \rho \to 0. \tag{28}$$

The energy of the vortex line in dimensionless units can be calculated from the equation

$$F'_v = 2\pi \int \left[2\big(F_s(f) - F_s(1)\big) - f^2 \frac{\partial F_s}{\partial (f^2)}\right]\rho\, d\rho \tag{29}$$

which, for the energy (4) gives

$$F'_v = \frac{\pi}{3}\int \big(1 - f^2\big)\Big[2(2+\theta) + (1-\theta)f^2\big(1+f^2\big)\Big]\rho\, d\rho. \tag{30}$$

It can easily be verified that equations (25) and (26) become essentially θ dependent when either $(1-f) \ll 1$ or $f \ll 1$ are satisfied. Consequently the dependence of f on ρ, in the asymptotic limit as ρ tends to 0 and as ρ tends to ∞, is insensitive to varying θ. Varying the value of θ influences the behaviour of f in the 'core' region $\rho \simeq 1/\kappa$.

We consider the most interesting situation in the sense of possible application, i.e. $\kappa \gg 1$. In such a case, we use simplifications arising from the difference in the characteristic scales of the variation of the magnetic field and the order parameter [2]. In the range of ρ in which the most significant contribution to the integral occurs, it is possible to equate f to unity in finding B from equation (26), and the asymptotic value of B, as ρ tends to 0 ($\rho \ll 1$), can be substituted into the equation determining f. Then one arrives at the following equation for f:

$$\left(1/\kappa^2\rho\right)(\mathrm{d}/\mathrm{d}\rho)(\rho\,\mathrm{d}f/\mathrm{d}\rho) - \left(1/\kappa^2\rho^2\right)f + \tfrac{1}{2}f\left(1-f^2\right)\left[(1+\theta)+(1-\theta)f^2\right] = 0. \qquad (31)$$

As in the usual case, the principal contribution to the integral in equation (30) comes from that region of ρ in which $1 \gg \rho \gg \kappa^{-1}$ is fulfilled. In that region, the proper solution of (31) is

$$f^2 = 1 - 1/\kappa^2\rho^2.$$

Substitution of this expression into equation (30) gives

$$F'_{\mathrm{v}} = \frac{2\pi}{\kappa^2}\int_{1/\kappa}^{1}\frac{\mathrm{d}\rho}{\rho} = \frac{2\pi}{\kappa^2}\ln\kappa$$

which in turn gives for H_{c1}

$$H_{c1} = \left(H_0/2x\right)\ln\kappa. \qquad (32)$$

As was discussed in the introduction, the field H_0 remains finite at T_c and becomes zero only when the limit of overheating is reached. This means that the line $H_{c1}(T)$ crosses the line $H_{cm}(T)$ at a finite field. Comparison of (22) with (32) reveals that the intersection of $H_{c1}(T)$ with $H_{cm}(T)$ does not coincide with the point where the surface energy is zero on H_{cm}. The latter point, i.e. the point where the surface energy turns to zero, is larger than the former point and the surface energy is still positive at the point at which $H_{c1}(T)$ intersects $H_{cm}(T)$. This reflects the fact that the geometry of a vortex is energetically more advantageous for the penetration of a magnetic field into a superconductor as opposed to the geometry of a plain wall.

4. Discussion

Both the surface energy and the characteristic features of temperature dependence of H_{c1} can be used as an experimental identification of superconductors with a TCP. The surface energy defines the structure of the intermediate state of superconductors. Such a state can be realized in a superconductor with a TCP if the sample under investigation is of a suitable form, and if the magnetic field at which transition takes place is smaller than H_{c1}. Observation of the intermediate state would show directly that σ_{ns} is positive, that the superconducting and normal phase coexist and that the phase transition is of the first order. Resolution of the structure of the intermediate state would make it possible to extract the values of the surface energy from experimental data and to compare it with the present calculations.

For H_{c1}, the qualitatively new feature in the curve of $H_{c1}(T)$ is its intersection with the curve $H_{cm}(T)$ at a finite H. For usual type-II superconductors, three curves $H_{c1}(T)$,

$H_{cm}(T)$ and $H_{c2}(T)$ intersect at one point $T = T_c$, where all three fields are zero. For a superconductor with a TCP, only $H_{cm} = 0$ at T_c; $H_{c2}(T)$ extrapolates into the point of overheating of the superconducting phase.

In [1], the possibility of UPt_3 being a superconductor with a TCP was discussed. The existing data on H_{c1} for this material [4] do not show the anomalies discussed above. It should be mentioned in that respect that, for observation of the anomalies, one needs particularly accurate measurement in the vicinity of T_c, where H_{c1} becomes smaller. The measurements in this region are not sufficiently accurate, which leaves room for further speculation. We mention here, for completeness, one more characteristic feature of the magnetic behaviour of a superconductor with a TCP, which can be used for its identification in low-field experiments, which is the vertical tangent of dependence of a critical field on temperature at T_c.

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