Free Energy and Torque for Superconductors with Different Anisotropies of H_{c2} and λ

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The free energy is evaluated for a uniaxial superconductor with the anisotropy of the upper critical field, $\gamma_H = H_{c2,a}/H_{c2,c}$, different from the anisotropy of the penetration depth $\gamma_\lambda = \lambda_c/\lambda_a$. With increasing difference between γ_H and γ_λ, the equilibrium orientation of the crystal relative to the applied field may shift from $\theta = \pi/2$ (θ is the angle between the field and the c axis) to lower angles and reach $\theta = 0$ for large enough γ_H. These effects are expected to take place in MgB_2.

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It is a common practice to characterize anisotropic superconductors by a single anisotropy parameter defined as $\gamma = \xi_a/\xi_c \equiv \lambda_c/\lambda_a$ (ξ is the coherence length, λ is the penetration depth, and a, c are principal directions of a uniaxial crystal of the interest here). The practice emerged after the anisotropic Ginzburg-Landau (GL) equations were derived for arbitrary gap and Fermi surface anisotropies by Gor'kov and Melik-Barkhudarov [1]. Formally, this came out because in the GL domain, the same "mass tensor" determines the anisotropy of both ξ (of the upper critical fields H_{c2}) and λ.

At arbitrary temperatures, however, the theoretical approach for calculating H_{c2} (the position of the second order phase transition in high fields) has little in common with evaluation of λ (the weak-field relation between the current and the vector potential), so that the anisotropies of these quantities are not necessarily the same. In fact, in materials with anisotropic Fermi surfaces and anisotropic gaps, not only the parameter $\gamma_H = H_{c2,a}/H_{c2,c}$ may strongly depend on T, but this ratio might differ considerably from $\gamma_\lambda = \lambda_c/\lambda_a$ at low T's. For MgB_2, $\gamma_H \approx 6$ at low temperatures [2–5]. There is no consensus yet on the low-T γ_λ. Zehetmayer *et al.* use the torque data to find $\gamma_\lambda \approx \gamma_H$; however, their procedure implies this equality to begin with (as discussed in detail below). Microscopic calculation for clean MgB_2 yields $\gamma_\lambda \approx 1.1$ [6,7]. With increasing T, $\gamma_H(T)$ decreases, the calculated $\gamma_\lambda(T)$ increases till they meet at $T = T_c$: $\gamma_H(T_c) = \gamma_\lambda(T_c) \approx 2.6$.

One of the most sensitive methods used to extract the anisotropy parameter γ is to measure the torque acting on a superconducting crystal in the mixed state with the applied field tilted relative to the crystal axes. In intermediate field domain, $H_{c1} \ll H \ll H_{c2}$, the demagnetization shape effects are weak, and the torque density can be evaluated [8,9]:

$$\tau = \frac{\phi_0 B(\gamma^2 - 1)\sin 2\theta}{64\pi^2\lambda^2\gamma^{1/3}\varepsilon(\theta)} \ln\frac{\eta H_{c2,a}}{B\varepsilon(\theta)}, \qquad (1)$$

where θ is the angle between the induction $\mathbf{B}$ and the crystal axis c,

$$\varepsilon(\theta) = \sqrt{\sin^2\theta + \gamma^2\cos^2\theta}, \qquad (2)$$

$\lambda^3 = \lambda_a^2\lambda_c$, and $\eta \sim 1$. This formula can be written as $\boldsymbol{\tau} = \boldsymbol{M} \times \boldsymbol{H}$; since in this field domain the magnetization $M \ll H$, one can disregard the distinction between $\boldsymbol{B}$ and $\boldsymbol{H}$. It has been assumed in the derivation of Eq. (1) that the anisotropies of H_{c2} and of the London penetration depth are the same: $\gamma_H = \gamma_\lambda = \gamma$.

Note that Eq. (1) describes the system with the stable equilibrium at $\theta = \pi/2$; i.e., the uniaxial crystal in the external field positions itself so that the field is parallel to ab (if $\gamma > 1$). It is worth noting that if one applies formally the expression (1) with $H_{c2}(\theta) = H_{c2,a}/\varepsilon(\theta)$ having the anisotropy different from γ_λ, one may obtain qualitatively different angular behavior of $\tau(\theta)$.

Expression (1) for the torque has been derived within the London approach by employing the cutoff at distances on the order of the coherence length ξ where this approach fails; that is how the upper critical field $H_{c2} \sim \phi_0/\xi^2$ enters the London formula. The formula, however, has been confirmed experimentally (for a few high-T_c materials) with a good accuracy as far as the angular dependencies of quantities involved are concerned [10]. Uncertainties of the London approach are incorporated in the parameter $\eta \sim 1$; discussion of those can be found, e.g., in Ref. [11].

Below, the free energy of the mixed state and the torque are derived for the general case of $\gamma_H \neq \gamma_\lambda$. The torque expression is shown to acquire new terms which describe a more complicated behavior as compared to that of Eq. (1). This implies that the analysis of the torque data might be misleading if Eq. (1) is employed to materials like MgB_2 [5,12,13].

Let us start with the London expression for the free energy valid for intermediate fields $H_{c1} \ll H \ll H_{c2}$ along z tilted with respect to the c crystal axis over the angle θ toward the crystal direction a [14]:

$$F = \frac{B^2}{8\pi} + \frac{B^2 m_{zz}}{8\pi\lambda^2 m_a}\sum_{\boldsymbol{G}}\frac{1}{m_{zz}G_x^2 + m_c G_y^2}; \qquad (3)$$

here $m_{zz} = m_a\sin^2\theta + m_c\cos^2\theta$, $m_c/m_a = \gamma_\lambda^2$, $m_a^2 m_c = 1$

for uniaxial crystals, and $\boldsymbol{G}$ form the reciprocal vortex lattice. The summation is extended over all nonzero $\boldsymbol{G}$.

As usual we evaluate the sum here by replacing it with an integral over the reciprocal plane, $\sum_{\boldsymbol{G}} \to (\phi_0/4\pi^2 B)\int dG_x dG_y$:

$$\tilde{F} = F - \frac{B^2}{8\pi} = \frac{\phi_0 B m_{zz}}{32\pi^3\lambda^2 m_a}\int \frac{dG_x dG_y}{m_{zz}G_x^2 + m_c G_y^2} = \frac{\phi_0 B\sqrt{m_{zz}}}{32\pi^3\lambda^2}\int_0^{2\pi} d\varphi \int \frac{dg}{g}, \tag{4}$$

where $g_x = \sqrt{m_{zz}}\,G_x$, $g_y = \sqrt{m_c}\,G_y$, and we use polar coordinates $g_x = g\sin\varphi$, $g_y = g\cos\varphi$.

To determine the limits of integration over g, one can recall that in fields $B \ll H_{c2}$ the vortex lattice structure is fixed by the anisotropy parameter γ_λ [14]. In intermediate fields, for all possible equilibrium London structures, the distance g_0 in the reciprocal space from the origin to the nearest neighbors is given by [15]

$$g_0^2 = m_{zz}G_x^2 + m_c G_y^2 = \frac{8\pi^2 B}{\sqrt{3}\phi_0}\sqrt{m_c m_{zz}}. \tag{5}$$

Therefore, one can take g_0 (multiplied by a number of order unity) as the lower limit in the logarithmically divergent integral over g.

The upper limit in this integral is affected by the form of the vortex core. To determine the core shape we note that the microscopic evaluation of H_{c2} (see Ref. [7]) shows that with a good accuracy the angular dependence of H_{c2} is given by the standard GL form at any T:

$$H_{c2} = \frac{\phi_0}{2\pi\xi^2\sqrt{\mu_a\sin^2\theta + \mu_c\cos^2\theta}} = \frac{\phi_0}{2\pi\xi^2\sqrt{\mu_{zz}}}. \tag{6}$$

This can be written as

$$H_{c2} = \frac{\phi_0}{2\pi\xi_x\xi_y}, \qquad \xi_x = \xi\sqrt{\mu_a\mu_{zz}}, \qquad \xi_y = \frac{\xi}{\sqrt{\mu_a}}, \tag{7}$$

where $\xi_{x,y}$ are semiaxes of the elliptical core. We stress that the "masses" μ_{ik} are different from m_{ik} which determine the anisotropy of λ; in particular, $\mu_a = \gamma_H^{-2/3}$, $\mu_c = \gamma_H^{4/3}$, whereas $m_a = \gamma_\lambda^{-2/3}$, $m_c = \gamma_\lambda^{4/3}$. Equation (7) gives maximum values of G_x and G_y:

$$G_{x,m} = \frac{2\pi}{\xi\sqrt{\mu_a\mu_{zz}}}, \qquad G_{y,m} = \frac{2\pi\sqrt{\mu_a}}{\xi}. \tag{8}$$

Thus, the domain of integration in the $\boldsymbol{G}$ plane is bound by an ellipse

$$\frac{G_x^2}{G_{x,m}^2} + \frac{G_y^2}{G_{y,m}^2} = 1. \tag{9}$$

In other words, at a given φ, the upper limit in the integral over g is

$$g_m(\varphi) = \frac{2\pi\sqrt{\mu_a m_c}}{\xi\sqrt{\beta^2\cos^2\varphi + \sin^2\varphi}}, \qquad \beta^2 = \frac{m_c\mu_{zz}}{m_{zz}\mu_c}, \tag{10}$$

and we obtain

$$\tilde{F} = \frac{\phi_0 B\sqrt{m_{zz}}}{32\pi^3\lambda^2}\int_0^{2\pi} d\varphi \ln\frac{g_m(\varphi)}{g_0} = \frac{\phi_0 B\sqrt{m_{zz}}}{32\pi^2\lambda^2}\left[\ln\frac{\sqrt{3m_c}\,\mu_a\phi_0}{2\xi^2 B\sqrt{m_{zz}}} - \frac{1}{2\pi}\int_0^{2\pi} d\varphi \ln(\beta^2\cos^2\varphi + \sin^2\varphi)\right]. \tag{11}$$

Note that $\beta = 1$ for coinciding anisotropies of H_{c2} and λ; the integral $J(\beta)$ over φ then vanishes, and we have the standard expression for the energy. To evaluate $J(\beta)$, we observe that the integral for $dJ/d\beta$ can be calculated by going to the complex plane with the help of residues: $dJ/d\beta = 4\pi/(\beta+1)$. Since $J(1) = 0$, we obtain

$$J = 4\pi\ln\frac{1+\beta}{2}. \tag{12}$$

Thus, we have

$$\tilde{F} = \frac{\phi_0 B\sqrt{m_{zz}}}{32\pi^2\lambda^2}\ln\frac{2\sqrt{3m_c}\,\mu_a\phi_0}{\xi^2 B\sqrt{m_{zz}}\,(1+\beta)^2}. \tag{13}$$

To write explicitly the angular dependence of F, it is convenient to use the angular functions

$$\Theta_{\lambda,H}(\theta) = \varepsilon_{\lambda,H}(\theta)/\gamma_{\lambda,H}, \tag{14}$$

where $\varepsilon_{\lambda,H}(\theta)$ are defined in Eq. (2) with corresponding γ's. In terms of these functions, $\beta = \Theta_H/\Theta_\lambda$ and

$$\tilde{F} = \frac{\phi_0 B\Theta_\lambda}{32\pi^2\lambda_a^2}\ln\frac{2\sqrt{3}\,\mu_a\phi_0\Theta_\lambda}{\xi^2 B\,(\Theta_\lambda+\Theta_H)^2}. \tag{15}$$

The torque density follows:

$$\tau = -\frac{\partial\tilde{F}}{\partial\theta} = -\frac{\phi_0 B}{32\pi^2\lambda_a^2}\left[\Theta_\lambda'\ln\frac{2e\sqrt{3}\,\mu_a\phi_0\Theta_\lambda}{\xi^2 B\,(\Theta_\lambda+\Theta_H)^2} - 2\Theta_\lambda\frac{\Theta_\lambda'+\Theta_H'}{\Theta_\lambda+\Theta_H}\right], \tag{16}$$

where $e = 2.718\ldots$. The torque is zero at $\theta = 0, \pi/2$ because

$$\Theta' = -\frac{(\gamma^2-1)\sin 2\theta}{2\gamma^2\Theta} \tag{17}$$

for both Θ_λ and Θ_H. In the standard case of $\gamma_H = \gamma_\lambda = \gamma$, Eq. (16) reduces to the result (1) if we set $\eta = \pi\sqrt{3}/e \approx 2$. We then can rewrite the torque in the form

$$\tau = \frac{\phi_0 B(\gamma_\lambda^2-1)\sin 2\theta}{64\pi^2\lambda^2\gamma_\lambda^{4/3}\Theta_\lambda}\left[\ln\left(\frac{\eta H_{c2,c}}{B}\frac{4e^2\Theta_\lambda}{(\Theta_\lambda+\Theta_H)^2}\right) - \frac{2\Theta_\lambda}{\Theta_\lambda+\Theta_H}\left(1+\frac{\Theta_H'}{\Theta_\lambda'}\right)\right]. \tag{18}$$

Since $\Theta'_{\lambda,H} < 0$, the second contribution to the torque (16) is negative, whereas the first one is positive. The positive torque implies that the system energy decreases with increasing θ, as in the case of $\gamma_H = \gamma_\lambda$ for which $\theta = \pi/2$ is the stable equilibrium.

The competing roles of these two contributions can be demonstrated by considering stability of equilibrium states at $\theta = 0$ and $\theta = \pi/2$. To do this one notes that $\Theta(0) = 1$, $\Theta(\pi/2) = 1/\gamma$, $\Theta'(0) = \Theta'(\pi/2) = 0$, and

$$\Theta''(0) = -\frac{\gamma^2 - 1}{\gamma}, \qquad \Theta''(\pi/2) = \frac{\gamma^2 - 1}{\gamma} \tag{19}$$

(for both Θ_λ and Θ_H). Then, one obtains

$$F''\left(\frac{\pi}{2}\right) = \frac{\gamma_\lambda^2 - 1}{\gamma_\lambda} \ln \frac{4\pi e\sqrt{3} H_{c2,a} \gamma_\lambda \gamma_H}{B(\gamma_H + \gamma_\lambda)^2} - 2\frac{\gamma_H \gamma_\lambda - 1}{\gamma_\lambda},$$
$$F''(0) = -\frac{\gamma_\lambda^2 - 1}{\gamma_\lambda} \ln \frac{\pi\sqrt{3} H_{c2,c}}{B} + \frac{\gamma_H^2 - 1}{\gamma_H}, \tag{20}$$

where the constant positive prefactor is omitted since we are interested only in the sign of F''. Clearly, $\theta = \pi/2$ corresponds to the stable equilibrium for $\gamma_H = \gamma_\lambda$. In the general case, however, there is no such a clear-cut result: for a fixed γ_λ and large enough γ_H, $\theta = \pi/2$ may become unstable. For example, for $\gamma_\lambda = 1$ and $\gamma_H > 1$, $F''(\pi/2) < 0$, whereas $F''(0) > 0$.

To illustrate how the angular dependence of the torque varies with anisotropies of H_{c2} and λ, we evaluate numerically the torque density (18) for parameters in the range of those for MgB_2. Figure 1 shows $\tau(\theta)$ for $\gamma_\lambda = 2.2$ and $\gamma_H = 3$, the values expected for temperatures somewhat below T_c. Qualitatively, the dependence is standard; the torque is positive in the whole angular domain; i.e., $\theta = \pi/2$ is the stable equilibrium.

With decreasing T, γ_H of MgB_2 increases, whereas γ_λ decreases. In Fig. 2 the torque (18) is plotted for $\gamma_\lambda = 2$, $\gamma_H = 5$ (the upper curve) and for $\gamma_\lambda = 1.7$, $\gamma_H = 5.3$ (the lower curve). These values correspond roughly to $0.7T_c$ and $0.6T_c$ according to Ref. [7]. Clearly, $\theta = \pi/2$ as well as $\theta = 0$ are unstable; the stable equilibrium is shifted to $0 < \theta < \pi/2$. Interestingly enough, Ref. [16] reports that a strong "peak-effect-like" irreversibility develops in the torque data at $\approx 77°$ at $T = 15$ K and $H = 7.5$ T. In layered materials this effect is commonly interpreted as manifestation of the "intrinsic pinning" in the small vicinity of the equilibrium orientation at $\theta = \pi/2$. From the point of view of this Letter, the peak should move to a position of the stable equilibrium, i.e., to lower angles. Moreover, the data show a *negative* torque above this angle ($77° < \theta < 90°$) in agreement with Fig. 2. Still, interpretation of these data within the London model should not be taken too literally: the applied field $H = 7.5$ T exceeds $H_{c2,c}(0)$, and in the θ domain where $H < H_{c2}(\theta)$, the London model should not be trusted.

Finally, we plot in Fig. 3 the torque density for parameters which correspond to low temperatures, where $\gamma_\lambda \approx 1.1$ and $\gamma_H \approx 6$. The torque is negative for all angles implying the stable equilibrium at $\theta = 0$.

Physically, the large low temperature anisotropy of H_{c2} in MgB_2 is caused by the large superconducting gap on the nearly two-dimensional sheets of the Fermi surface of this material [17–19]. With increasing T, thermal mixing with the states at the three-dimensional part of the Fermi surface suppresses this anisotropy to about $\gamma_H(T_c) \approx 2.6$. The anisotropy of the London λ (or of the superfluid density) at $T = 0$ of clean materials does not depend on the gap at all ("Galilean invariance of the superflow") and therefore is determined by the whole Fermi surface; i.e., it is weak for MgB_2 (see discussions in Refs. [6,7]). The calculation [6] shows that $\gamma_\lambda(T = 0) \approx 1.1$ and grows to ≈ 2.6 as $T \to T_c$.

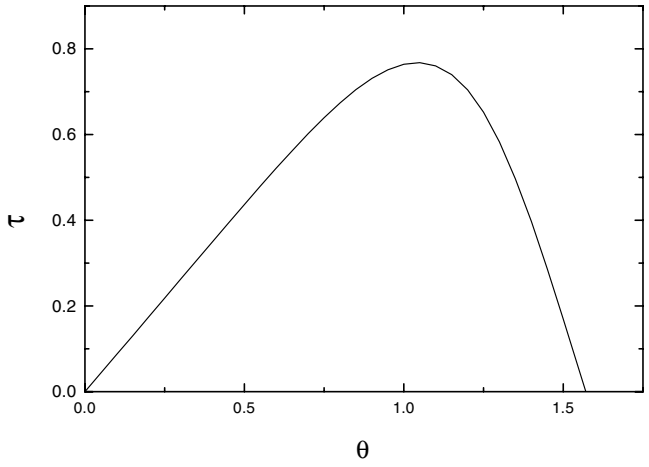

FIG. 1. The torque τ in units of $\phi_0 B/32\pi^2\lambda_{ab}^2$ versus angle $0 < \theta < \pi/2$ for $\gamma_\lambda = 2.2$, $\gamma_H = 3$, and $4e^2\eta H_{c2,c}/B = 100$.

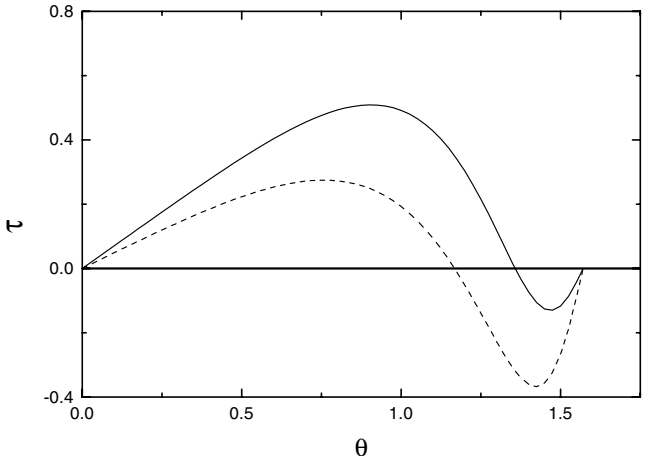

FIG. 2. The same as in Fig. 1. The solid curve is calculated with Eq. (18) for $\gamma_\lambda = 2$ and $\gamma_H = 5$; the dashed curve corresponds to $\gamma_\lambda = 1.7$ and $\gamma_H = 5.3$.

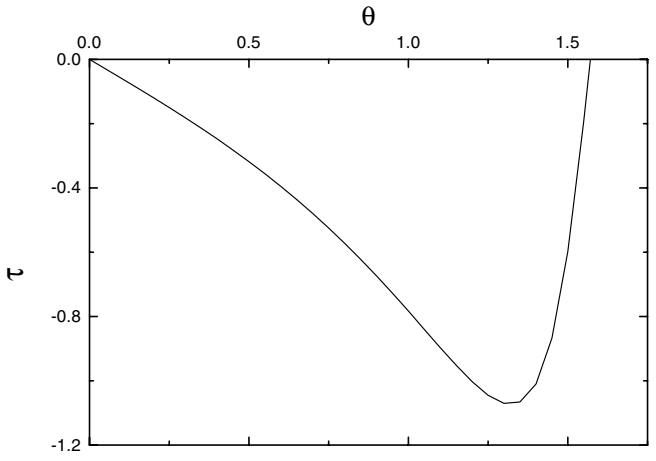

FIG. 3. The same as in Fig. 1, but $\gamma_\lambda = 1.1$ and $\gamma_H = 6$.

Thus, different gaps at different Fermi surface pieces of MgB_2 (or, generally, anisotropic gaps on anisotropic Fermi surfaces) may lead to profound macroscopic consequences such as those considered above. Since γ_H determines the anisotropy of the coherence length and, therefore, of the vortex core, whereas γ_λ describes the ellipticity of the current distribution far from the core, the symmetry of the intervortex interaction should depend on the intervortex spacing, i.e., on the field B and its direction. In MgB_2 at low temperatures in fields along ab, one expects to have the standard triangular (hexagonal) vortex lattice in low fields ($\gamma_\lambda \sim 1$), which should evolve to a distorted triangular (orthorhombic) lattice in increasing fields when the core ellipticity ($\gamma_H \approx 6$) becomes relevant for the vortex current distribution. The field dependence of the vortex lattice structure should become weaker at elevated temperatures and disappear near T_c. Possibility of a peak effect near the field orientation other than $H \parallel ab$ is an example of peculiar dynamic phenomena which might be related to the shift in the minimum of the energy angular dependence for certain values of γ's. This possibility calls for further study.

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