d-wave-induced angular dependence of surface superconductivity

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(Received 23 June 1997; revised manuscript received 17 February 1998)

The Ginzburg-Landau theory is used to estimate the d-wave correction to the critical field H_{c2} and to H_{c3}, the superconducting critical field in the presence of a surface. The correction to H_{c3} is dependent on the angle of orientation of the crystal lattice with respect to the surface of the sample while that due to H_{c2} is a constant. This angular-dependent shift in H_{c3}, if experimentally observable, would be an indication of the pairing state of the superconductor. [S0163-1829(98)06026-3]

In recent years the pairing state of high-temperature superconductors has been the subject of great theoretical and experimental interest. There have been numerous recent studies regarding the nature of the pairing state and its relationship to vortex structure.[1–5]

In this paper it will be shown in the spirit of the Ginzburg-Landau theory that there is a d-wave-induced shift in the critical field H_{c2} of high-temperature superconductors. More importantly, the critical field in the presence of a surface H_{c3} has a characteristic dependence on the angle of orientation of the crystal lattice to the sample surface. Given bulk samples with various specific orientations of the crystal lattice to the surface (specific, as there are preferred directions to be able to form smooth, well characterized surfaces), this effect should, in principle, be experimentally observable giving an indication of the pairing state.

The contents of the paper will now be summarized. Firstly the extended Ginzburg-Landau equation with an anisotropic term is presented. The critical fields H_{c2} and H_{c3} in the absence of the anisotropic term are then obtained by a standard variational procedure. Thereafter, the corrections to the critical fields associated with the extended Ginzburg-Landau equation are obtained perturbatively assuming the prefactor (D) of the anisotropic term to be small. This assumption is justified later in the paper. The next step is to study the effect of diffuse scattering due to surface quality; the calculation is extended for general boundary conditions incorporating a phenomenological parameter γ. The cosinusoidal angular dependence of H_{c3} is seen to persist over a significant range of γ enhancing the possibility of experimental observation. The dimensionless prefactor D is next estimated from the microscopic theory of Maki *et al.*[6,7] D is seen to be small in the regime where the Ginzburg-Landau theory is valid, justifying the perturbation theory used. An examination of the microscopic results[6,7] shows that D increases significantly as temperature decreases suggesting that a substantial effect might exist at low temperatures. In conclusion, the results of the paper are summarized and experimental issues are briefly discussed.

The first step is to write the Ginzburg-Landau free-energy density with a term incorporating d-wave contributions. Such a term could arise from a treatment involving s and d-wave order parameters simultaneously,[1,8–10] or from higher-order Ginzburg-Landau free energy terms:[11,12,18]

$$f=\beta|\psi|^2+\frac{1}{2m^*}|\Pi\psi|^2+\frac{D}{2m^*}\frac{\xi^2}{2\hbar^2}|(\hat{\Pi}_x^2-\hat{\Pi}_y^2)\psi|^2, \quad (1)$$

where

$$\hat{\Pi}=\left(-i\hbar\nabla-\frac{2e\vec{A}}{c}\right), \quad (2)$$

$m^*=2m_e$, m_e being the electron mass, and $e=$electron charge. Also,

$$\beta=\alpha\left(\frac{T}{T_c}-1\right)=\frac{\hbar^2}{2m^*\xi^2}, \quad (3)$$

where ξ is the coherence length. The factor $\xi^2/2\hbar^2$ is chosen for later convenience and to make D, the prefactor of the d-wave term, dimensionless. Equation (1) may be rewritten as

$$f=\beta|\psi|^2+\frac{1}{2m^*}|\Pi\psi|^2+\frac{D}{2m^*}\frac{\xi^2}{\hbar^2}\left[|\hat{\Pi}_x^2\psi|^2+|\hat{\Pi}_y^2\psi|^2-\frac{1}{2}|(\hat{\Pi}_x^2+\hat{\Pi}_y^2)\psi|^2\right]. \quad (4)$$

The third term with the prefactor D in Eq. (4) is an isotropic term of higher order while the first and second terms give rise to the angular dependence of H_{c3}.

Let us consider first the case where $D=0$ (the standard linearized Ginzburg-Landau free energy), the corresponding wave function being called ψ_o. The boundary condition appropriate to ψ_o is

$$\left(-i\hbar\nabla-\frac{2e\vec{A}}{c}\right)\psi_o|_{\text{surface}}=0. \quad (5)$$

Consider a semi-infinite superconductor with a single surface in the yz plane. The x axis is chosen perpendicular to the surface as shown in Fig. 1. Furthermore, the analysis in this paper is restricted to the case where the external magnetic field is directed along the c axis which is chosen parallel to the z coordinate axis. Proceeding along the usual lines,[13–15] the gauge is chosen such that $\vec{A}$ is parallel to the y axis:

$$\vec{A}=H(x-x_o)\hat{y}. \quad (6)$$

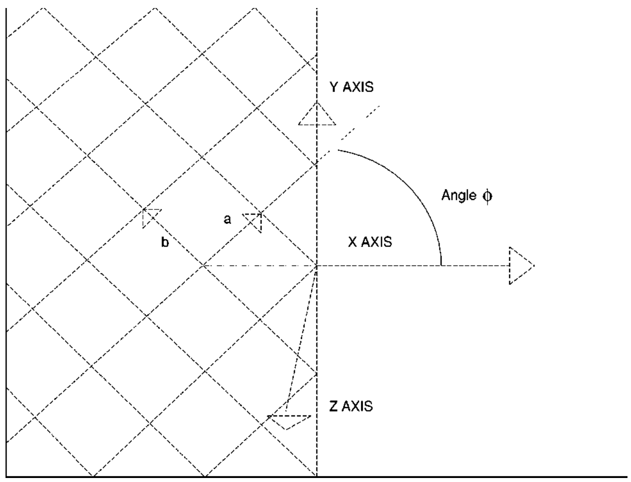

FIG. 1. The orientation of the crystal planes to the surface and the coordinate axes. $\hat{a}$ and $\hat{b}$ are unit vectors along the crystal axes.

The wave function of the superconducting nucleus can then be chosen to be a function of x alone. The boundary condition then reduces to

$$\left.\frac{d\psi_o}{dx}\right|_{\text{surface}}=0. \tag{7}$$

Obtaining the critical field can be treated as a variational problem[16] of minimizing the quantity:

$$\beta_o=\frac{\hbar^2}{2m^*\xi^2}=\frac{\hbar^2}{2m^*}\frac{\int_0^\infty[(d\psi_o/dx)^2+(4\pi^2A^2/\phi_o^2)|\psi_o|^2]dx}{\int_0^\infty|\psi_o|^2dx}, \tag{8}$$

where $\phi_o=hc/2e$ is the flux quantum. The appropriate wave function is

$$\psi_o=e^{-Cx^2/2}, \tag{9}$$

which satisfies the boundary conditions $\psi_o(\infty)=0$ and Eq. (7). Thereupon

$$\beta_o=\beta_o(C,x_o)=\left(\frac{\hbar^2}{2m^*}\right)\left\{\frac{1}{2}\left[C+\left(\frac{2\pi H}{\phi_o}\right)^2\frac{1}{C}\right]+\left(\frac{2\pi H}{\phi_o}\right)^2x_o^2-2\left(\frac{2\pi H}{\phi_o}\right)^2\frac{x_o}{\sqrt{\pi C}}\right\}. \tag{10}$$

The upper critical field H_{c2} for the bulk can be obtained by setting $x_o=0$ in Eq. (10) and minimizing with respect to C. One obtains

$$C=\left(\frac{2\pi H}{\phi_o}\right), \tag{11}$$

$$\beta_o=\frac{\hbar^2}{2m^*}\left(\frac{2\pi H}{\phi_o}\right). \tag{12}$$

In view of Eq. (3) one obtains

$$(H_{c2})_o=\frac{\phi_o}{2\pi\xi^2}, \tag{13}$$

where the subscript ''o'' in $(H_{c2})_o$ will serve to differentiate the above critical field from the one incorporating the d-wave corrections.

The critical field of surface superconductivity, H_{c3} can be obtained by minimizing Eq. (10) with respect to x_o and C in turn, whereupon one obtains

$$C=\left(\frac{2\pi H}{\phi_o}\right)b, \tag{14}$$

$$x_o=\frac{1}{\sqrt{\pi C}}, \tag{15}$$

$$\beta_o=\frac{\hbar^2}{2m^*}\left(\frac{2\pi H}{\phi_o}\right)b. \tag{16}$$

Proceeding as above one now obtains

$$(H_{c3})_0=\frac{\phi_o}{2\pi\xi^2b}=\frac{\phi_o}{2\pi\xi^2}\frac{1}{(1-2/\pi)^{1/2}}. \tag{17}$$

Now let us return to the extended Ginzburg-Landau of Eq. (4). Assuming D to be small, the correction to β_o can be obtained perturbatively with C and x_o retaining the values corresponding to the unperturbed case with $D=0$.

For the above system with the coordinate axes chosen as in Fig. 1, the perturbative correction to β is

$$\beta_1=\beta_{s2}+\beta_d, \tag{18}$$

where

$$\beta_{s2}=\frac{D}{2m^*}\left(-\frac{\xi^2}{2\hbar^2}\right)\frac{\int_0^\infty|[(\Pi\cdot\hat{a})^2\psi_o+(\Pi\cdot\hat{b})^2\psi_o]|^2dx}{\int_0^\infty|\psi_o|^2dx} \tag{19}$$

and

$$\beta_d=\frac{D}{2m^*}\frac{\xi^2}{\hbar^2}\frac{\int_0^\infty[|(\Pi\cdot\hat{a})^2\psi_o|^2+|(\Pi\cdot\hat{b})^2\psi_o|^2]dx}{\int_0^\infty|\psi_o|^2dx}. \tag{20}$$

In the above $\hat{a}$ and $\hat{b}$ are orthogonal unit vectors along the crystal axes, $\hat{a}$ making an angle ϕ with respect to the x axis. Thus we have

$$\hat{a}=\cos(\phi)\hat{x}+\sin(\phi)\hat{y}, \tag{21}$$

$$\hat{b}=-\sin(\phi)\hat{x}+\cos(\phi)\hat{y}. \tag{22}$$

Equations (19) and (20) may be rewritten as

$$\beta_{s2}=\frac{\hbar^2}{2m^*}\left(-\frac{1}{2}\right)\frac{D\xi^2}{\int_0^\infty e^{-cx^2}dx}\left[\int_0^\infty\left|\left(\cos(\phi)\frac{d}{dx}+\sin(\phi)\frac{d}{dy}+iQ(x-x_o)\sin(\phi)\right)^2 e^{-(c/2)x^2}\right.\right.$$
$$\left.\left.+\left(-\sin(\phi)\frac{d}{dx}+\cos(\phi)\frac{d}{dy}+iQ(x-x_o)\cos(\phi)\right)^2 e^{-(c/2)x^2}\right|^2 dx\right] \tag{23}$$

and

$$\beta_d=\frac{\hbar^2}{2m^*}\frac{D\xi^2}{\int_0^\infty e^{-cx^2}dx}\left[\int_0^\infty\left|\left(\cos(\phi)\frac{d}{dx}+\sin(\phi)\frac{d}{dy}+iQ(x-x_o)\sin(\phi)\right)^2 e^{-(c/2)x^2}\right|^2 dx\right.$$
$$\left.+\int_0^\infty\left|\left(-\sin(\phi)\frac{d}{dx}+\cos(\phi)\frac{d}{dy}+iQ(x-x_o)\cos(\phi)\right)^2 e^{-(c/2)x^2}\right|^2 dx\right], \tag{24}$$

where $Q=-2\pi H/\phi_o$. After some algebra one obtains for the surface critical field

$$\beta_{s2}=-\left(\frac{\hbar^2}{2m^*}\right)D\xi^2\left(\frac{2\pi H}{\phi_o}\right)^2\left(\frac{1}{2}\right)\left(1+\frac{1}{\pi}-\frac{1}{\pi b^2}\right) \tag{25}$$

$$=-\left(\frac{\hbar^2}{2m^*}\right)D\xi^2\left(\frac{2\pi H}{\phi_o}\right)^2(0.2217) \tag{26}$$

and

$$\beta_d=\frac{\hbar^2}{2m^*}D\xi^2\left(\frac{2\pi H}{\phi_o}\right)^2\left\{\frac{1}{16}\left[9b^2+6-\frac{4}{\pi}+\frac{1}{b^2}\left(9-\frac{12}{\pi}-\frac{36}{\pi^2}\right)\right]+\frac{1}{16}\left[3b^2+\frac{4}{\pi}-6+\frac{1}{b^2}\left(3-\frac{4}{\pi}-\frac{12}{\pi^2}\right)\right]\cos(4\phi)\right\} \tag{27}$$

$$=\frac{\hbar^2}{2m^*}D\xi^2\left(\frac{2\pi H}{\phi_o}\right)^2[b_1+b_2\cos(4\phi)], \tag{28}$$

where $b_1=0.763\,446$ and $b_2=-0.139\,415$.

Again assuming the D-wave term to be small, one can make an expansion in D to obtain

$$H_{c3}=(H_{c3})_0\{1-D[1.490\,85-0.383\,708\cos(4\phi)]+O(D^2)\}. \tag{29}$$

Thus the d-wave correction induces an angular dependence in the surface superconducting field which lends itself to experimental observation.

Proceeding in an analogous fashion with $x_o=0$ and $Q=-C$ one obtains the critical field H_{c2}

$$H_{c2}=(H_{c2})_o[1-D+O(D^2)]. \tag{30}$$

Thus, in this case, there is no angular dependence in the correction. The ratio of the critical fields is

$$\frac{H_{c3}}{H_{c2}}=\left(\frac{1}{b}\right)\{1+D[-0.490\,85+0.383\,708\cos(4\phi)]+\cdots\} \tag{31}$$

$$=1.6589+D[-0.814\,271+0.636\,532\cos(4\phi)]+O(D^2). \tag{32}$$

The quality of the crystal surface is an issue as regards experimental studies. Pair breaking due to diffuse scattering at imperfect surfaces can suppress surface superconductivity. To study this effect, the calculation is now performed for general boundary conditions incorporating a phenomenological parameter γ describing the structure of the junction between the superconductor and the vacuum.

As a first step, it is necessary to obtain the critical field H_{c3} in the absence of the d-wave term of interest. In the

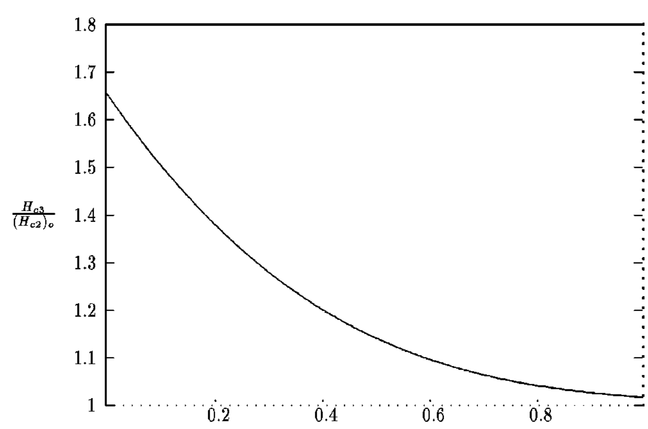

FIG. 2. The dependence of $H_{c3}(\eta_1)/(H_{c2})_o$ on η_1 for $D=0$.

presence of a magnetic field parallel to the surface, we have the following Ginzburg-Landau equation valid in the superconducting region:

$$-\frac{d^2\psi_o}{dx^2}+\left(\frac{2\pi H}{\phi_o}\right)^2(x-x_o)^2\psi_o=\frac{\psi_o}{\xi^2}. \tag{33}$$

The boundary condition is now given by

$$\frac{d\psi_o}{dx}=\frac{\psi_o}{\gamma}, \tag{34}$$

where the wave function is now

$$\psi_o=e^{-(x-x_1)^2/2\xi^2}. \tag{35}$$

The eigenvalue of the operator

$$-\frac{d^2}{dx^2}+\left(\frac{2\pi H}{\phi_o}\right)^2(x-x_o)^2 \tag{36}$$

being $1/\xi^2$, we obtain[17]

$$\frac{1}{\xi^2}=\frac{\int_0^\infty e^{-(1/2)\,[(x-x_1)/\xi]^2}(-d^2/dx^2+(2\pi H/\phi_o)^2(x-x_o)^2)e^{-(1/2)\,[(x-x_1)/\xi]^2}dx}{\int_0^\infty e^{-1/2\,[(x-x_1)/\xi]^2}dx}. \tag{37}$$

Writing $\xi/\gamma=\eta_1$, this leads to

$$\left[\frac{H_{c3}(\eta_1)}{(H_{c2})_o}\right]^2=\frac{[U(\eta_1)/2-(\eta_1/2)\,e^{-\eta_1^2}]}{\{U(\eta_1)/2-(\eta_1/2)\,e^{-\eta_1^2}-[1/4U(\eta_1)]\,e^{-2\eta_1^2}\}}=\frac{g_1(\eta_1)}{g_2(\eta_1)}, \tag{38}$$

where $U(\eta_1)=\int_{-\eta_1}^{\infty}e^{-x^2}dx$ and $x_o=x_1+[\xi/2U(\eta_1]\,e^{-\eta_1^2}$. The dependence of $H_{c3}(\eta_1)/(H_{c2})_o$ on η_1 is shown in Fig. 2.

The effect of the d-wave term is now studied by a perturbative analysis as before. The correction to the eigenvalue is determined from Eqs. (19) and (20) to be

$$\beta_d(\eta_1)+\beta_{s2}(\eta_1)=\frac{\hbar^2}{2m^*}\frac{D}{\xi^2}\left[f_3(\eta_1,\phi)+\left(\frac{H_{c3}(\eta_1)}{(H_{c2})_o}\right)^2f_2(\eta_1,\phi)+\left(\frac{H_{c3}(\eta_1)}{(H_{c2})_o}\right)^4f_1(\eta_1,\phi)\right], \tag{39}$$

where f_1, f_2, and f_3 are known functions of η_1 and ϕ:

$$f_1(\eta_1)=\frac{-\{\eta_1[2+\sqrt{\pi}\sin(2\,\phi)^2+\sqrt{\pi}\mathrm{Erf}(\eta 1)\sin(2\,\phi)^2]\}}{2\,e^{3\,\eta_1{}^2}\pi^{3/2}[1+\mathrm{Erf}(\eta_1)]^3}-\frac{(1+4\,\eta_1{}^2)[2+\sqrt{\pi}\sin(2\,\phi)^2+\sqrt{\pi}\mathrm{Erf}(\eta_1)\sin(2\,\phi)^2]\}}{4\,e^{2\,\eta_1{}^2}\pi^{3/2}[1+\mathrm{Erf}(\eta_1)]^2}$$
$$-\frac{\eta_1(1+2\,\eta_1{}^2)[2+\sqrt{\pi}\sin(2\,\phi)^2+\sqrt{\pi}\mathrm{Erf}(\eta_1)\sin(2\,\phi)^2]}{4\,e^{\eta_1{}^2}\sqrt{\pi}[1+\mathrm{Erf}(\eta_1)]}+\frac{2+3\,\sqrt{\pi}\sin(2\,\phi)^2+3\,\sqrt{\pi}\mathrm{Erf}(\eta_1)\sin(2\,\phi)^2}{8}, \tag{40}$$

$$f_2(\eta_1)=\frac{3\,[4-3\,\sqrt{\pi}-\sqrt{\pi}\cos(4\,\phi)-3\,\sqrt{\pi}\mathrm{Erf}(\eta_1)-\sqrt{\pi}\cos(4\,\phi)\mathrm{Erf}(\eta_1)]}{8\,e^{4\,\eta_1{}^2}\pi^2[1+\mathrm{Erf}(\eta_1)]^4}$$
$$+\frac{3\,\eta_1[4-3\,\sqrt{\pi}-\sqrt{\pi}\cos(4\,\phi)-3\,\sqrt{\pi}\mathrm{Erf}(\eta_1)-\sqrt{\pi}\cos(4\,\phi)\mathrm{Erf}(\eta_1)]}{4e^{3\eta_1{}^2}\pi^{3/2}[1+\mathrm{Erf}(\eta_1)]^3}$$
$$+\frac{(1+4\,\eta_1{}^2)[4-3\,\sqrt{\pi}-\sqrt{\pi}\cos(4\,\phi)-3\,\sqrt{\pi}\mathrm{Erf}(\eta_1)-\sqrt{\pi}\cos(4\,\phi)\mathrm{Erf}(\eta_1)]}{8\,e^{2\,\eta_1{}^2}\pi[1+\mathrm{Erf}(\eta_1)]^2}$$
$$+\frac{\eta_1(3+2\,\eta_1{}^2)[4-3\,\sqrt{\pi}-\sqrt{\pi}\cos(4\,\phi)-3\,\sqrt{\pi}\mathrm{Erf}(\eta_1)-\sqrt{\pi}\cos(4\,\phi)\mathrm{Erf}(\eta_1)]}{16\,e^{\eta_1{}^2}\sqrt{\pi}[1+\mathrm{Erf}(\eta_1)]}$$
$$+\frac{3\,[-4+3\,\sqrt{\pi}+\sqrt{\pi}\cos(4\,\phi)+3\,\sqrt{\pi}\mathrm{Erf}(\eta_1)+\sqrt{\pi}\cos(4\,\phi)\mathrm{Erf}(\eta_1)]}{32} \tag{41}$$

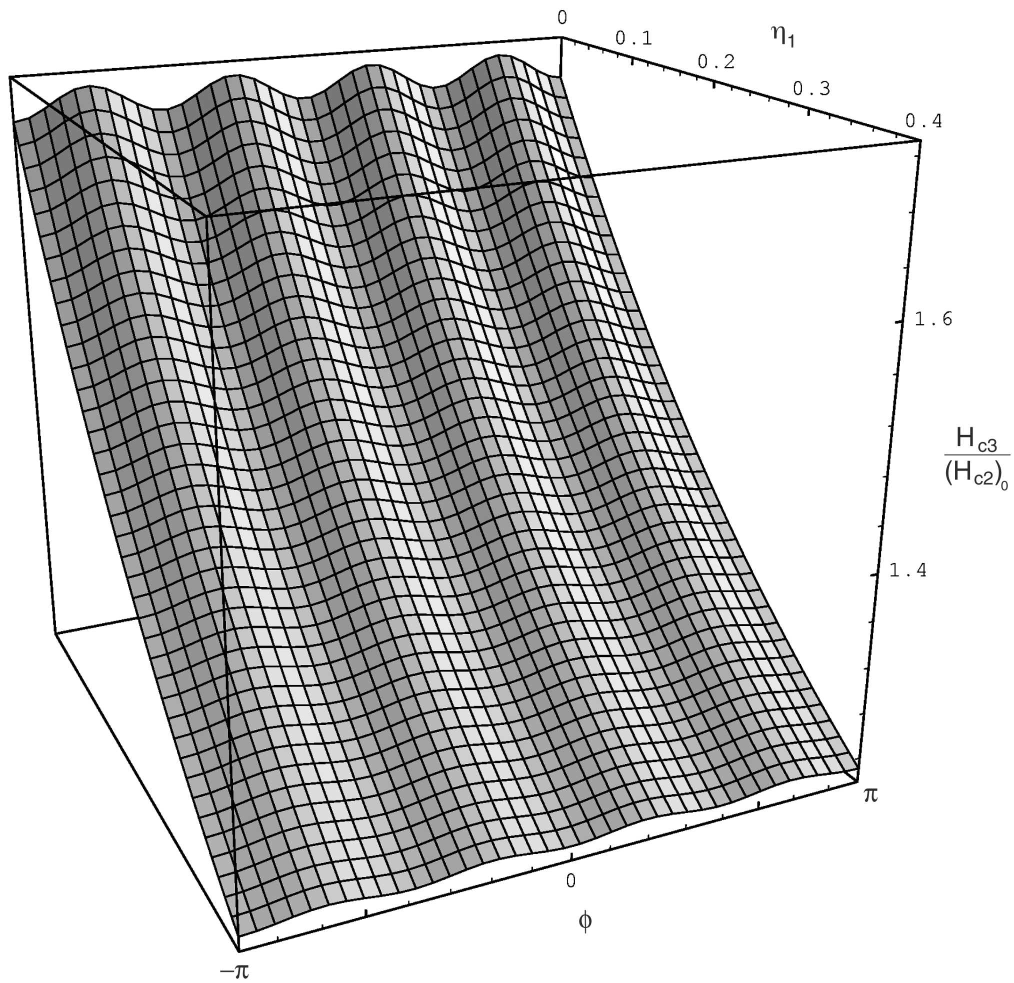

FIG. 3. The plot of $[H_{c3}/(H_{c2})_o]$ as a function of η_1 and ϕ is shown for $D=-0.02$. The parameter η_1 is plotted over a range from 0 to 0.4 and ϕ from $-\pi$ to π.

$$f_3(\eta_1)=\frac{\eta_1(-1+2\,\eta_1{}^2)[4-3\sqrt{\pi}-\sqrt{\pi}\cos(4\,\phi)-3\sqrt{\pi}\mathrm{Erf}(\eta_1)-\sqrt{\pi}\cos(4\,\phi)\mathrm{Erf}(\eta_1)]}{16\,e^{\eta_1{}^2}\sqrt{\pi}[1+\mathrm{Erf}(\eta_1)]}+\frac{3\,[-4+3\sqrt{\pi}+\sqrt{\pi}\cos(4\,\phi)+3\sqrt{\pi}\mathrm{Erf}(\eta_1)+\sqrt{\pi}\cos(4\,\phi)\mathrm{Erf}(\eta_1)]}{32}. \tag{42}$$

In the above expressions, $\mathrm{Erf}(\eta_1)$ is the error function.

Proceeding as in the unperturbed case, we obtain

$$\left[\frac{H_{c3}}{(H_{c2})_o{}^2}\right]^2=\frac{g_1(\eta_1)}{g_2(\eta_1)}-\frac{D}{g_2^3}[f_3(\eta_1)g_2^2+f_2(\eta_1)g_1^2+f_1(\eta_1)g_1g_2]+O(D^2). \tag{43}$$

Maki *et al.*[6,7] have studied the upper critical field of d-wave superconductors within the weak-coupling model. They have obtained, among other results, the critical field for the bulk case with the field parallel to the c axis. An estimate of D can be obtained by comparing with this microscopic model. Following Maki *et al.*,[7] the upper critical field for a bulk d-wave superconductor can be obtained by solving the coupled equations:

$$-\ln t=\int_0^\infty\frac{du}{\sinh(u)}[1-e^{-\rho u^2}(1+2\rho^2u^4c_1)], \tag{44}$$

$$-c_1\ln t=\int_0^\infty\frac{du}{\sinh(u)}\left\{c_1-e^{-\rho u^2}\left[\frac{\rho^2u^4}{12}+c_1\left(1-8\rho u^2+12\rho^2u^4-\frac{16}{3}\rho^3u^6+\frac{2}{3}\rho^4u^8\right)\right]\right\}, \tag{45}$$

where $\rho = 2ev^2 H_{c2}(T)/(4\pi T)^2$, v being the Fermi velocity in the ab plane. In the neighborhood of the transition temperature, ρ is small and the above equations can be solved to obtain approximate analytic expressions for the upper critical fields for d- and s-wave superconductors. Then using Eq. (30) $D \approx -0.02$ in the temperature where the Ginzburg-Landau theory is valid. (It should be emphasized that this value of D is an underestimate due to the approximations made. Further, D is seen from the exact results of the microscopic theory, to increase substantially at lower temperatures suggesting an enhanced effect.) The plot of $[H_{c3}/(H_{c2})_o]$ as a function of η_1 and ϕ is shown in Fig. 3 for this value of D. It can be seen that the cosinusoidal variation that is the d-wave signature persists over a significant range of the parameter γ.

In conclusion, it has been shown that the above d-wave contribution to the free energy generates an angle dependence of the surface superconducting field. The ϕ dependence of H_{c3} provides, in principle, a method for experimentally detecting a d-wave contribution without knowledge of the s-d coupling strength.

Surface quality is of significance in observing this effect. For diffuse surfaces with indentations comparable to the interparticle spacing, η_1 is of order unity for short coherence length superconductors[19] and the effect could be substantially suppressed (it should be noted that if η_1 is different for two crystals with different cleaving directions, corrections can be made to the observed H_{c3}/H_{c2} ratio using the known dependence of large angle-independent component of the ratio on η_1). However, for high symmetry directions along which atomically smooth surfaces can be cleaved, the effect should be observable. The same would be true for cleavage angles where the step size is large (step formation can be induced under certain conditions[20]). There have been some experimental efforts where some degree of control in obtaining cleavage angles other than along the c and a axis has been demonstrated.[21,22]

The high magnitude of H_{c3} for high-T_c superconductors makes experiments difficult, but measurements near T_c would make H_{c3} accessible. Furthermore, this particular problem is far less severe in the case of organic superconductors [such as the κ-(BEDT-TTF)$_2$ salts] which also possess layered structures. Hence this analysis could be applied to other superconducting systems apart from the high-temperature superconductors, where the nature of the pairing state is not well established.

I would like to express my sincere gratitude to Professor A. I. Larkin for his guidance, to Professor O. T. Valls for his invaluable insights, and to Professor A. M. Goldman for his comments.

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