Upper critical field in the extended saddle-point model

A. A. Abrikosov
Materials Science Division, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439
(Received 10 April 1997)

The dependence of the upper critical field on temperature for all temperatures is calculated in the framework of the extended saddle-point model. A discussion is given of the present experimental situation. [S0163-1829(97)00634-6]

I. Introduction. In the previous paper[1] the Ginzburg-Landau (GL) equations for the model based on the dominance of extended saddle points in the electron spectrum were derived and, as an example, the critical magnetic field H_{c2} parallel to the c axis was calculated. Its temperature dependence had a positive curvature, which was attributed to the fact that in the model under consideration, the motion of Cooper pairs becomes increasingly one-dimensional with departure from T_c. This feature reproduced the experimental trend for different high-T_c cuprates, provided that their critical temperature was sufficiently suppressed by underdoping, overdoping, or strongly scattering impurities. It was believed that H_{c2} could be defined from the resistive transition, because the latter was rather sharp even in magnetic field. Since then measurements of specific heat in magnetic field were performed, and the curve $H_{c2}(T)$, defined from the step in $C(T)$, differed from the one obtained by the resistive transition. Unfortunately, these data were available only for temperatures in the vicinity of T_c.

In the paper[1] we did not attempt to make a numerical comparison with experiment, since the latter would require the knowledge of the curve $H_{c2}(T)$ at all temperatures, from zero to T_c, and the GL equations were applicable only in the vicinity of T_c. From what was said it follows that the existing experimental data are controversial, and hence, now is not the best time to perform such a comparison. Nevertheless, we believe that it is useful to derive the complete dependence $H_{c2}(T)$ and to discuss the existing situation together with some additional options.

In the paper[1] it was shown that, if the coefficient η, defining the connection between different ''one-dimensional'' momentum regions, is small enough, H_{c2} becomes infinite within the limits of applicability of the GL theory. This conclusion did not take into account the paramagnetic mechanism of the destruction of Cooper pairs; hence, in order to obtain meaningful results, this mechanism has also to be considered.

II. Quasiclassical Equations. We will base our calculation on the method developed by Gor'kov for isotropic superconductors.[2] The difference will be that we have to consider two vicinities of singular regions, a and b. The linear equations defining an infinitesimal nucleus of the superconducting phase will be (see Refs. 1, 2):

$$\Phi_a^*(\rho)=T\sum_\omega \int G^a_{-\omega 11}(\rho',\rho)G^a_{\omega 22}(\rho',\rho)[\lambda_1\Phi_a^*(\rho') +\lambda_2\Phi_b^*(\rho')]d\rho', \tag{1a}$$

$$\Phi_b^*(\rho)=T\sum_\omega \int G^b_{-\omega 11}(\rho',\rho)G^b_{\omega 22}(\rho',\rho)[\lambda_1\Phi_b^*(\rho') +\lambda_2\Phi_a^*(\rho')]d\rho', \tag{1b}$$

where $G^a_{-\omega 11}(\rho',\rho)$ means the normal-metal Green function for the vicinity a and spin projection 1/2, and similarly for G^b; $\rho=(x,y)$; the definitions of Φ_a, Φ_b, λ_1, and λ_2 are given in Ref. 1. The functions $G^{a,b}(\rho',\rho)$ satisfy the equations

$$[i\omega-v_1(-i\partial/\partial x)+\beta H\sigma_z]G^a_\omega(\rho,\rho')=\delta(\rho-\rho'), \tag{2a}$$

$$[i\omega-v_1(-i\partial/\partial y-eHx/c)+\beta H\sigma_z]G^b_\omega(\rho,\rho')=\delta(\rho-\rho'), \tag{2b}$$

where β is the Bohr magneton, and we introduced the vector potential $A_y=Hx$. From these equations we see that G^a is proportional to $\delta(y-y')$, and G^b to $\delta(x-x')$. Now we will use the transformation proposed in Ref. 2:

$$G^{a,b}(\rho,\rho')=\exp[i(eH/2c)(y-y')(x+x')]\widetilde{G}^{a,b}(\rho-\rho'). \tag{3}$$

Taking into account the factors $\delta(x-x')$ and $\delta(y-y')$ in the corresponding G, we obtain

$$G^a(\rho,\rho')=\widetilde{G}^a(x-x')\,\delta(y-y'), \tag{4a}$$

$$G^b(\rho,\rho')=\exp[i(eH/c)(y-y')x]\widetilde{G}^b(y-y')\,\delta(x-x'). \tag{4b}$$

Substituting these expressions into Eqs. (2a), (2b) we get ''free'' one-dimensional equations for $\widetilde{G}^a(x-x')$ and $\widetilde{G}^b(y-y')$, and hence we may conclude that they correspond to Green functions in the absence of magnetic field, except for the paramagnetic term.

As in Ref. 1, we assume that $\Phi_{a,b}$ depend only on x, and introduce the notations

$$Q(x,x')=\int G^a_{-\omega 11}(\rho',\rho)G^a_{\omega 22}(\rho',\rho)dy', \tag{5a}$$

$$R(x,x')=\int G^b_{-\omega 11}(\rho',\rho)G^b_{\omega 22}(\rho',\rho)dy'. \tag{5b}$$

We will consider for definiteness the more common case with an odd order parameter, $\lambda_2<0$ (d wave), and rewrite Eqs. (1) in the form

$$\left[\int Q_0(x-x')dx'-(\lambda_1+|\lambda_2|)^{-1}\right]\Phi_a^*(x)-\eta[\Phi_a^*(x)+\Phi_b^*(x)]+\int Q_1(x'-x)\Phi_a^*(x')dx'=0, \tag{6a}$$

$$\left[\int Q_0(x-x')dx'-(\lambda_1+|\lambda_2|)^{-1}\right]\Phi_b^*(x)-\eta[\Phi_a^*(x)+\Phi_b^*(x)]+\int R_1(x'-x)\Phi_b^*(x')dx'=0, \tag{6b}$$

where $Q_0\equiv R_0$ are the kernels in absence of the magnetic field, $Q_1=Q-Q_0$, $R_1=R-Q_0$, $\eta=|\lambda_2|/(\lambda_1+|\lambda_2|)^2$. We assumed that $|\lambda_2|\ll(\lambda_1+|\lambda_2|)$, and substituted in the second term of Eqs. (6) Q and R by Q_0, which to the first approximation is defined by neglecting the second and third terms in Eqs. (6). According to Ref. 1 and the previous papers on the same model quoted therein, the square bracket in the first term of Eqs. (6) can be replaced by $\tau=\ln(T_c/T)$.

III. Variational Principle. Both Eqs. (6) can be obtained from a variational principle by defining the minimum of

$$\tau=\left[-\int\Phi_a^*(x')Q_1(x'-x)\Phi_a(x)dx\,dx'-\int\Phi_b^*(x')R_1(x'-x)\Phi_b(x)dx\,dx'+\eta\int|\Phi_a(x)+\Phi_b(x)|^2dx\right]\Big/\int[|\Phi_a(x)|^2+|\Phi_b(x)|^2]dx. \tag{7}$$

Now everything becomes rather similar to the case $\tau\ll1$, considered in Ref. 1.

Let us first calculate Q_1 and R_1. The Fourier component of Q_1 is

$$Q_1(k)=T\sum_{-\infty<\omega<\infty}\int_{-\infty}^{\infty}d\xi\times\left[\frac{1}{(-i\omega-\xi+\beta H+v_1k)(i\omega-\xi-\beta H)}-\frac{1}{\omega^2+\xi^2}\right]=\psi\left(\frac{1}{2}\right)-\mathrm{Re}\;\psi\left(\frac{1}{2}+\frac{iv_1k}{4\pi T}+\frac{i\beta H}{2\pi T}\right), \tag{8}$$

where $\psi(x)$ is the digamma function. Compared to the value in the absence of the field the function R contains a factor $\exp[(2ieH/c)x(y'-y)]$, which can be considered as resulting from the change in the p_y momentum. Therefore, similarly to Q_1, we obtain

$$R_1(x)=\psi\left(\frac{1}{2}\right)-\mathrm{Re}\;\psi\left(\frac{1}{2}-\frac{ieHv_1x}{2\pi Tc}+\frac{i\beta H}{2\pi T}\right). \tag{9}$$

Since this case is more difficult than $\tau\ll1$, considered in Ref. 1, we will use trial functions from the start and take them the same, as in Ref. 1:

$$\Phi_a(x)=\exp[-(2eH\gamma_a/c)x^2], \tag{10a}$$

$$\Phi_b(x)=-q\,\exp[-(2eH\gamma_b/c)x^2]. \tag{10b}$$

The calculation of the term with Q_1 in the functional (7) is easier to perform in Fourier components, whereas for the term with R_1 it is simpler to use formulas (10). The ψ functions can be presented in the integral form:

$$\psi(z)=\int_0^{\infty}\left(\frac{e^{-t}}{t}-\frac{e^{-zt}}{1-e^{-t}}\right)dt, \tag{11}$$

and hence,

$$\psi\left(\frac{1}{2}\right)-\psi\left(\frac{1}{2}+x\right)=\int_0^{\infty}\frac{e^{-xt}-1}{2\sinh(t/2)}\,dt. \tag{12}$$

After straightforward calculations we obtain from Eq. (7)

$$\tau=\eta-\frac{2\sqrt{2}\,\eta qs}{(1+s^2)^{1/2}(1+q^2s)}+\frac{1}{2(1+q^2s)}\int_0^{\infty}\frac{1-\exp[-v_1^2(eH/c)s^2\gamma_bt^2/(4\pi T)^2]\cos(\beta Ht/2\pi T)}{\sinh(t/2)}\,dt+\frac{q^2s}{2(1+q^2s)}\int_0^{\infty}\frac{1-\exp[-v_1^2(eH/c)t^2/(8\pi T)^2\gamma_b]\cos(\beta Ht/2\pi T)}{\sinh(t/2)}\,dt, \tag{13}$$

where we introduced $s=(\gamma_a/\gamma_b)^{1/2}$ (in Ref. 1 we used the notation β for this quantity but here we keep β as the standard symbol for the Bohr magneton).

Expression (13) has to be minimized over three parameters: γ_b, q, and s. The task is easier than it seems from the start. If we denote the integrals in the two last terms by $F(s^2\gamma_b)$ and $F(1/4\gamma_b)$ and look for extrema with respect to γ_b and q, we get very easily

$$\gamma_b=1/(2s),\quad q^2s=1. \tag{14}$$

After that the functional τ acquires the form

$$\tau=\eta\left[1-\left(\frac{2s}{1+s^2}\right)^{1/2}\right]+\frac{1}{2}\int_0^\infty \frac{1-\exp[-\mu_1(eH/m_xc)st^2/(4\pi T)^2]\cos(\beta Ht/2\pi T)}{\sinh(t/2)}\,dt, \tag{15}$$

and only minimization with respect to s remains (here we introduced $\mu_1=m_xv_1^2/2$ as the chemical potential, calculated with respect to the extended saddle-point energy). Close to T_c we can set $\cos(\beta Ht/2\pi T)\approx 1$ and expand $\exp[-\mu_1(eH/m_xc)st^2/(4\pi T)^2]$. After that we obtain

$$\tau=\eta\left[1-\left(\frac{2s}{1+s^2}\right)^{1/2}\right]+\frac{7\zeta(3)}{8}\frac{\mu_1 eH}{m_xc(\pi T)^2}\,s. \tag{16}$$

If we put in the last term $T=T_c$, this coincides with Eq. (33) in Ref. 1 from which $H_{c2}(T)$ was obtained. Since the GL equations are derived under the assumption $\tau\approx(T_c-T)/T_c \ll 1$, the conclusion about the positive curvature can be done, strictly speaking, only for $\eta\ll 1$. It is rather evident that for sufficiently large η the problem will be two-dimensional up to $\tau=0$. This can be established by expansion of the integral in Eq. (15) up to second order and accurate calculation of $H_{c2}(T)$ up to terms $\sim\tau^2$. We will not reproduce here this simple but cumbersome calculation; the curvature at $\tau\to 0$ will be negative, if $\eta>7.25$. Such large values are unrealistic, and therefore we can conclude that for our model the curvature will always be positive in the vicinity of T_c.

In the general case we can denote

$$f=\frac{\mu_1 eH}{m_xc(4\pi T)^2},\quad g=\frac{\beta H}{2\pi T},\quad r=\frac{g}{\sqrt{fs}}. \tag{17}$$

Introducing in the integral term of Eq. (15) a new variable $u=t\sqrt{fs}$, and differentiating with respect to r we obtain

$$\tau=\eta\left[1-\left(\frac{2s}{1+s^2}\right)^{1/2}\right]+\frac{1}{2}\int_0^\infty\frac{1-e^{-fst^2}}{\sinh(t/2)}\,dt$$
$$+\frac{1}{2\sqrt{fs}}\int_0^r dr_1\int_0^\infty \frac{ue^{-u^2}\sin(r_1u)}{\sinh(u/2\sqrt{fs})}\,du. \tag{18}$$

IV. Limiting Cases. Let us consider the case of low temperatures. We will see that in this case the parameter s corresponding to H_{c2} will be small but finite, and $fs\gg 1$. The second term on the right-hand side of Eq. (18) up to terms of the order $1/(fs)$ is then

$$(1/2)\ln(16\gamma fs)+1/(48fs), \tag{19}$$

where $\gamma=e^C=1.78$. The third term is in the same case and with the same accuracy

$$\int_0^r Q\left(\frac{r_1}{2}\right)dr_1+\frac{1}{48fs}\left[\left(\frac{r^2}{2}-1\right)Q\left(\frac{r}{2}\right)-\frac{r}{2}\right], \tag{20}$$

where

$$Q(x)=e^{-x^2}\int_0^x e^{u^2}du. \tag{21}$$

This function can be expressed in terms of the error function, namely,

$$Q(x)=-(\sqrt{\pi}/2)\; ie^{-x^2}\Phi(ix).$$

In order to find the necessary value of s, we neglect first the terms proportional to $1/(fs)$ and express s in terms of r, see Eq. (17):

$$\frac{1}{2}\ln\left[\frac{\gamma\mu_1(eH/m_xc)}{(\pi T_c)^2}\right]=-\eta+\ln\frac{\sqrt{f}}{g}+\ln r$$
$$-\int_0^r dr_1 e^{-r_1^2/4}\int_0^{r_1/2}e^{u^2}du. \tag{22}$$

The maximum of the right-hand side is reached at $r=1.86$, and at this value the sum of the last two terms on the right is equal to -0.0433. If we substitute the definitions of f and g into the term $\ln(\sqrt{f}/g)$ we get $(1/2)\ln[(\mu_1/2\beta H)(m/m_x)]$. This term does not depend explicitly on temperature. Transferring it to the left-hand side of Eq. (22) and remembering that the maximum value of the r-dependent term is -0.0433 we get the ''paramagnetic'' critical field at zero temperature

$$\beta H_{c2}(0)/T_c=1.127e^{-\eta}. \tag{23}$$

One sees from here that in case the singularities in the electron spectrum are not connected, i.e., $\eta=0$, the only mechanism of destruction of superconductivity is the paramagnetic effect. With increasing η, however, the role of orbital motion becomes rapidly very important.

The temperature dependence at low temperatures is defined by the terms of the order $1/(fs)$ in formulas (19), (20), and we get

$$\frac{H_{c2}(T)-H_{c2}(0)}{H_{c2}(0)}=-1.04e^{2\eta}\left(\frac{T}{T_c}\right)^2. \tag{24}$$

The conditions of applicability of this approximation are $s \ll 1$ and $fs\gg 1$. Since $s\sim g^2/f$, we get $T\ll\beta H\ll\mu_1$, or $T \ll T_ce^{-\eta}$.

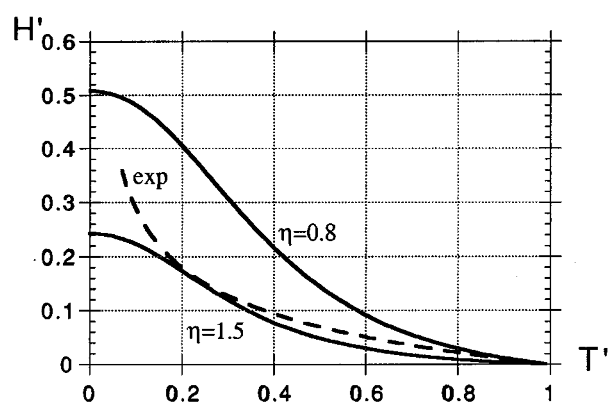

FIG. 1. The theoretical dependences of $H'=\beta H_{c2}/T_c$ on $T'=T/T_c$ for $\eta=0.8$ and $\eta=1.5$ together with the experimental curve obtained from the resistive transition (Ref. 3).

In order to trace the crossover from the regime close to T_c, where H_{c2} is defined by the orbital motion, to the paramagnetic regime, it will be more convenient to consider the case of small η, despite the fact that it, most likely, does not describe the true substances. As we know from Ref. 1, in this case the rapid increase of $H_{c2}(T)$ happens in the vicinity of T_c, and we can suppose that the most important region is not far from this point. Both coefficients, f and g, can be assumed to be small, and we expand the last term in Eq. (15). We get

$$\tau=\eta\left[1-\left(\frac{2s}{1+s^2}\right)^{1/2}\right]+\frac{7\zeta(3)}{4(\pi T_c)^2}\left[\mu_1\beta_x Hs+(\beta H)^2\right], \quad (25)$$

where $\beta_x=e/(2m_x c)=\beta(m/m_x)$. Minimizing over s and considering limiting cases we obtain

$$\beta H_{c2}(T)=\begin{cases}\dfrac{2(\pi T_c)^2(m_x/m)}{7\zeta(3)\mu_1}\dfrac{\eta^2}{\eta-\tau} \quad \eta-\tau>0, \quad \eta-\tau\gg(T_c/\mu_1)^{2/3}\eta^{4/3} & (26a)\\ \dfrac{2\pi}{\sqrt{7\zeta(3)}}T_c(\tau-\eta)^{1/2} \quad \tau-\eta>0, \quad |\eta-\tau|\gg(T_c/\mu_1)^{2/3}\eta^{4/3} & (26b)\end{cases}$$

and

$$\beta H_{c2}(T)=2\left(\frac{(\pi T_c)^4\eta^2(m_x/m)}{[7\zeta(3)]^2\mu_1}\right)^{1/3}\times\left[1+\frac{1}{3}\left(\frac{\mu_1^2[7\zeta(3)]}{(\pi T_c)^2(m_x/m)^2\eta^4}\right)^{1/3}(\tau-\eta)\right],$$
$$|\eta-\tau|\ll(T_c/\mu_1)^{2/3}\eta^{4/3} \quad (27)$$

(m is the free-electron mass). From this example we see that the crossover between the two regimes (26a) and (26b), happens smoothly.

V. Discussion. If we introduce the variables $T'=T/T_c$ and $H'=\beta H/T_c$, then Eq. (15) depends on two fitting parameters. They can be established from the behavior of H' at $T'\to 0$ [η can be found from Eqs. (23) or (24)] and at $T'\to 1$; the slope at this point is

$$-\left(\frac{dH'}{dT'}\right)_{T'=1}=\frac{4\pi^2 T_c(m_x/m)}{7\zeta(3)\mu_1}. \quad (28)$$

The comparison with experiment, until recently, was easy, since there existed numerous experimental data on $H_{c2}(T)$, and the best of them were the data by Mackenzie *et al.*[3] for $Tl_2Ba_2CuO_{6+\delta}$, where $H_{c2}(T)$ was measured down to less than 20 mK. Unfortunately, these data, with $H_{c2}(T)$ defined from the resistive transition, were not confirmed by subsequent measurements of specific heat for the same substance,[4] and that caused suspicions that the resistive transition measures the melting field of the vortex array rather than the real H_{c2}. Moreover, measurements of the specific heat on extremely pure samples of $YBa_2Cu_3O_7$ in a magnetic field[5] clearly showed two features: a step at a higher temperature and a peak at a lower one; the latter depended on the field similarly to the resistive transition. The step, which could be interpreted as evidence of the true H_{c2}, corresponded to significantly higher fields at a given temperature. Unfortunately, this step is smeared out and reduced at low temperatures, and, therefore, it cannot be used for a detailed comparison of theory with experiment. In Fig. 1 we placed two theoretical curves, for $\eta=0.8$ (upper curve) and $\eta=1.5$ (lower curve) and experimental data for the resistive transition from Ref. 3 (dashed curve). The slope at $T'=1$ was adjusted to the experimental curve. Nevertheless, the trends are quite different.

Even without experimental data on the specific heat one could become suspicious, because in the low-temperature region the critical field obtained in Ref. 3 was of the order of the paramagnetic limit ($H'\sim 1$), and in this case the curve must become flat close to $T=0$.

Therefore it is very desirable to find a reliable method to measure $H_{c2}(T)$. In this connection the experiments on Josephson plasmons in high-T_c cuprates (see Refs. 6–8) may be of considerable interest due to the fact that such plasmons exist only in the superconducting state, and they do not disappear even in the melted vortex regime. The latter was shown theoretically and confirmed by experiment. One can hope that the disappearance of such plasmons happens at H_{c2}, or somewhere close to this field.

I would like to express my gratitude to Dr. A. P. Mckenzie and Dr. A. Carrington for useful discussions. This work was supported by the U.S. Department of Energy under Contract No. W-31-109-ENG-38.

[1] A. A. Abrikosov, Phys. Rev. B **56,** 446 (1997).
[2] L. P. Gor'kov, Sov. Phys. JETP **37**, 593 (1960).
[3] A. P. Mackenzie *et al.*, Phys. Rev. Lett. **71**, 1238 (1993).
[4] A. Carrington, A. P. Mackenzie, and A. Tyler, Phys. Rev. B **54**, R3788 (1996).
[5] A. Junod *et al.*, Physica C **27**, 245 (1997).
[6] N. P. Ong *et al.*, Phys. Rev. Lett. **73**, 724 (1994).
[7] Y. Matsuda *et al.*, Phys. Rev. Lett. **75**, 4512 (1995).
[8] Y. Matsuda *et al.*, Phys. Rev. Lett. **78**, 1972 (1997).