Anisotropy parameters of superconducting MgB$_2$

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Abstract

Data on macroscopic superconducting anisotropy of MgB$_2$ are reviewed. The data are described within a weak coupling two-gaps anisotropic s-wave model of superconductivity. The calculated ratio of the upper critical fields $\gamma_H = H_{c2,ab}/H_{c2,c}$ increases with decreasing temperature in agreement with available data, whereas the calculated ratio of London penetration depths $\gamma_\lambda = \lambda_c/\lambda_{ab}$ decreases to reach $\approx 1.1$ at $T = 0$. Possible macroscopic consequences of $\gamma_\lambda \neq \gamma_H$ are discussed.

Key words: magnesium diboride, upper critical field, penetration depth, anisotropy, torque
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1 Introduction

Physics and applications of new superconducting materials cannot be properly understood and developed without careful characterization of possible anisotropies. High-$T_c$ materials are one of the best examples of relevance of the superconducting anisotropy to all aspects of physics and possible applications.

It is a common practice to characterize anisotropic superconductors by a single anisotropy parameter defined as $\gamma = \xi_a/\xi_c \equiv \lambda_c/\lambda_a$. Here, $\xi$ is the coherence length, $\lambda$ is the penetration depth, and $a, c$ are principal directions of a uniaxial crystal of the interest here. Often $\xi_a = \xi_b$ are denoted in literature as

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\(\xi_{ab}\); for formal reasons we prefer a single subscript notation. Since the upper critical fields, \(H_{c2,c} = \frac{\phi_0}{2\pi\xi_0^2}\) and \(H_{c2,a} = \frac{\phi_0}{2\pi\xi_a\xi_c}\), the anisotropy parameter can also be written as \(\gamma = \frac{H_{c2,a}}{H_{c2,c}}\). Historically, the practice to assign a single anisotropy parameter to each material emerged after the anisotropic Ginzburg-Landau (GL) equations were proposed phenomenologically by Ginzburg [1] and derived microscopically for arbitrary gap and Fermi surface anisotropies by Gor’kov and Melik-Barkhudarov [2]. Formally, this came out because near the critical temperature \(T_c\), the same “mass tensor” \(m_{ik}\) determines the anisotropy of both \(\xi\) (of the upper critical fields \(H_{c2}\) and of \(\lambda\):

\[
\begin{align*}
(\xi^2)_{ik} &\propto m_{ik}^{-1}, \\
(\lambda^2)_{ik} &\propto m_{ik}.
\end{align*}
\]

Therefore,

\[
\gamma_{\lambda}^2 = \frac{\lambda^2}{\lambda_a^2} = \frac{m_{cc}}{m_{aa}} = \frac{\xi_a^2}{\xi_c^2} = \gamma^2_{\xi}.
\]

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 \(\lambda\) (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 \(\gamma_H = \frac{H_{c2,a}}{H_{c2,c}}\) may strongly depend on \(T\), but this ratio might differ considerably from \(\gamma_{\lambda} = \frac{\lambda_c}{\lambda_a}\) at low temperatures [3,4].

In this brief review we collect data on anisotropy of MgB\(_2\) available to us, discuss briefly the methods used and the results obtained. Then we outline the weak-coupling microscopic approach which can be used to evaluate the anisotropy parameters and their \(T\) dependence. We conclude with discussion of macroscopic consequences of different \(H_{c2}\) and \(\lambda\) anisotropies focussing on the torque problem, the quantity commonly measured to extract the anisotropy parameters.

2 Data review

Experimentally, superconducting anisotropy of MgB\(_2\) was under scrutiny right away after the discovery of this material. Almost all experimental studies were concerned with the \(H_{c2}\) anisotropy, \(\gamma_H = \frac{H_{c2,ab}}{H_{c2,c}}\).

Based on the AC susceptibility and the field dependent magnetization measurements on sorted powders, magnesium diboride was claimed to be an
isotropic superconductor [5]. The $H_{c2}$ anisotropy for separate particles settled on a flat surface was reported as $\gamma_H \approx 1.73$ [6]. For a hot-pressed bulk samples values of $\gamma_H$ up to 1.2 were obtained from susceptibility and resistance measurements [7]. Magnetotransport measurements on MgB$_2$ thin films with different degrees of c-axis orientation yielded $\gamma_H = 1.8 - 2$ ($T_c = 31-37$ K) with higher anisotropy for films of higher resistivity [8]. The temperature-independent $\gamma_H = 1.2$ ($T_c = 39$ K) was reported for c-oriented films, Ref. [9]. Similar results ($\gamma_H = 1.2 - 1.8$) were later obtained for a set of three films pulsed laser deposited (PLD) on different substrates ($T_c = 31-37$ K) [10,11]. In this case no apparent correlation was observed between the $H_{c2}$ anisotropy and residual resistance ratio (RRR) or superconducting transition temperature of the films. Quite different values, $\gamma_H = 9 - 13$, were reported for in-situ grown PLD films with $T_c$ suppressed down to 24 - 27 K [12].

In a different approach, the $H_{c2}$ anisotropy of magnesium diboride was evaluated from a number of measurements on randomly oriented powders. Analysis of the conduction electron spin resonance (CESR) data on fine MgB$_2$ powders taken in a wide temperature range yielded an estimate of $\gamma_H \approx 8$ [13]. Similar idea (deconvoluting the signal in a certain temperature range in two components, one corresponding to superconducting state and the other originating from the normal state) was later used for interpretation of the $^{11}$B nuclear magnetic resonance (NMR) data in the mixed state of MgB$_2$ [14]. These measurements resulted in $\gamma_H \approx 6$. Subsequent $^{11}$B NMR and magnetization studies on Mg$_{1-x}$Al$_x$B$_2$ ($x \leq 0.025$) reveal a considerable decrease of the anisotropy with Al doping [15].

In addition to local NMR and CESR probes, global measurements on samples with randomly oriented grains were used for the anisotropy studies. High field reversible DC magnetization data were well described assuming that MgB$_2$ is an anisotropic superconductor with $\gamma_H = 6 - 9$ and using the available experimental estimates of the average penetration depth $\lambda(0) = (\lambda_{ab}^2 \lambda_c)^{1/3} = 110 - 140$ nm [13]. The $H_{c2}$ anisotropy was also evaluated from the broadening of the resistive transition in applied magnetic field. Two slightly different theoretical approaches to this problem, [16] and [17], based on the anisotropic Ginzburg-Landau and percolation theories for randomly oriented anisotropic superconducting grains, were developed more than a decade ago in early days of the high $T_c$ superconductivity. They require somewhat different analysis of the resistivity data but result in similar estimates: $\gamma_H = 5 - 7$ [18].

The aforementioned determinations of the $H_{c2}$ anisotropy utilized traditional techniques, with the exception of those based on CESR and NMR. About a year ago a robust and a simple way to extract this anisotropy from the data on $T$ dependence of the magnetization of random powders taken in various fixed fields has been suggested [19]. The method is based on two features in $(\partial M/\partial T)_H$: the onset of diamagnetism at $T_c^{\text{max}}$, which is commonly associated
with $H_{c2}$ and which is, in fact, $H_{c2,max} \equiv H_{c2,a}$, and a kink in $\partial M/\partial T$ at a lower temperature $T_{c,\text{min}}$ (see Fig. 1). The origin of these two features can be understood as follows.

Upon cooling a powder sample in a fixed $H$, there is a deviation from a roughly $T$ independent normal state magnetization (for non-magnetic materials as is the case of MgB$_2$) to an increasingly diamagnetic signal at $T = T_{c,max}$. On the $H - T$ diagram, the point $(H, T_{c,max})$ lies at the phase boundary $H_{c2,max}(T)$. Repeating this measurement at various fixed field one recovers the full curve $H_{c2,max}(T) \equiv H_{c2,a}(T)$. This line coincides with the upper critical field determined for polycrystalline samples by, e.g., the standard resistivity measurements. A second sharp feature occurs in $\partial M/\partial T$ when the sample temperature passes through $T_{c,\text{min}}$. This can be readily understood by considering what happens to the sample upon warming. For $T < T_{c,\text{min}}$ all randomly oriented grains are superconducting, whereas for $T > T_{c,\text{min}}$ part of them are normal, depending upon their orientation with respect to the applied magnetic field. Therefore, upon warming through $T_{c,\text{min}}$ we expect some peculiarity, or a kink in $\partial M/\partial T$ associated with the onset of normal state properties in an increasing number of appropriately oriented grains. In a similar spirit the field dependent magnetization can be analyzed. This method constitutes a robust procedure independent either of a particular model for describing the anisotropy or of a degree of powder randomness. A kink in $\partial M/\partial T$ at $T = T_{c,\text{min}}$ should be present for any angular distribution of the grains (as long as it is continuous, although not necessarily random).

It should be noted that in superconductors with strong fluctuations (like HTSC) or in the samples with a distribution of $T_c$’s or other physical properties due to chemical or/and structural inhomogeneities the region of superconductornormal transition and the kink in $\partial M/\partial T$ may be smeared. In such cases this simple method may not work. Still, given difficulties in growing single crystals of a sufficient size often encountered when a new material is synthesized, the method may prove useful and sometimes the only one available for determination of the $H_{c2}$ anisotropy.

The analysis of detailed temperature and field dependent magnetization measurements on MgB$_2$ powders together with the data on polycrystalline $H_{c2}$ ($= H_{c2,\text{max}}^{\text{polycrystalline}}$) obtained from high field magnetotransport measurements on similar samples yielded a complete anisotropic $H_{c2}(T)$ phase diagram [20], see Fig. 2.

A number of direct measurements of the $H_{c2}$ anisotropy on single crystals was reported. Magnetoresistance data on small MgB$_2$ single crystalline platelets [21,22,23,24] gave $\gamma_H = 2.6 - 3.0$ (in these samples $T_c = 38.0-38.6$ K, $RRR = 5 - 8$). It is argued in Ref. [25] that electrical transport measurements are not well suited to probe bulk upper critical field of MgB$_2$ due to possible presence
The torque magnetometry was also employed to study superconducting anisotropy on single crystals [26]. From angular dependent torque measurements taken in different applied fields the anisotropy of the upper critical field was found to be temperature dependent: it decreases from \( \gamma_H \approx 6 \) at 15 K to \( \approx 2.8 \) at 35 K. Reversible angular dependent torque measurements (with a vortex shaking process [27]) performed in the temperature range 27 - 36 K and in fields up to 10 kOe were analyzed using a formula derived in [28] for \( \gamma_H = \gamma_\lambda \), see Eq. (15) below. As a result, nearly linear field dependence of \( \gamma \) has been extracted with \( \gamma(H \to 0) \approx 2 \) and \( \gamma(10 \text{ kOe}) \approx 3.7 \) with practically no \( T \) dependence between 27 K and 36 K. Extensive torque data of Ref. [29] were also interpreted assuming \( \gamma_H = \gamma_\lambda = \gamma \) and produced estimates \( \gamma \approx 3 - 4 \) which vary somewhat with \( T \) and \( H \).

Subsequent analysis [20] of the anisotropic \( H_{c2}(T) \) data obtained on random MgB\(_2\) powders (Fig. 2) showed \( \gamma_{H}(T) \) dependence consistent (Fig. 3) with the one observed in the single crystals [26]. Similar temperature-dependent \( \gamma_H \) behavior was extracted from magnetotransport, magnetization, ac susceptibility and specific heat in applied magnetic field measurements on single-crystalline platelets [30,31,32] and in thin films [11].

Summarizing, the reported anisotropy of the upper critical field in magnesium diboride range from \( \gamma_H \approx 1 \) to \( \gamma_H \approx 13 \). There are some concerns related to the spread of these results such as purity and homogeneity of materials used, degree of alignment of crystallites/grains, possible sharp angular dependence of \( H_{c2} \) so that correct evaluation of the anisotropy may suffer from even slight misorientations in measurements on single crystallites, and, last but not least, adequacy of models used to analyze the data on polycrystals and crystals. Even for similar small single crystals different apparently direct measurements give somewhat different estimates of \( \gamma_H \) (see e.g. [26,25]). On the other hand, there is an apparent consistence between recent data on the temperature dependence of \( \gamma_H \) obtained by at least two groups on single crystals and on high quality powders, similar ”convergence” emerges in data for other physical properties. This indicates that we are coming closer to measuring the intrinsic properties of MgB\(_2\). As a side remark it should be mentioned that temperature dependent \( H_{c2} \) anisotropy is not unique for MgB\(_2\), it was observed, for example, in NbSe\(_2\) [33].

For sub-mm size MgB\(_2\) single crystal, an anisotropic lower critical field, \( H_{c1} \), was estimated from the \( M(H) \) data [21]. The \( H_{c1}^{ab}(T) \) dependence was reported as near linear with \( H_{c1}^{ab}(0) \approx 384 \text{ G} \), while the \( H_{c1}^{c}(T) \) appeared to be non-linear
with and $H_{c1}^c(0) \approx 272 \text{ G}$. Another estimate of the temperature dependent anisotropic $H_{c1}$ from magnetization measurements on MgB$_2$ single crystallites [32] gave close to linear $H_{c1}(T)$ for both directions with extrapolated to $T = 0$ values $H_{c1}^c(0) \approx 2800 \text{ G}$ and $H_{c1}^{ab}(0) \approx 1300 \text{ G}$ and near $T$ independent ratio $H_{c1}^c / H_{c1}^{ab} \approx 2.2$.

Apparently more work on sample quality, measurement procedures, measurements analysis, and modelling is required to obtain a better physical picture of the superconducting anisotropy of MgB$_2$. Reliable data on the temperature dependence of the anisotropy of the London penetration depth, when available, will serve as an important test of existing models.

3 Theory of anisotropies of $\lambda$ and $H_{c2}$

To address theoretically the question of anisotropy at arbitrary temperatures one has to turn to a microscopic model. The most complete and sophisticated approach is based on taking into account the actual Fermi surface, the phonon distribution, and the electron-phonon interaction (all of which are anisotropic) in the frame of the Eliashberg theory. This can be and has been done numerically by a few groups, which evaluated the Fermi surfaces [34,35] and the gap distribution [36,37].

As is shown in Fig. 4, the Fermi surface of MgB$_2$ consists of two nearly cylindrical sheets, ”2D $\sigma$-bands”, and two others corresponding to the ”3D $\pi$-bands”. The gap on the four Fermi surface sheets of this material has two sharp maxima: $\Delta_1 \approx 1.7 \text{ meV}$ at the two $\pi$-bands and $\Delta_2 \approx 7 \text{ meV}$ at the two $\sigma$-bands, see Fig. 5. Within each of these groups, the spread of the gap values is small, and the gaps can be considered as constants, the ratio of which is nearly $T$ independent. In this situation, a model with only two Fermi surface sheets and two gaps may prove useful in relating various macroscopic properties of MgB$_2$. Starting with Ref. [38], the two-band models were studied by many, see, e.g., Ref. [39] and references therein. We outline below the results of evaluation of the London penetration depth and the upper critical fields within a relatively simple two-gap weak-coupling model which provides consistent physical picture of superconducting anisotropies. We also discuss possible consequences of different anisotropies of $\lambda$ and $H_{c2}$ upon macroscopic magnetic properties of MgB$_2$.  

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3.1 Two gap model

We begin with the notion that within the weak-coupling BSC theory the macroscopic characteristics of superconductors such as the coherence length and the penetration depth are expressed in terms of quantities averaged over the Fermi surface. This basic consequence of the collective nature of the superconducting condensate is formally expressed by the self-consistency (or gap) equation:

\[ \Delta(\mathbf{r}, \mathbf{v}, T) = 2\pi T N(0) \sum_{\omega > 0} \omega \langle V(\mathbf{v}, \mathbf{v}') f(\mathbf{r}, \mathbf{v}', \omega) \rangle_{\mathbf{v}'}. \tag{3} \]

Here, \( N(0) \) is the total density of states at the Fermi level per one spin; the Fermi velocity \( \mathbf{v} \) relates to a certain position on the Fermi surface, \( \Delta \) is the gap function, \( f(\mathbf{r}, \mathbf{v}, \omega) \) is Eilenberger Green’s function which describes the condensate, and \( \hbar \omega = \pi T(2n + 1) \) with an integer \( n \). In the uniform zero-field situation \( f = \Delta/\sqrt{\Delta^2 + \hbar^2 \omega^2} \). Substituting this in Eq. (3) one can evaluate how the gap depends on temperature and on position at the Fermi surface provided the pair-pair interaction \( V(\mathbf{v}, \mathbf{v}') \) is known.

The averages over the Fermi surface weighted with the local density of states \( \propto 1/\mathbf{v} \) are defined as

\[ \langle X \rangle = \int \frac{d^2 \mathbf{k}_F}{(2\pi)^3 \hbar N(0) \mathbf{v}} X(\mathbf{v}). \tag{4} \]

Commonly, the interaction \( V \) is assumed factorizable \([40], V(\mathbf{v}, \mathbf{v}') = V_0 \Omega(\mathbf{v}) \Omega(\mathbf{v}') \) (the assumption with far reaching consequences for the two-gap model, see below). Then, one looks for \( \Delta(\mathbf{r}, T; \mathbf{v}) = \Psi(\mathbf{r}, T) \Omega(\mathbf{v}) \). The self-consistency Eq. (3) for the uniform condensate takes the form:

\[ 1 = 2\pi T N(0) V_0 \sum_{\omega > 0} \langle \frac{\Omega^2(\mathbf{v})}{\sqrt{\Psi^2 \Omega^2(\mathbf{v}) + \hbar^2 \omega^2}} \rangle. \tag{5} \]

Consider now a model material with the gap anisotropy given by

\[ \Omega(\mathbf{v}) = \Omega_{1,2}, \quad \mathbf{v} \in F_{1,2}, \tag{6} \]

where \( F_1, F_2 \) are two sheets of the Fermi surface. Denoting the densities of states on the two parts as \( N_{1,2} \), and assuming the quantity \( X \) being constant
at each sheet, we obtain for the general averaging:

\[
\langle X \rangle = \frac{\langle X \rangle_1 N_1 + \langle X \rangle_2 N_2}{N(0)} = \nu_1 \langle X \rangle_1 + \nu_2 \langle X \rangle_2 ,
\]

where we use normalized densities of state \( \nu_{1,2} = N_{1,2}/N(0) \) for brevity. The Fermi relief of the gap, \( \Omega \), can be normalized so that \( \langle \Omega^2 \rangle = 1 \) which gives for the two-gap model:

\[
\Omega_1^2 \nu_1 + \Omega_2^2 \nu_2 = 1 , \quad \nu_1 + \nu_2 = 1 .
\]

Within this model, the interaction \( V \) now takes the form of a \( 2 \times 2 \) symmetric matrix \( V_{ij}/V_0 \) with diagonal components \( \Omega_1^2 \) and \( \Omega_2^2 \), and the two equal off-diagonal elements \( \Omega_1 \Omega_2 \). It is worth noting that if \( V_{12} = 0 \), i.e., there is no interband interaction at all, the general gap equation (3) splits in two independent equations for the independent order parameters, \( \Delta_1 \) on \( F_1 \) and \( \Delta_2 \) on \( F_2 \). Such a model would imply different, in general, critical temperatures for \( \Delta \)'s, different phases with many macroscopic consequences [41,42]. The factorizable interaction \( V_{ij} = V_0 \Omega_i \Omega_j \) excludes such possibilities and automatically implies the single \( T_c \) for both gaps, the feature in fact seen in many tunneling experiments on MgB\(_2\) [43,44,45].

### 3.2 T dependence of the two gaps

The self consistency equation (5) for the order parameter \( \Psi(T) \) can be solved for known \( \Omega_{1,2} \) and the densities of states \( \nu_{1,2} \). Based on the band structure calculations, the relative densities of states \( \nu_1 \) and \( \nu_2 \) of our model are \( \approx 0.56 \) and \( 0.44 \) [46,36]. The ratio \( \Delta_2/\Delta_1 = \Omega_2/\Omega_1 \approx 4 \), if one takes the averages of 6.8 and 1.7 meV for the two groups of distributed gaps as calculated in Ref. [36]. Then, the normalization (8) yields \( \Omega_1 = 0.36 \) and \( \Omega_2 = 1.45 \). It should be noted that the tunneling data provide somewhat lower ratio \( \Delta_2/\Delta_1 \) [43,44,45].

We have now all parameters needed to solve the self-consistency equation (5) for \( \Psi(T) \) (the clean case). This is done numerically and the result is shown in Fig. 6 along with two gaps \( \Delta_{1,2}(T) \).

The parameter \( \Delta/T_c \) commonly used to distinguish strong and weak coupling materials, has a "strong coupling" value of \( \approx 4 \) for \( \Delta_2/T_c \), whereas \( \Delta_1/T_c \approx 1 \), which is less than the BCS weak coupling value of 3.5. Thus, this parameter cannot be used to characterize coupling for materials like MgB\(_2\). The \( T \) dependence of the two gaps similar to shown in Fig. 8 has been reported by a number of groups [43,44,45].
3.3 Anisotropy of $\lambda$

Having obtained the temperature dependence of both gaps, one can turn to calculation of the weak-field penetration depth $\lambda(T)$. To this end, one first solves equations of superconductivity for the zero-field case and then employs the perturbation theory to evaluate the small corrections due to small currents. In this manner one obtains the London relation between the current and the vector potential,

$$\frac{4\pi}{c} j_i = -(\lambda^2)^{-1}_{ik} \left( \frac{2\pi}{\phi_0} \frac{\partial \theta}{\partial x_k} + A_k \right)$$  \hspace{1cm} (9)

where $\theta$ is the phase, $\phi_0$ is the flux quantum, $\mathbf{A}$ is the vector potential, and

$$\lambda^2_{ik} = \frac{16\pi^2 c^2 T}{c^2} N(0) \sum_\omega \left\{ \frac{\Delta_i^2 v_i v_k}{\beta^3} \right\}$$  \hspace{1cm} (10)

is the tensor of the inverse squared penetration depth. Here, $i, k = x, y, z$ and

$$\beta^2 = \Delta^2 + \hbar^2 \omega^2$$

(the reader may find details of this calculation in Ref. [3]). This general expression for the tensor of squared penetration depth is valid for clean superconductors with an arbitrary Fermi surface and gap anisotropies.

The anisotropy parameter now reads:

$$\gamma^2_{\lambda} = \frac{\lambda^2_{cc}}{\lambda^2_{aa}} = \frac{\langle v^2_a \Delta_a^2 \sum_\omega \beta^{-3} \rangle}{\langle v^2_c \Delta_c^2 \sum_\omega \beta^{-3} \rangle}.$$  \hspace{1cm} (11)

As $T \to 0$, we have $2\pi T \Delta^2_0 \sum_\omega \beta^{-3} \to 1$, and

$$\gamma^2_{\lambda}(0) = \frac{\langle v^2_a \rangle}{\langle v^2_c \rangle}.$$  \hspace{1cm} (12)

Note that the gap and its anisotropy do not enter this result. The physical reason for this is in the Galilean invariance of the superfluid flow in the absence of scattering: all charged particles take part in the supercurrent.

Near $T_c$, the sum over $\omega$ in Eq. (11) is is a $\mathbf{k}_F$ independent constant because $\beta \approx \hbar \omega$, and we obtain the GL result of Ref. [2]:

$$\gamma^2_{\lambda}(T_c) = \frac{\lambda^2_{cc}}{\lambda^2_{aa}} = \frac{\langle \Omega^2 v^2_a \rangle}{\langle \Omega^2 v^2_c \rangle}.$$  \hspace{1cm} (13)

We observe that near $T_c$, the gap anisotropy amplifies contribution of the large gap Fermi surface pieces to the anisotropy parameter $\gamma_{\lambda}$. We also see that for
isotropic gaps, \( \gamma_{\lambda}(T_c) = \gamma_{\lambda}(0) \) (which is not true for the general case). Thus, the anisotropy parameter depends on \( T \), the feature absent in superconductors with isotropic gaps.

To apply these results to MgB\textsubscript{2}, one has to know averages of squared Fermi velocities not only over the whole Fermi surface (as for \( \gamma_{\lambda}(0) \) of Eq. (12)), but also the averages over the separate Fermi sheets. These can be taken from the band structure calculations of Ref. [46]:

\[
\begin{align*}
\langle v^2_a \rangle_1 &= 33.2, & \langle v^2_c \rangle_1 &= 42.2, \\
\langle v^2_a \rangle_2 &= 23, & \langle v^2_c \rangle_2 &= 0.5 \times 10^{14} \text{ cm}^2/\text{s}^2.
\end{align*}
\]

The numerical results for \( \gamma_{\lambda}(T) \) are shown in Fig. 7.

Thus, we expect the London penetration depth of clean MgB\textsubscript{2} to be nearly isotropic at low temperatures; \( \gamma_{\lambda}(T) \) increases on heating and reaches \( \approx 2.6 \) at \( T_c \). Qualitatively similar behavior of \( \gamma_{\lambda}(T) \) is predicted within a more general Eliashberg scheme [47]. As up to date, there is no published data on direct measurements of the \( \lambda \) anisotropy and its \( T \) dependence. It is pointed out below that the data on the angular dependence of the torque acting on the anisotropic superconducting crystal in tilted fields cannot provide information about \( \gamma_{\lambda}(T) \) without taking into account the \( H_{c2} \) anisotropy which for MgB\textsubscript{2} might be quite different from \( \gamma_{\lambda}(T) \). In principle, one can extract \( \gamma_{\lambda} \) from the data on the vortex lattice structure in fields tilted relative to the \( c \) axis of MgB\textsubscript{2}. These, however, are difficult to acquire and to our knowledge are not yet available.

### 3.4 Anisotropy of \( H_{c2} \)

Unlike the case of London \( \lambda \), the evaluation of \( H_{c2} \) is more complicated a problem because one has to deal with the high-field phase transition from the normal to the superconducting mixed state. Still, major behavior of \( H_{c2}(T) \) can be obtained within a simplified scheme: Since the actual band structure enters equations for \( H_{c2} \) via Fermi-surface averages, one can further model the sheets \( F_{1,2} \) by two spheroids with average Fermi velocities close to the band-structure generated values. As a result one obtains qualitatively (and - given the spread of existing data - quantitatively) correct behaviors of \( H_{c2}(T) \) for both principal directions. Details of this evaluation can be found in Ref. [4].

The result for the anisotropy parameter \( \gamma_{H}(T) = \frac{H_{c2,ab}}{H_{c2,c}} \) obtained within the scenario of two constant gaps on two Fermi surface sheets, the same used for \( \gamma_{\lambda}(T) \) and with the same input parameters, is shown in Fig. 7.
The drop of the $H_{c2}$ anisotropy with increasing $T$ has been recorded in measurements on single crystals of MgB$_2$ [26]. Nearly the same behavior has been extracted from the data on random polycrystals in the whole temperature range using the $T$ dependence of the magnetization of random powders [20]. Recent specific heat measurements [31] and magnetization data [30] on single crystals produced similar results. All these data show qualitatively similar behavior to that of the upper curve of Fig. 7.

Physically, the large anisotropy of $H_{c2}$ at low temperatures ($\approx 6$ in our calculation) is related to the large gap value at the Fermi sheet which is nearly two-dimensional. With increasing $T$, the thermal mixing with the small-gap states on the three-dimensional Fermi sheet suppresses the anisotropy down to 2.6 at $T_c$.

3.5 Free energy and torque in materials with different anisotropies of $\lambda$ and $H_{c2}$

One of the most sensitive methods used to extract the anisotropy parameter $\gamma$ 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: [28,48]

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

(15)

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

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

(16)

$\lambda^3 = \lambda_0^3 \lambda_c$, and $\eta \sim 1$. This formula can be written as $\tau = \mathbf{M} \times \mathbf{H}$; since in this field domain the magnetization $M \ll H$, one can disregard the distinction between $\mathbf{B}$ and $\mathbf{H}$. It has been assumed in the derivation of Eq. (15) that the anisotropies of $H_{c2}$ and of the London penetration depth are the same: $\gamma_H = \gamma_\lambda = \gamma$. It is worth noting that Eq. (15) 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 $\gamma > 1$).

Expression (15) for the torque has been derived within the London approach by employing the cutoff at distances on the order of the coherence length $\xi$ where this approach fails. The formula, however, has been confirmed experimentally (for a few high-$T_c$ materials close to their $T_c$) with a good accuracy as far as the
angular dependencies of quantities involved are concerned \[49\]. Uncertainties of the London approach are incorporated in the parameter \(\eta \sim 1\); discussion of those can be found, e.g., in Ref. \[50\].

We now outline possible effects of different anisotropies of \(\lambda\) and \(H_{c2}\) on the torque angular dependence. To this end, we first recall 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 \(\theta\) toward the crystal direction \(a\) \[51\]:

\[
F = \frac{B^2}{8\pi} + \frac{B^2 m_{zz}}{8\pi\lambda^2 m_a} \sum_{\mathbf{G}} \frac{1}{m_{zz} G_x^2 + m_c G_y^2}; \tag{17}
\]

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 \(\mathbf{G}\) form the reciprocal vortex lattice. The summation is extended over all nonzero \(\mathbf{G}\).

For isotropic case, all reduced masses in Eq.\( (17)\) are unity. The sum \(\sum G^{-2}\) can be approximated by an integral \((\phi_0/4\pi^2 B) \int dG_x dG_y / G^2\) which diverges logarithmically and should be cut off at a circle in the reciprocal space of a radius \(\sim 1/\xi\) where \(\xi\) is the radius of the circular vortex core.

In anisotropic material with \(\gamma_\lambda = \gamma_H\), calculation of this sum is reduced to the isotropic case by rescaling

\[
g_x = \sqrt{m_{zz}} G_x, \quad g_y = \sqrt{m_c} G_y. \tag{18}\]

In this manner one can derive the free energy of a superconductor in an applied field of a certain direction; the torque formula \((15)\) is obtain differentiating the energy with respect to the angle \(\theta\).

However, for \(\gamma_\lambda \neq \gamma_H\), the masses in the sum \((17)\) correspond to the anisotropy \(\gamma_\lambda\) (in other words, the vortex-vortex interaction is determined by the \(\lambda\) anisotropy) whereas the cut-off reflects the shape of the core (it is determined by the anisotropy of the coherence length \(\xi\), i.e., by the parameter \(\gamma_H\)). In this situation, the scaling \((18)\) which transforms the summand of Eq. \((17)\) to the isotropic-like form, leaves the shape of the cut-off contour elliptical. Therefore, the energy \(F\) and its angular dependence acquire extra terms and so does the torque which can be measured.

We refer the reader to the original work \[52\] for the details of this calculation and give here only the result. To write explicitly the angular dependence of \(F\), it is convenient to use the angular functions

\[
\Theta_{\lambda,H}(\theta) = \varepsilon_{\lambda,H}(\theta)/\gamma_{\lambda,H}\tag{19}
\]
where $\varepsilon_{\lambda,H}(\theta)$ are defined in Eq. (16) with corresponding $\gamma$'s. In terms of these functions,

$$
F = \frac{B^2}{8\pi} + \frac{\phi_0 B_{\lambda}}{32\pi^2 \lambda^2_{ab}} \ln \frac{2\sqrt{3} \mu_a \phi_0 \Theta_{\lambda}}{\xi^2 B (\Theta_{\lambda} + \Theta_H)^2},
$$

where $\mu_a = \gamma_{H}^{-2/3}$. The torque density $\tau = -\partial F/\partial \theta$ follows:

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

(21)

where $e = 2.718...$. In the standard case of $\gamma_H = \gamma_{\lambda} = \gamma$, Eq. (21) reduces to the result (15).

Since both $\Theta'_{\lambda,H} < 0$, the second contribution to the torque (21) is negative whereas the first one is positive. The positive torque implies that the system energy decreases with increasing $\theta$, as in the standard case of $\gamma_H = \gamma_{\lambda}$ for which $\theta = \pi/2$ is the stable equilibrium.

On the other hand, it is straightforward to see that for large enough $\gamma_H$ and fixed $\gamma_{\lambda}$ (e.g., set $\gamma_{\lambda} = 1$ and leave $\gamma_H > 1$) Eq. (21) yields a negative torque, which means that in the equilibrium the crystal c axis is parallel to the applied field. This strange behavior can be tracked down to the angular dependence of the line energy of a single vortex: the energy cost of having an elliptical core for vortices along $ab$ for which the current distribution far from the core is near isotropic (as for the example with $\gamma_{\lambda} = 1$) is too high.

To illustrate how the angular dependence of the torque varies with anisotropies of $H_{c2}$ and $\lambda$, we evaluate numerically the torque density (21) for parameters in the range of those for clean MgB$_2$. Fig. 8 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 $T$, $\gamma_H$ of MgB$_2$ increases whereas $\gamma_{\lambda}$ decreases. In Fig. 9 the torque (21) 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 0.7 and 0.6 $T_c$ according to Ref. [4]. Clearly, $\theta = \pi/2$ as well as $\theta = 0$ are unstable; the stable equilibrium is shifted to $0 < \theta < \pi/2$.

Finally, we plot in Fig. 10 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 $\theta = 0$.

4 Conclusions

Hence, 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. Moreover, since $\gamma_H$ determines the anisotropy of the coherence length and, therefore, of the vortex core, whereas $\gamma_\lambda$ 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 clean 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 $T_c$ where $\gamma_\lambda \to \gamma_H$. In intermediate temperature range where the equilibrium vortex lattice orientation shifts from $\theta = \pi/2$ to lower angles, one may expect peculiar vortex dynamics (as for fields near parallel to the layers of high-$T_c$ materials). This possibility calls for further study.

Thus, the question “what is the anisotropy parameter of MgB$_2$?” does not have a unique answer. To pose the question properly one should specify the quantity of interest. If this is $H_{c2}$, the answer is given by the upper curve of Fig. 7 for a clean material; if this is $\lambda$, see the dashed line. If this is the magnetization in intermediate fields, $M \propto (\phi_0/\lambda^2) \ln(H_{c2}/H)$, the main contribution to anisotropy comes from $\lambda$; however, the $H_{c2}$ anisotropy contributes as well (being smoothed by the logarithm). The last situation should be taken into account while extracting anisotropy from the torque data in tilted fields [26,29]. It should be noted in closing, that all anisotropies discussed here might be suppressed by impurities.

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Fig. 1. Sketch of the maximum $H_{c2,\text{max}}(T) \equiv H_{c2,a}$ and the minimum $H_{c2,\text{min}}(T) \equiv H_{c2,c}$ upper critical fields. For a given applied field $H$, the relation $H = H_{c2,\text{min}}(T_{c}^{\text{min}}) = H_{c2,\text{max}}(T_{c}^{\text{max}})$ defines temperatures $T_{c}^{\text{min}}, T_{c}^{\text{max}}$. The open (shaded) rectangles represent superconducting (normal) grains.
Fig. 2. The $H - T$ phase diagram for anisotropic MgB$_2$. Symbols: circles (open and filled) are extracted from $M(T)|_H$, triangles - from $M(H)|_T$, asterisks - from resistivity data on polycrystalline MgB$_2$. 
Fig. 3. Temperature-dependent anisotropy of the upper critical field. The range of data from Ref. [26] is shown for comparison as a hatched area between dashed lines.
Fig. 4. Fermi surface of MgB$_2$ calculated in Ref. [36].
Fig. 5. The energy distribution of the gap values calculated in Ref. [36].
Fig. 6. The gaps $\Delta_{1,2} = \Psi(T) \Omega_{1,2}$ versus $T/T_c$. The upper curve is $\Delta_2/T_c$, the lower one is $\Delta_1/T_c$, and the middle curve is $\Psi(T)/T_c$ evaluated as described in the text.
Fig. 7. Anisotropy ratio $\gamma_H = H_{c2,ab}/H_{c2,c}$ versus $T/T_c$ calculated with parameters for MgB$_2$ given in the text. Dashed line is $\gamma_\lambda(T) = \lambda_c/\lambda_{ab}$. 
Fig. 8. The torque $\tau$ in units of $\phi_0 B / 32\pi^2 \lambda_0^2$ versus angle $0 < \theta < \pi/2$ for $\gamma_\lambda = 2.2$, $\gamma_H = 3$, and $4e^2 \eta H_{c2,c}/B = 100.$
Fig. 9. The same as in Fig. 8. The solid curve is calculated with Eq. (21) for $\gamma_\lambda = 2$ and $\gamma_H = 5$; the dashed curve corresponds to $\gamma_\lambda = 1.7$ and $\gamma_H = 5.3$. 
Fig. 10. The same as in Fig. 8, but $\gamma_\lambda = 1.1$ and $\gamma_H = 6$. 