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Lower critical field of a superconductor with uniaxial anisotropy

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Exact transformation of the Ginzburg-Landau free energy with uniaxial anisotropy and a variational procedure are used to calculate accurately the line energy of a single magnetic vortex for arbitrary stiffness $\kappa_\perp$ and anisotropy γ. The lower critical field $H_{c1}(\theta_H)$ can exhibit a discontinuity, a kink, or be monotonic. Comparisons with experiment are made, and materials likely to exhibit such anomalies are suggested. The effective core cross section in the anisotropic London model is found.

The two most commonly studied phenomenological models of anisotropic superconductors are the anisotropic London and Ginzburg-Landau (GL) models. The anisotropic GL model contains the anisotropy of the order parameter as well as of the local magnetic induction **b**, but has been solved previously *only* in certain simplified situations. Letting θ and θ_H be the angles the macroscopic magnetic induction **B** and the external magnetic field **H** make with the c axis, these cases are: at the upper critical field[1,2] $H_{c2}(\theta)$, where $\theta=\theta_H$, and at the lower critical field H_{c1} when **H** is along a crystal symmetry direction,[2,3] i.e., $\theta_H=0$ or $\pi/2$. Very few results for the intermediate state have been obtained,[4] except for $\theta_H=0$ or $\pi/2$.[5]

The anisotropic London model is much simpler to use than the anisotropic GL model in calculations relevant to the intermediate state. However, because it neglects variations of the order parameter, it is inapplicable near to H_{c2}. In addition, some of the intermediate state anisotropic London results are questionable, since in calculating the vortex line energy, cutoffs at the vortex cores must be introduced. Treatments in the literature have generally *ignored* the precise form of such cutoffs.

In this paper, we report on results of an accurate GL calculation of the line energy of a single vortex at an arbitrary direction and $H_{c1}(\theta_H)$ in a superconductor with uniaxial anisotropy, the details of which will be published elsewhere.[6] Depending upon the material parameters, as θ_H is increased, $H_{c1}(\theta_H)$ can exhibit a *discontinuity*, a *kink*, or be monotonic. Fits to existing data are presented, and materials likely to exhibit such behaviors are suggested. In addition, the *exact* form of the core cross section appropriate for the London model is found, leading to essentially identical results for $H_{c1}(\theta_H)$.

We use the standard[2] dimensionless units, in which $m=(m_1m_2m_3)^{1/3}$, $\xi^2=\hbar^2/(2m|\alpha_{\rm GL}(T)|)$, $\lambda^2=mc^2/(16\pi e^2|\psi_0|^2)$ are the geometric-mean effective mass, coherence length squared, and penetration depth squared, and measure lengths in units of λ, magnetic fields in units of $\sqrt{2}H_c=\Phi_0/(2\pi\xi\lambda)$, vector potential in units of $\Phi_0/(2\pi\xi)$, and energy density in units of $H_c^2/(4\pi)$, where $\Phi_0=hc/(2e)$ is the flux quantum and H_c is the bulk thermodynamic critical field. We assume uniaxial anisotropy $m_1=m_2<m_3$. Letting the order parameter $\psi=|\psi_0|f\exp(i\varphi)$, and making the standard choice of gauge, the Gibbs free energy difference between the superconducting and normal states is

$$\mathcal{G}=\int d^3\mathbf{r}\left\{-f^2+\frac{1}{2}f^4+\sum_{\mu=1}^{3}\frac{1}{\overline{m}_\mu}\left[\frac{1}{\kappa^2}\left[\frac{\partial f}{\partial x_\mu}\right]^2+a_\mu^2f^2\right]+(\mathbf{b}-\mathbf{h})^2\right\}, \quad (1)$$

where $\overline{m}_\mu=m_\mu/m$, $\kappa=\lambda/\xi$ is the geometric-mean GL parameter, and $\mathbf{b}=\mathrm{curl}\,\mathbf{a}$. We write the components of **B** as $B_1=B\sin\theta\cos\phi$, $B_2=B\sin\theta\sin\phi$, and $B_3=B\cos\theta$.

We then employ the Klemm-Clem transformations,[2] which consist of an anisotropic scale transformation [scaling the x_μ, the b_μ, and the h_μ by $(\overline{m}_\mu)^{-1/2}$], a rotation of the axes to the scale-transformed magnetic induction direction $\hat{\mathbf{B}}'$, and an isotropic scale transformation of the lengths by $\alpha(\theta)=\gamma^{2/3}\mathcal{A}(\theta)$, where $\gamma=(m_3/m_1)^{1/2}$ is the uniaxial anisotropy factor[7] and $\mathcal{A}^2(\theta)=\cos^2\theta+\gamma^{-2}\sin^2\theta$ is the square of the angular anisotropy factor present in $H_{c2}(\theta)$.[1,2]

With these transformations, the transformed Gibbs free energy difference becomes[2,6]

$$\tilde{\mathcal{G}}=\alpha(\theta)^{-3}\int d^3\tilde{\mathbf{r}}\left[-f^2+\frac{1}{2}f^4+\frac{1}{\tilde{\kappa}^2}(\tilde{\nabla}f)^2+\tilde{\mathbf{a}}^2f^2+(\tilde{\mathbf{b}}-\tilde{\mathbf{h}})\cdot\overleftrightarrow{K}\cdot(\tilde{\mathbf{b}}-\tilde{\mathbf{h}})\right], \quad (2)$$

where $\tilde{\kappa}=\kappa/\alpha(\theta)=\kappa_\perp/\mathcal{A}(\theta)$, $\kappa_\perp=\lambda_\parallel/\xi_\parallel$ is the GL parameter for $\mathbf{B}\|\hat{\mathbf{c}}$, $\tilde{\mathbf{b}}=\tilde{\nabla}\times\tilde{\mathbf{a}}$, and the symmetric matrix $\overleftrightarrow{K}$ is given for unaxial anisotropy by $K_{11}=\gamma^2\mathcal{A}^2(\theta)$, $K_{22}=\gamma^2\cos^2\theta+\gamma^{-2}\sin^2\theta$, $K_{23}=(\gamma-\gamma^{-1})\sin\theta\cos\theta$, $K_{33}=1$, and $K_{12}=K_{13}=0$. Klemm and Clem[2] inadvertendly omitted all of the K_{ij} except $K_{33}=1$. Nevertheless, (2) is *exact* for arbitrary **B**, and is valid in the critical as well as mean-field regions. Recently,[4,8] only the anisotropic scale transformation was used. Below H_{c2}, K_{23} leads to $\theta\neq\theta_H$, modifies the θ dependence of the vortex lattice,[4] and yields the magnetic torque first predicted in the anisotropic London model.[7,9] In Ref. 8, it was *assumed* that $\tilde{\mathbf{b}}=\tilde{\mathbf{h}}$, which is only true at the mean-field upper critical field $H_{c2}(\theta)$. This assumption inherently neglects K_{23} and the resulting magnetic torque, and is therefore questionable for $H<H_{c2}$.

Minimization of (2) with respect to f and $\tilde{\mathbf{a}}$ gives the transformed GL (mean-field) equations. Using $\tilde{\mathbf{b}}=\tilde{\nabla}\times\tilde{\mathbf{a}}$, $\tilde{\mathbf{a}}$ may be eliminated, leading to

$$-(1/\tilde{\kappa}^2)\tilde{\nabla}^2 f+(1/f^3)(\tilde{\nabla}\times\overleftrightarrow{K}\cdot\tilde{\mathbf{b}})^2=f(1-f^2)\ ,\quad(3)$$

$$\tilde{\mathbf{b}}+\tilde{\nabla}\times[(1/f^2)\tilde{\nabla}\times\overleftrightarrow{K}\cdot\tilde{\mathbf{b}}]=\hat{\tilde{\mathbf{e}}}_3(2\pi/\tilde{\kappa})\delta^{(2)}(\tilde{\mathbf{r}})\ ,\quad(4)$$

where we have introduced a straight, singly quantized vortex along the line $\tilde{x}_3=0$, satisfying the boundary condition $\int_{\tilde{S}_2} d^2\mathbf{r}\,\tilde{b}_3=2\pi/\tilde{\kappa}$. Outside the core region $\tilde{\rho}=[\tilde{x}_1^2+\tilde{x}_2^2]^{1/2}>1/\tilde{\kappa}$, it suffices from (3) to set $f=1$ in (4). The resulting equation is linear in the $\tilde{b}_i$, and can be solved by Fourier transformation. By combining (4) and (2), the combination of the b_i relevant to the vortex line energy is $g=\tilde{\mathbf{b}}\cdot\overleftrightarrow{K}\cdot\hat{\tilde{\mathbf{e}}}_3$. The Fourier transform g_k of g is readily found to be

$$g_k=2\pi[1+C(\theta_k)k^2]/\tilde{\kappa}[1+A(\theta_k)k^2+C(\theta_k)k^4]\ ,\quad(5)$$

where $k_x=k\cos\theta_k$, $k_y=k\sin\theta_k$, $A(\theta_k)=1+A_+ + A_-\cos2\theta_k$, $A_\pm=(K_{11}\pm K_{22})/2$, $C(\theta_k)=C_+ + C_-\cos2\theta_k$, and $C_\pm=A_\pm-K_{23}^2/2$. As $k\to\infty$, $g_k\to2\pi/(k^2\tilde{\kappa})$, so that $g(\tilde{\rho},\tilde{\phi})$ has an isotropic core cross section, independent of $\tilde{\phi}$.

The single vortex line energy $\tilde{\epsilon}_1$ per unit length L is obtained from the difference between the Helmoholtz free energies of the Meissner state (with $\mathbf{b}=0$ and $f=1$) and the intermediate state, using the transformed $\tilde{L}=L\alpha^2(\theta)$ and $\tilde{B}=2\pi/\tilde{\kappa}$.[2] From (2)–(4), $\tilde{\epsilon}_1=\tilde{\epsilon}_{11}+\tilde{\epsilon}_{12}$, where

$$\tilde{\epsilon}_{11}=\int_0^{2\pi}\frac{d\theta_k}{2\pi}\int_0^{\eta\tilde{\kappa}/\zeta}\frac{k\,dk}{2\pi}g_k\ ,\quad(6)$$

$$\tilde{\epsilon}_{12}=\frac{\tilde{\kappa}}{2\pi}\int_0^{2\pi}d\tilde{\varphi}\int_0^{\infty}\tilde{\rho}\,d\tilde{\rho}\left[\frac{1}{2}(1-f^2)^2+\frac{1}{\tilde{\kappa}^2}(\tilde{\nabla}f)^2\right]\ ,\quad(7)$$

and ζ is a variational parameter of order unity. The parameter $\eta\approx1.1$ should approximate $2/\gamma_E$, where $\gamma_E=1.781$, in order that the integral reduce to the real-space result[3] $K_0(\zeta/\tilde{\kappa})$ as $\tilde{\kappa}\to\infty$, where $K_0(z)$ is a modified Bessel function.

We then evaluate (6) for $\tilde{\epsilon}_{11}$ exactly, and use the variational form[3] for f in (7), $f=\tilde{\rho}/[\tilde{\rho}^2+(\zeta/\tilde{\kappa})^2]^{1/2}$, leading to $\tilde{\epsilon}_{12}=(\zeta^2+1)/(4\tilde{\kappa})$. Combining these results, we obtain $\tilde{\epsilon}_1=\epsilon/\kappa_\perp$, where

$$\epsilon=\mathcal{A}(\theta)[\,\ln R(\eta\kappa_\parallel/\zeta)+(\zeta^2+1)/4]$$
$$-|\cos\theta|\ln\left[\frac{R(\eta\kappa_\parallel/\zeta)[\mathcal{A}(\theta)+|\cos\theta|]}{D(\eta\kappa_\perp/\zeta,\theta)}\right]\ ,\quad(8)$$

$R^2(z)=1+z^2$, $\kappa_\parallel=\gamma\kappa_\perp$, $D(z,\theta)=S(z,\theta)+|\cos\theta|R(z)$, and $S^2(z,\theta)=z^2+\mathcal{A}^2(\theta)$.

Minimizing $\epsilon(\zeta,\kappa_\perp,\gamma,\theta)$ with respect to ζ gives $\zeta^*(\kappa_\perp,\gamma,\theta)$ and $\epsilon^*\equiv\epsilon(\zeta^*,\kappa_\perp,\gamma,\theta)$. It is necessary to perform the variational calculation at each angle θ for fixed $\kappa_\perp$ and γ values. As $\kappa_\perp\to\infty$, $\zeta^*\to\sqrt{2}$, independent of θ and γ. By choosing $\eta=1.098$, the large $\kappa_\perp$ limit of ϵ^* is set equal to the exact numerical result of Hu[10] for a large κ, isotropic superconductor, $\epsilon\to\ln\kappa+0.497$. For $\kappa_\perp\gg1$ and $\theta=0(\pi/2)$, ϵ^* reduces to the expression of Klemm and Clem,[2] and agrees with the variational calculation of Clem *et al.*[3] for arbitrary $\kappa_\perp$ ($\kappa_\parallel$). In the limits $\gamma\to\infty$ and $\kappa_\perp\gg1$, ϵ^* agrees quantitatively with the expression of Clem[11] for a tilted stack of pancake vortices, provided that one modifies Clem's solution to include Hu's constant 0.497.[11] In the worst case we consider, $\kappa_\perp\to1\sqrt{2}$ [at which $H_{c1}(0)$ should equal H_c], the error in ϵ^* is 3.5%. In short, ϵ^* is quantitatively accurate in *all* limits available in the literature.

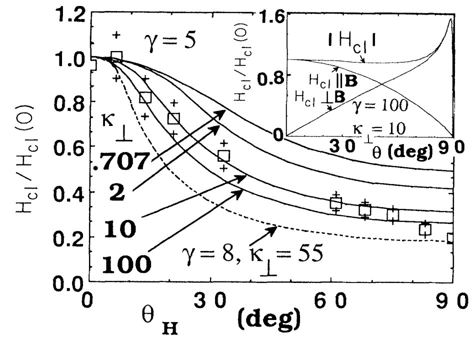

FIG. 1. Plots of $H_{c1}(\theta_H)/H_{c1}(0)$ for $\gamma=5$ and $\kappa_\perp=1/\sqrt{2},2,10,100$. □,+: Y 1:2:3 data, error bars (Ref. 12). Dashed curve: $\gamma=8$, $\kappa_\perp=55$. Inset: Plots of $H_{c1,\parallel\mathbf{B}}(\theta)$, $H_{c1,\perp\mathbf{B}}(\theta)$, and $H_{c1}(\theta)$, relative to $H_{c1}(0)$, for $\gamma=100$, $\kappa_\perp=10$.

The lower critical field is then found from $\mathbf{H}_{c1}=\hat{\mathbf{B}}H_{c1,\parallel\mathbf{B}}+\hat{\theta}H_{c1,\perp\mathbf{B}}$, where $H_{c1,\parallel\mathbf{B}}=\Phi_0\epsilon^*/(4\pi\lambda_\parallel^2)$, $H_{c1,\perp\mathbf{B}}=\partial H_{c1,\parallel\mathbf{B}}/\partial\theta$, and $\hat{\theta}=d\hat{\mathbf{B}}/d\theta$ is a unit vector normal to $\mathbf{B}$. The angles θ_H and θ are related by

$$\tan\theta_H=(\tan\theta+\epsilon'^*)/(1-\epsilon'^*\tan\theta)\ ,$$

where $\epsilon'^*=\partial\epsilon^*/\partial\theta$. Just above H_{c1}, the torque $\vec{\tau}=\mathbf{M}\times\mathbf{H}$ is proportional to $H_{c1,\perp\mathbf{B}}$.

It is elementary to minimize ϵ and evaluate the components of $\mathbf{H}_{c1}$ numerically. In the inset of Fig. 1, we have plotted $H_{c1,\parallel\mathbf{B}}$, $H_{c1,\perp\mathbf{B}}$, and $H_{c1}=|\mathbf{H}_{c1}|$, as functions of θ, for the case $\gamma=100$ and $\kappa_\perp=10$. While $H_{c1,\parallel\mathbf{B}}$ decreases monotonically with increasing θ, $H_{c1,\perp\mathbf{B}}$ exhibits a sharp peak at $\theta_p=88.6°$. The resulting H_{c1} has a shallow minimum at intermediate θ values, a sharp peak at θ_p, and an absolute minimum at $\theta=90°$. Hence, for fixed $H=H_{c1}$, multiple values of θ are possible.

Experimentally, one controls θ_H, provided that one has a reasonably good idea of the demagnetization factors relevant for the particular sample shape. In Fig. 2, we

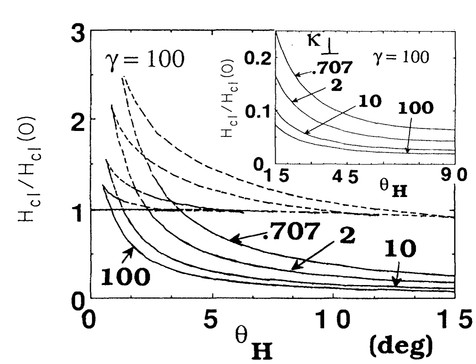

FIG. 2. Plots of $H_{c1}(\theta_H)/H_{c1}(0)$ for $\gamma=100$, $\kappa_\perp=1/\sqrt{2},2,10,100$, and $0°\le\theta_H\le15°$. Dashed curves are spurious, solid curves are real. Inset: $15°\le\theta_H\le90°$.

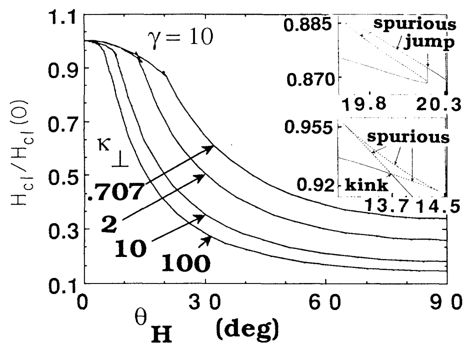

FIG. 3. Plots of $H_{c1}(\theta_H)/H_{c1}(0)$ for $\gamma=10$ and $\kappa_\perp=1/\sqrt{2}$, 2, 10, 100. Top inset: Jump in the $\kappa_\perp=1/\sqrt{2}$ curve. Lower inset: Kink in the $\kappa_\perp=2$ curve.

have plotted $H_{c1}(\theta_H)$ for $\gamma=100$ and $\kappa_\perp$ values between $1/\sqrt{2}$ and 100. The region $15°\leq\theta_H\leq 90°$ shown in the inset is innocuous, as $\theta_p<\theta\approx 90°$. For $0\leq\theta_H\leq 15°$, there can be three H_{c1} values at fixed θ_H. The actual H_{c1} is the minimum of these. Hence, the dashed curves are spurious, and the actual $H_{c1}(\theta_H)$ (solid) curves each exhibit a *kink* at a small θ_H value. These kinks arise as the vortex direction θ jumps from one side of θ_p to the other. Note that as $\kappa_\perp$ increases, the height of the (spurious) maximum decreases, but the (real) change in slope at the kink increases. Hence such kinks should be observable in the most anisotropic cuprates such as $Bi_2Sr_2CaCu_2O_{8+\delta}$ and $Tl_2Ba_2CaCu_2O_x$, as well as in the organic layered superconductors κ-$(ET)_2Cu(NCS)_2$ and κ-$(ET)_2Cu[N(CN)_2]Br$, for which $\gamma\geq 100$ from torque measurements.[9]

In Fig. 1, we have plotted $H_{c1}(\theta_H)$ for $\gamma=5$ and $\kappa_\perp$ values ranging from $1/\sqrt{2}$ to 100, along with the experimental data of Senoussi and Aguillon[12] for $YBa_2Cu_3O_{7-\delta}$ (Y 1:2:3) at $T\ll T_c$. In addition, the dashed curve is evaluated for $\gamma=8$ and $\kappa_\perp=55$, as obtained by Farrell *et al.*[9] from Torque measurements on a different crystal of Y 1:2:3. For these low γ values, $H_{c1}(\theta_H)$ decreases *monotonically* as θ_H increases. The experimental data are mostly consistent with $\gamma=5$ and $\kappa_\perp$ between 10 and 100, dropping below the theoretical curves for θ_H near to 90°. This latter deviation may be due to dimensional crossover effects[13] in H_{c1}, not present in the anisotropic GL model.

In Fig. 3, $H_{c1}(\theta_H)$ is shown for $\gamma=10$ and $\kappa_\perp$ values between $1/\sqrt{2}$ and 100. For $\kappa_\perp=1/\sqrt{2}$, $H_{c1}(\theta_H)$ is S shaped, with the minimum value exhibiting a *jump*, as shown in detail in the top inset. For $\kappa_\perp=2, 10$ a kink in $H_{c1}(\theta_H)$ is found, detailed in the lower inset for $\kappa_\perp=2$. For $\kappa_\perp=100$, the behavior is monotonic. Some of the graphite intercalation compounds, e.g., C_8K and C_4KHg, have γ and $\kappa_\perp$ values[14] appropriate for experimental investigations of the jump, as well as the kink. Other materials that could exhibit the kink are the transition metal dichalcogenides and their intercalates. Such behavior may have been observed[15] in $NbSe_2$, although the parameters for that material are such that a kink is not predicted. However, in the intercalated material $K_{0.33}(H_2O)_{0.66}TaS_2$, the apparent observation[15] of such a kink is consistent with this theory.

A calculation of H_{c1} in the anisotropic London model was made by Balatskiĭ *et al.*[16] However, those authors[16] implicity assumed $\ln\kappa_\parallel\gg\ln\gamma$, *neglecting* the term proportional to $|\cos\theta|$, and used an isotropic core cutoff. The correct core cutoff can be derived rigorously from the isotropic ($\tilde{\rho}$=const) vortex core cross section in the transformed GL frame. Then inverting the Klemm-Clem transformations to the laboratory frame, and rotating $\hat{\mathbf{c}}$ to $\hat{\mathbf{B}}$ in the anisotropic London frame, we obtain

$$k_x^2+k_y^2\mathcal{A}(\theta)\leq\xi_\parallel^{-2}\ . \tag{9}$$

When the integral analogous to (6) in the anisotropic London calculation[16] with the core cutoff (9) is performed *exactly*, the correct anisotropic London line energy can be precisely obtained from (8) by setting $\eta=\zeta=1$ [and dropping the $\mathcal{A}(\theta)(\zeta^2+1)/4$ term arising from $f\neq 1$]. Hence the anisotropic GL and London models are essentially *equivalent* for arbitrary $\kappa_\perp$ and γ.

Inclusion of the elliptical core cutoff (9) modifies many of the anisotropic London calculations of the intermediate state for $0<\theta<\pi/2$. Such corrections will be presented elsewhere.[6] In two London calculations, the correct elliptical cutoff was used.[17] In these papers, the (correct) cutoff cross section was assumed to be concentric to the streamlines of constant current, and the $\ln\kappa_\perp\gg 1$ limit of the vortex line energy was correctly obtained. We have thus proven that such a cutoff is rigorous for arbitrary $\kappa_\perp$.

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