Vortex lattice structures in uniaxial superconductors

L. J. Campbell
Theoretical Division, MS-B262, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

M. M. Doria*
Center for Nonlinear Studies, MS-B258, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

V. G. Kogan
Ames Laboratory and Department of Physics, Iowa State University, Ames, Iowa 50011
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The structure of the vortex lattice in anisotropic, unaxial superconductors in the domain $H_{c1} \ll H \ll H_{c2}$ is considered within the London approach. To first order in the small parameter $(L/\lambda)^2$, where L is the average intervortex spacing and λ is the average penetration depth, there exists a continuum of different lattices with the same free energy for any direction of the magnetic induction $\mathbf{B}$ with respect to the crystal. It is shown that the degeneracy is removed if terms in the free energy of order $(L/\lambda)^4$ are taken into account, yielding both a unique structure and a preferred orientation of the vortex lattice with respect to the direction of $\mathbf{B}$ within the crystal. Parameters of the primitive cell for this structure are obtained and evaluated for known values of the anisotropy of $YBa_2Cu_3O_7$. For the particular case of vortices parallel to the Cu-O planes the degeneracy remains exact (within the London approach), which should make this lattice more susceptible to disorder. The magnetization is shown to be almost parallel to the $\hat{\mathbf{c}}$ crystal direction for all orientations of the external field $\mathbf{H}_0$, except in a narrow domain where $\mathbf{H}_0$ is nearly normal to $\hat{\mathbf{c}}$.

It is well established that all known high-T_c superconductors are strongly anisotropic. In the orthorhombic $Y_1Ba_2Cu_3O_7$, the $\hat{\mathbf{c}}$ axis of the primitive cell is about 3 times larger than either the $\hat{\mathbf{a}}$ or $\hat{\mathbf{b}}$ dimensions in the basal Cu-O plane. The "in-plane" anisotropy is relatively weak: the $\hat{\mathbf{a}}$ and $\hat{\mathbf{b}}$ sizes differ by about 1%. Therefore, major anisotropy effects can be described within a uniaxial model, which simplifies the matter considerably. The decoration experiments[1] done in a magnetic field parallel to $\hat{\mathbf{c}}$ revealed a predominantly hexagonal arrangement of the Abrikosov vortices—a feature of a uniaxial superconductor. Hence, the uniaxial approximation is a reasonable first step in a description of the anisotropy of 1:2:3-type materials. The equilibrium vortex lattice structure for an *arbitrary field orientation* with respect to the uniaxial crystal is a subject of this paper.

The coherence length ξ of the materials in question is considerably shorter than the magnetic field penetration depth λ. This means that the vortex core size is small with respect to the characteristic size λ of the current and field distributions (unless the external field H approaches the upper critical field H_{c2}, a domain that is hardly attainable). Thus, the London equations are applicable in a wide domain $H \ll H_{c2}$.

Major effects of a strong uniaxial anisotropy can be taken into account by replacing the scalar $\lambda^2(\mathrm{curl}\mathbf{h})^2$ in the London free-energy density of an isotropic material with an invariant combination $\lambda^2 m_{ik}\mathrm{curl}_i\mathbf{h}\,\mathrm{curl}_k\mathbf{h}$ (for details the reader may turn to Refs. 2 and 3). Here λ^2 is proportional to the "average mass" $M_{\mathrm{av}}=(M_1M_2M_3)^{1/3}$ with M_a being the principal values of the "mass tensor" M_{ik}; $m_{ik}=M_{ik}/M_{\mathrm{av}}$. Although m_{ik} is often called "the effective-mass tensor," the tensor $\lambda^2 m_{ik}$ presumably includes all possible sources of anisotropy of the tensor type. The free energy (per unit length in the direction of vortices) then reads

$$F=\int(\mathbf{h}^2+\lambda^2 m_{ik}\mathrm{curl}_i\mathbf{h}\,\mathrm{curl}_k\mathbf{h})\,dxdy/8\pi\,, \qquad (1)$$

where $\mathbf{h}(x,y)$ is the local magnetic field and $dxdy$ is an element of area in the plane normal to the direction $\hat{\mathbf{z}}$ of vortex axes. For a vortex along $\hat{\mathbf{z}}$, the field $\mathbf{h}$ in an anisotropic material has h_x and h_y nonzero components, unless the vortex axis coincides with one of the principal crystal directions.[2]

We wish to consider vortices oriented arbitrarily with respect to the crystal frame (X,Y,Z) defined in Fig. 1, and therefore we transform m_{ik} from the crystal frame

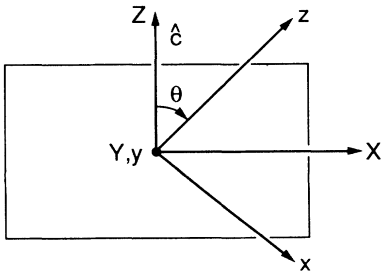

FIG. 1. In the crystal frame (X,Y,Z) the plane XY coincides with the basal Cu-O planes. Axis z is parallel to the vortex axes. The frame (x,y,z) is obtained by a rotation θ of the (X,Y,Z) system about the Y axis.

(where $m_{XX}=m_{YY}=m_1$, $m_{ZZ}=m_3$) to the "vortex frame" (x,y,z):

$$m_{xx}=m_1\cos^2\theta+m_3\sin^2\theta,\ m_{xy}=m_{yz}=0,$$
$$m_{yy}=m_1,\ m_{zz}=m_1\sin^2\theta+m_3\cos^2\theta, \tag{2}$$
$$m_{xz}=(m_1-m_3)\sin\theta\cos\theta,$$

where θ is the angle between $\hat{\mathbf{c}}$ (or $\hat{\mathbf{Z}}$) and the vortex axes $\hat{\mathbf{z}}$. The London equations are obtained by varying F with respect to $\mathbf{h}(x,y)$; they are given, e.g., in Refs. 2-4. For a vortex lattice, $\mathbf{h}(x,y)$ is a periodic function with nonzero Fourier components $h(\mathbf{G})$, where $\mathbf{G}$'s form the reciprocal lattice. After straightforward algebra one obtains for the free-energy density f:[4]

$$8\pi f=B^2\sum_{\mathbf{G}}\frac{1+\lambda^2 m_{zz}G^2}{(1+\lambda^2 m_{zz}G_x^2+\lambda^2 m_3 G_y^2)(1+\lambda^2 m_1 G^2)}. \tag{3}$$

Here the induction $B=\phi_0 N$, where ϕ_0 is the flux quantum and N is the number density of vortices.

In the field domain $H_{c1}\ll H\ll H_{c2}$, the average vortex spacing L satisfies $\xi\ll L\ll\lambda$. Then one can expand the free energy (3) in powers of the small parameter $L^2/\lambda^2\ll 1$. To obtain this expansion we introduce dimensionless reciprocal-lattice vectors $\mathbf{g}=L\mathbf{G}$ with $L=(\phi_0/B)^{1/2}$ and write, e.g.,

$$(1+\lambda^2 m_1 G^2)^{-1}=(L/\lambda)^2(m_1 g^2)^{-1}\times(1-L^2/\lambda^2 m_1 g^2+\cdots).$$

The zero- and the first-order terms then read[4]

$$8\pi(f_0+f_1)=B^2+B^2\frac{m_{zz}}{m_1}\frac{L^2}{\lambda^2}\sum{}'(m_{zz}g_x^2+m_3 g_y^2)^{-1}, \tag{4}$$

where $\sum'$ denotes the summation over all nonzero $\mathbf{g}$'s. The second-order term is readily obtained:

$$8\pi f_2=B^2\frac{m_{zz}}{m_1}\frac{L^4}{\lambda^4}\left[\frac{m_1-m_{zz}}{m_1 m_{zz}}\sum{}'g^{-2}g_1^{-2}-\sum{}'g_1^{-4}\right], \tag{5}$$

where we have introduced $g_1^2=m_{zz}g_x^2+m_3 g_y^2$ for brevity.

It was shown in Ref. 4, that the free energy (4) is the same for two different types of lattices, shown as (B)1 and (B)3 in Fig. 2. We are going to show now that, in fact, there exists a *continuous set* of structures, which all have the same free energy (4) in the *first approximation in* L^2/λ^2.

To this end we first notice that in the isotropic material there exists a continuous set of hexagonal lattices, which differ only in orientation of their primitive cells with respect to an arbitrary system of axes xy. Each one of these lattices can be labeled with the angle α of one of its basis vectors, say, $\mathbf{a}_1$ of Fig. 2(A), with respect to the x axis. All essentially different lattices correspond to $0<\alpha<\pi/6$ [choose primitive cells as hexagons centered at the origin for cases (A)1 and (A)3]. The basis lattice

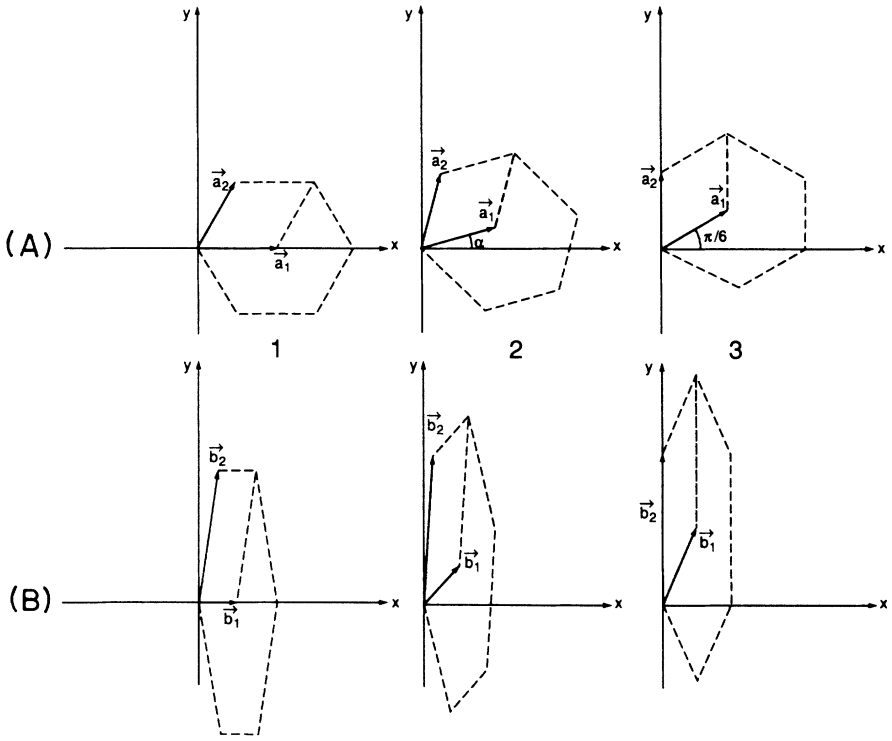

FIG. 2. (A) All possible orientations of a triangular lattice with respect to the x axis can be described by the angle α between x and one of the unit vectors a_1, where $0<\alpha<\pi/6$. (B) Lattice structures obtained with (A)1, (A)2, (A)3 above by uniform deformations (different in the x and y directions) which conserve the unit-cell area. The lowest free energy corresponds to the case (B)1.

vectors of this set are

$$\mathbf{a}_1 = L_\Delta(\hat{\mathbf{x}}\cos\alpha + \hat{\mathbf{y}}\sin\alpha)\,,$$
$$\mathbf{a}_2 = L_\Delta[\hat{\mathbf{x}}\cos(\alpha+\pi/3) + \hat{\mathbf{y}}\sin(\alpha+\pi/3)]\,, \tag{6}$$

where L_Δ is the side of the equilateral triangle with the area $\phi_0/2B$.

Let us now "turn on" the anisotropy so that the deformation γ_x in the x direction differs from γ_y. The deformations are assumed uniform; the deformed structures are still periodic. The triangular primitive cell (6) then transforms to

$$\mathbf{b}_1 = L_\Delta(\hat{\mathbf{x}}\gamma_x\cos\alpha + \hat{\mathbf{y}}\gamma_y\sin\alpha)\,,$$
$$\mathbf{b}_2 = L_\Delta[\hat{\mathbf{x}}\gamma_x\cos(\alpha+\pi/3) + \hat{\mathbf{y}}\gamma_y\sin(\alpha+\pi/3)]\,. \tag{7}$$

Due to the flux quantization, the unit-cell area should be conserved; this yields $\gamma_x\gamma_y = 1$ and we denote $\gamma = \gamma_x = 1/\gamma_y$. The reciprocal lattice corresponding to the cell (7) is given by

$$g_x = g_0[p\sin(\alpha+\pi/3) - q\sin\alpha]/\gamma\,,$$
$$g_y = g_0[-p\cos(\alpha+\pi/3) + q\cos\alpha]\gamma\,, \tag{8}$$

where $g_0 = 2^{3/2}\pi/3^{1/4}$ and $p,q = 0, \pm 1, \ldots$. It is now easy to verify that the combination $g_1^2 = m_{zz}g_x^2 + m_3 g_y^2$, which enters the energy (4), is α *independent*, if

$$\gamma = (m_{zz}/m_3)^{1/4}\,. \tag{9}$$

Thus, we have proved that all lattices (7) labeled by α (which may take any value between 0 and $\pi/6$) with parameter γ of Eq. (9), belong to the same free energy,[5] if the terms (5) of the order L^4/λ^4 are neglected.

In order to find out which of these structures is actually realized, one can consider the small correction $f_2 \propto L^4/\lambda^4$ as a perturbation, which may remove the above degeneracy. Hence, one should evaluate f_2 for the "lowest-order solution" given in Eqs. (7) and (9). The sum $\sum' g_1^{-4}$ cannot contribute to possible energy differences, because g_1 is α independent. The α-dependent part of f_2 is given by

$$8\pi f_2(\alpha) = B^2\frac{L^4}{\lambda^4}\frac{m_1 - m_{zz}}{m_1^2}\sum{}' g_1^{-2}g^{-2}(\alpha)\,. \tag{10}$$

The results of numerical evaluation of the sum in this equation are given in Fig. 3, where the free energy $f_2(\alpha)$ normalized on $B^2L^4/8\pi\lambda^4$ is plotted as a function of parameter α for two different directions θ of the magnetic induction (or vortex axes) with respect to the $\hat{\mathbf{c}}$ axis of the crystal. It is seen clearly that the minimum free energy corresponds to $\alpha = 0$ for all θ's. Because the angle θ enters the calculation only through the "effective" masses, one concludes that this is the case ($\alpha = 0$) for any ratio m_3/m_1. [In fact, one can show that the *exact* free energy (3) has extremums at $\alpha = 0$ and $\pi/6$]. Thus, the structure (B)1 of Fig. 2, which corresponds to $\alpha = 0$, has the lowest free energy. This structure should be realized in a uniform magnetic field (in a pinning free material).

It is worth noting that this result agrees with that given in Ref. 3. However, Ref. 6 states that only the $\alpha = \pi/6$ case [(B)3 lattice] is observed in experiment (with uniaxial materials).

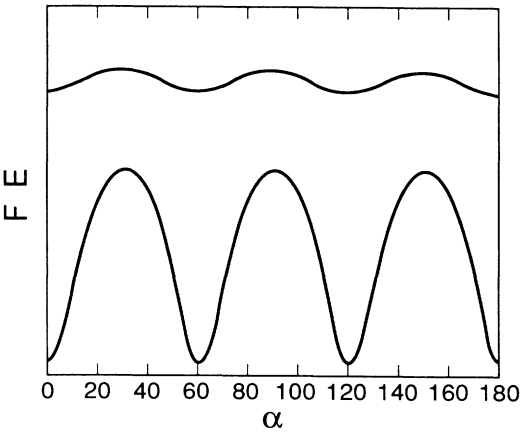

FIG. 3. Numerical results for the α-dependent part of the free energy (FE) given by Eq. (10). The magnetic induction is inclined to the c axis by $\theta = 60°$ for the upper curve and by $\theta = 75°$ for the lower. In both cases $m_3/m_1 = 50$. The summation in Eq. (10) was taken over 100 lattices sites in each direction, which seem sufficient. (Summing over only 10 lattice sites caused a variation of 0.4% in the value of the free energy for both curves, with the position of the minimum remaining an integral multiple of 60°.)

Having found the equilibrium parameter $\alpha = 0$, one obtains the unit-cell parameters for an arbitrary orientation θ of the magnetic induction, using Eqs. (7) and (9):

$$\mathbf{b}_1 = L_\Delta\gamma\hat{\mathbf{x}},\quad \mathbf{b}_2 = L_\Delta(\hat{\mathbf{x}}\gamma + \hat{\mathbf{y}}\sqrt{3}/\gamma)/2\,. \tag{11}$$

The side-to-base ratio b_2/b_1 of the isosceles triangle (11) and the angle ϕ between $\mathbf{b}_1$ and $\mathbf{b}_2$ are readily found:[7]

$$2b_2/b_1 = (1+3m_3/m_{zz})^{1/2},\quad \tan\phi = (3m_3/m_{zz})^{1/2}\,. \tag{12}$$

Thus, when the orientation of vortices changes from $\theta = 0$ (parallel to $\hat{\mathbf{c}}$) to $\theta = \pi/2$, the ratio b_2/b_1 changes from unity to $0.5(1+3m_3/m_1)^{1/2}$, while the angle ϕ increases from $\pi/3$ to $\tan^{-1}(3m_3/m_1)^{1/2}$.

Note that the primitive cell of Eqs. (11) and (12) describes the flux line lattice in the plane (x,y) normal to $\mathbf{B}$ (or to $\mathbf{H}_0$ in high enough fields). Crystals of high-T_c materials (available to date) usually have smooth-plane surfaces normal[1] or parallel[8] to the $\hat{\mathbf{c}}$ axis. Having in mind possible decoration experiments for an *arbitrary field orientation* within the crystal, we project the cell (11) upon the plane normal to $\hat{\mathbf{c}}$, denoted with subscript n and on the plane parallel to $\hat{\mathbf{c}}$ and perpendicular to the $\mathbf{B},\hat{\mathbf{c}}$ plane, p:

$$\mathbf{b}_{1n} = L_\Delta\gamma\hat{\mathbf{x}}/\cos\theta,\quad \mathbf{b}_{2n} = L_\Delta(\hat{\mathbf{x}}\gamma/\cos\theta + \hat{\mathbf{y}}\sqrt{3}/\gamma)/2\,,$$
$$\mathbf{b}_{1p} = L_\Delta\gamma\hat{\mathbf{x}}/\sin\theta,\quad \mathbf{b}_{2p} = L_\Delta(\hat{\mathbf{x}}\gamma/\sin\theta + \hat{\mathbf{y}}\sqrt{3}/\gamma)/2\,. \tag{13}$$

The ratio m_3/m_1 for single crystals of $YBa_2Cu_3O_7$ can be estimated from the upper critical fields ratio:

$$H_{c2}(\pi/2)/H_{c2}(0) = (m_3/m_1)^{1/2}\,,$$

which ranges from 6 (Ref. 9) to about 10 (Ref. 8). Tak-

ing for an estimate $m_3/m_1 \simeq 50$, we obtain for vortices in Cu-O planes $b_2/b_1 \simeq 6$ and $\phi \simeq 85°$. Thus, the flux line lattice in this material should be strongly distorted with respect to the equilateral triangle unless the magnetic induction $\mathbf{B}$ is parallel to $\hat{\mathbf{c}}$. This distortion, in turn, should influence such features of the vortex lattice as elastic moduli and the response to transport currents.[10]

The case $\theta = \pi/2$, i.e., vortices aligned with the basal Cu-O plane, calls for separate consideration, because as is seen from Eq. (10), the "perturbation" energy vanishes at this orientation: $m_{zz}(\pi/2) = m_1$. In fact, the perturbation argument is not needed in this case; one can work with the exact free energy (3), which simplifies to

$$8\pi f(\pi/2) = B^2 \sum [1 + (\lambda^2/L^2) g_\Gamma^2]^{-1}, \tag{14}$$

where $g_\Gamma^2 = m_1 g_x^2 + m_3 g_y^2$ at this orientation. As was pointed out above, g_1 is α independent, which means that all structures (7) [Fig. 2(B)] with $\gamma_x = 1/\gamma_y = (m_1/m_3)^{1/4}$ belong to the same London free energy.

A simple way to see this degeneracy is to note that Eq. (14) is equivalent to the expansion in reciprocal-lattice space of the pairwise vortex interactions $K_0(r_{ij}/\lambda)$, where K_0 is the modified Bessel function and

$$r_{ij}^2 = (x_i - x_j)^2/m_1 + (y_i - y_j)^2/m_3 .$$

It is obvious that any change in the anisotropy m_1/m_3 can be canceled by rescaling the coordinates, and therefore the degeneracy of the continuum of orientations of the equilateral triangular lattice that occurs for $m_1/m_3 = 1$ is maintained for the corresponding continuum of inequivalent distortions of the triangular lattice for $m_1/m_3 \neq 1$. For an arbitrary field orientation this observation is true provided $L^2/\lambda^2 \ll 1$.

Given the free energy for $H \gg H_{c1}$, Eq. (4), one can find the constitutive relation $\mathbf{H} = 4\pi \partial f/\partial \mathbf{B}$ in this domain. To this end, we note first that a cutoff at $G_{\max} \sim 1/\xi$ (or $g_{\max} \sim L/\xi$) should be introduced in the logarithmically divergent sum of Eq. (4) (see, e.g., Ref. 11). Then, we write explicitly the quantity g_Γ^2 [for any lattice (7)] in order to extract the θ dependence:

$$g_\Gamma^2 = g_0^2 (m_3 m_{zz})^{1/2} (p^2 + q^2 - pq) .$$

We obtain

$$8\pi f = B^2 + (\eta \phi_0 B \sqrt{m_{zz}}/\lambda^2) \ln(H_{c2}/B) , \tag{15}$$

where η is a number of the order unity. The angular dependence of H_{c2} (or ξ) is ignored in (15); this would amount to an addition to a large $\ln(H_{c2}/B)$, which is beyond the accuracy of the London approximation. In the crystal frame (X,Y,Z), $B_X = B\sin\theta$, $B_Z = B\cos\theta$, and $m_{zz}B^2 = m_1 B_X^2 + m_3 B_Z^2$. Thus, the free energy (15) assumes the form

$$8\pi f = B^2 + (\eta \phi_0/\lambda^2) \sqrt{m_1 B_X^2 + m_3 B_Z^2} \ln(H_{c2}/B) , \tag{16}$$

and we obtain

$$H_Z = B_Z + \frac{\eta \phi_0}{2\lambda^2} \frac{m_3 B_Z}{B\sqrt{m_{zz}}} \ln\left(\frac{H_{c2}}{B}\right),$$
$$H_X = B_X + \frac{\eta \phi_0}{2\lambda^2} \frac{m_1 B_X}{B\sqrt{m_{zz}}} \ln\left(\frac{H_{c2}}{B}\right). \tag{17}$$

The quantity $\phi_0 \eta/\lambda^2$ is of order of H_{c1}; it is, therefore, small with respect to both H and B in the field domain of interest. Equations (17) then show that $\mathbf{B}$ is almost parallel to the thermodynamic field $\mathbf{H}$ inside the sample.[3] The reversible magnetization $\mathbf{M} = (\mathbf{B} - \mathbf{H})/4\pi$ is small (of the order H_{c1}); its orientation θ_M with respect to the $\hat{\mathbf{c}}$ axis is given by

$$\frac{M_X}{M_Z} = \tan\theta_M \frac{m_1}{m_3} \tan\theta \tag{18}$$

(recall: θ is the angle between $\mathbf{B}$ and $\hat{\mathbf{c}}$).

It is worth noting that for an arbitrarily shaped sample in a homogeneous external field $\mathbf{H}_0$, the internal fields $\mathbf{H}$ and $\mathbf{B}$ are not uniform. For a general ellipsoid, however, $\mathbf{B}$ and $\mathbf{H}$ are uniform and linearly related to the external field $\mathbf{H}_0$:[10]

$$H_{0\beta} = B_\beta - 4\pi(1 - n_\beta) M_\beta , \tag{19}$$

where β denotes the principal ellipsoid directions and n_β are the corresponding demagnetization coefficients. As we pointed out, in the domain $H_0 \gg H_{c1}$, M is small; Eq. (19) then shows that $\mathbf{B}$ is close to $\mathbf{H}_0$. One can, therefore, replace θ in Eq. (18) with θ_0, which gives the orientation of $\mathbf{H}_0$ with respect to $\hat{\mathbf{c}}$:

$$\frac{M_X}{M_Z} = \frac{m_1}{m_3} \frac{H_{0X}}{H_{0Z}} . \tag{20}$$

This remarkably simple and shape-dependent result means that for $m_3/m_1 \gg 1$ the direction of $\mathbf{M}$ is close to $\hat{\mathbf{c}}$ for almost any orientation of the external field $\mathbf{H}_0$ (if $H_0 \gg H_{c1}$). A substantial deviation of the $\mathbf{M}$ direction from that of $\hat{\mathbf{c}}$ occurs only if $\mathbf{H}_0$ is close to the a-b plane:

$$\theta_0 \sim \tan^{-1}(m_3/m_1) \simeq \pi/2 \pm m_1/m_3 .$$

It is interesting to observe that the same relation (20) holds in high fields near H_{c2} (see Ref. 12), so that the validity domain for (20) might be broader than the London region. The situation, however, is different in the field domain close to H_{c1}.[3] At H_{c1}, $-4\pi M_\beta = H_\beta = H_{0\beta}/(1 - n_\beta)$. For a spherical particle, for example, $\mathbf{M}$ is antiparallel to $\mathbf{H}_0$. Therefore, when $\mathbf{H}_0$—in a certain direction—increases from H_{c1}, the magnetization direction changes from being antiparallel to $\mathbf{H}_0$ to that of Eq. (20) (i.e., to $\hat{\mathbf{c}}$ for all orientations of $\mathbf{H}_0$ except a narrow domain $\theta_0 \sim \pi/2 \pm m_1/m_3$).

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*After December 1, 1988 will be at Instituto de Física, Universidade de São Paulo, Caixa Postal 20 516, 01 498 São Paulo, São Paulo, Brazil.

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