Macroscopic anisotropy in superconductors with anisotropic gaps

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It is shown within the weak-coupling model that the macroscopic superconducting anisotropy for materials with the gap varying on the Fermi surface cannot be characterized by a single number, unlike the case of clean materials with isotropic gaps. For clean uniaxial materials, the anisotropy parameter $\gamma(T)$ defined as the ratio of London penetration depths, $\lambda_\parallel/\lambda_\perp$, is evaluated for all $T$’s. Within the two-gap model of MgB$_2$, $\gamma(T)$ is an increasing function of $T$.

A remarkable confirmation for the observed two-gap structure of superconducting MgB$_2$ came from solving the Eliashberg equations for the gap distribution on the Fermi surface. According to this, the gap on the four Fermi sheet surfaces 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. 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 $1.7/7$, with two gaps on two parts of the Fermi surface may prove useful in relating various macroscopic properties of MgB$_2$. Starting with Ref. 8, the two-band models were studied by many, see, e.g., Ref. 9 and references therein. The focus of this work is on the macroscopic superconducting anisotropy $\gamma$. To a large extent, motivation for this work was to understand why experiments on different samples of MgB$_2$ done with different techniques yield widely varying values for $\gamma$.

The anisotropic Ginzburg-Landau (GL) equations, derived for clean superconductors with an arbitrary gap anisotropy in the seminal work by L.Gor’kov and T.Melik-Barkhudarov, led to the commonly used concept of a single parameter $\gamma$ defined as $\xi_\parallel/\xi_\perp \equiv \lambda_\parallel/\lambda_\perp$ ($\xi$ is the coherence length, $\lambda$ is the penetration depth, and $a, c$ are principal crystal directions). Formally, this came out because the same mass tensor enters both the first GL equation which determines the anisotropy of $\xi$ (and of the upper critical fields $H_{c2}$) and the equation for the current which defines the anisotropy of $\lambda$. However, it has been later shown by S.Pokrovsky and V.Pokrovsky in the work on the GL equations for anisotropic gaps in the presence of impurities, that $\gamma$ in fact depends on the impurity scattering, i.e., it might be sample dependent.

In the following the near-$T_c$ result of Ref. 13 is reproduced using the Eilenberger formalism. Moreover, the ratio $\lambda_\parallel/\lambda_\perp$ for arbitrary temperatures $T$ is derived for the clean case. It is shown that for MgB$_2$, $\lambda_\parallel/\lambda_\perp$ should increase with increasing $T$, the result which calls for experimental verification.

We begin with the quasiclassical version of the BCS theory for a general anisotropic Fermi surface:

\begin{align}
\mathbf{v} \Pi f &= 2\Delta g/h - 2\omega f + (g(f) - f(g))/\tau , \\
-\mathbf{v} \Pi^* f^+ &= 2\Delta^* g/h - 2\omega f^+ + (g(f^+) - f^+(g))/\tau ,
\end{align}

where $\Delta(T) = 2\pi T N(0) \sum_{\omega>0} \langle \Omega(\omega) f(\mathbf{v}, \mathbf{r}, \omega) \rangle$. Then, the self-consistency Eq. (4) takes the form:

\begin{equation}
\bar{\Psi}(\mathbf{r}, T) = 2\pi T N(0) V_0 \sum_{\omega>0} \langle \Omega(\omega) f(\mathbf{v}, \mathbf{r}, \omega) \rangle.
\end{equation}

The function $\Omega(\omega)$ can be normalized by requiring that the critical temperature $T_{c0}$ for the clean material ($\tau \to \infty$) is given by the standard isotropic weak-coupling model with the effective interaction $V_0$: $T_{c0} = 1/k_f^2$. As usual, we incorporate $T_{c0}$ in the Eilenberger system using the identity

\begin{equation}
\frac{1}{N(0)V_0} = \ln \frac{T}{T_{c0}} + 2\pi T \sum_{\omega>0} \frac{1}{h\omega}.
\end{equation}

Substitute this in Eq. (5) and replace $\omega_D$ with infinity due to the fast convergence:

\begin{equation}
\frac{\Psi}{2\pi T} \ln \frac{T_{c0}}{T} = \sum_{\omega>0} \left( \frac{\Psi}{\omega} - \langle \Omega f \rangle \right).
\end{equation}

Here $\mathbf{v}$ is the Fermi velocity, $\Pi = \nabla + 2\pi i A/\phi_0$; $\Delta$ is the gap function, $f(\mathbf{v}, \mathbf{r}, \omega)$, $f^+$, and $g$ are Eilenberger Green’s functions, $N(0)$ is the total density of states at the Fermi level per one spin; $h\omega = \pi T(2n + 1)$ with an integer $n$. Further, $\tau$ is the scattering time on non-magnetic impurities and $\omega_D$ is the Debye frequency. The averages over the Fermi surface weighted with the local density of states $\propto 1/|\mathbf{v}|$ are defined as

\begin{equation}
\langle X \rangle = \int \frac{d^2 k_F}{(2\pi)^3 h N(0)} |\mathbf{v}| X.
\end{equation}
Effect of nonmagnetic impurities on $T_c$. It is long known that scattering by nonmagnetic impurities suppresses $T_c$, and this is done in the clean case by expanding for the d-wave symmetry $\langle \Delta \rangle = 0$ and $\Omega' = \Omega$ unless $\Omega = 0$ as, e.g., for the d-wave on the order parameter symmetry. For large $\mu$'s, unlike the case of the magnetic pair-breaking, we obtain

$$T_c = T_{c,0} \left[ \Delta_0(0) \tau / h \right]^{(\Omega)^{-2} - 1},$$

where $\Delta_0(0) = 1.76 T_{c,0}$. Therefore, $T_c$ does not turn zero at a finite $\tau$, unless $\Omega = 0$ as, e.g., for the d-wave superconductors. 

Anisotropy near $T_c$. As is seen from Eq. (11), impurities cause isotropization of amplitudes $f$, and one expects the macroscopic anisotropy to be suppressed by scattering. To address this question, one has to derive the GL equations in the presence of impurities following basically the work for clean superconductors. As mentioned above, the same mass tensor enters both the first and the second GL equations. We focus on the current equation because this is an easier task. Within Eilenberger formalism this is done in the clean case by expanding for the d-wave symmetry $\langle \Delta \rangle = 0$ and $\Omega' = \Omega$ unless $\Omega = 0$ as, e.g., for the d-wave superconductors. 

Substituting this in Eq. (1) one obtains $a = -1/2$. The second GL equation follows by using Eq. (11) in which we substitute $g \approx 1 - f^2/2$ with $f$'s of Eq. (16):

$$j_i = -\frac{7 \zeta(3) e^2}{4 \pi^2 T_{c,0}^2} \langle \Omega^2 v_i v_k \rangle \Im \Psi^* \Pi_k \Psi.$$

In the London limit $\Psi = \Psi_0 e^{i \theta}$ with a constant $\Psi_0$, and

$$j_i = -\frac{c_0}{4 \pi^2} \left( \lambda^2 \right)_{ik}^{-1} \left( \nabla \theta + \frac{2 \pi}{\phi_0} A \right)_k,$$

with

$$\left( \lambda^2 \right)_{ik}^{-1} = \frac{14 \zeta(3) e^2 N(0)}{\pi c^2 T_{c,0}} \Psi_0^2 \langle \Omega^2 v_i v_k \rangle .$$

The anisotropy parameter follows:

$$\gamma^2(T_c) = \frac{\lambda_{cc}}{\lambda_{aa}} = \frac{\langle \Omega^2 v_a v_a \rangle}{\langle \Omega^2 v^2 \rangle}.$$
Hence, in the dirty limit, all parts of the Fermi surface contribute evenly to the anisotropy parameter as is the case for isotropic gaps.

$T$ dependence of $\gamma = \lambda_c / \lambda_a$. To address this question in the full temperature range one has to study weak supercurrents, i.e., turn to Eq. (2). We consider only the clean case for which $f_0, g_0$ in the absence of currents are:

$$f_0 = f_0^* = \frac{\Delta_0}{\beta}, \quad g_0 = \frac{h\omega}{\beta}, \quad \beta^2 = \Delta_0^2 + h^2 \omega^2; \quad (27)$$

in general, both $\Delta_0$ and $\beta$ depend on $k_F$. A weak supercurrent causes the order parameter $\Delta$ and the amplitudes $f$ to acquire an overall phase $\theta$ on the surface pieces with large gap to the parameter $\lambda$. The GL result (20) which amplifies contribution of the Fermi surface pieces with large gap to the parameter $\gamma$. Thus, the anisotropy parameter depends on $T$, the feature absent in superconductors with isotropic gaps.

It is worth noting that in literature the superconducting anisotropy is commonly referred to as the ratio $H_{c2,a}/H_{c2,c}$, an important figure for applications, but a difficult quantity to evaluate for anisotropic Fermi surfaces, not to speak about anisotropic gaps. On the other hand, measurements of the $\lambda$-anisotropy such as, e.g., the high-field torque technique is more demanding than the resistive determination of $H_{c2}$ since one has to work in the reversible domain. One should also note that, theoretically, the ratios of $H_{c2}$’s and of $\lambda$’s are not necessarily the same, except near $T_c$ where their equality is provided by the GL theory.

It is of interest to examine the consequences of our results for $MgB_2$. The reported $\gamma$’s vary from 1.7 to 8 [13] or even higher as in Ref. [14]. In all these reports, different techniques for extracting the anisotropy and samples with different resistivity ratios were used.

Consider a model material with the gap anisotropy given by

$$\Omega = \Omega_{1,2}, \quad v \in F_{1,2}, \quad (34)$$

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 [36]:

$$\langle X \rangle = \langle X_1 N_1 + X_2 N_2 \rangle / N(0) = \nu_1 X_1 + \nu_2 X_2, \quad (35)$$

where we introduce normalized densities of state $\nu_{1,2} = N_{1,2}/N(0)$ for brevity. We have then instead of Eq. (36):

$$\Omega_1^2 \nu_1 + \Omega_2^2 \nu_2 = 1, \quad \nu_1 + \nu_2 = 1. \quad (36)$$

We also assume that the two parts of the Fermi surface have the symmetries of the total, e.g., $\langle v \rangle_1 = 0$ where the average is performed only over the first Fermi sheet. Within this model, Eq. (37) reads:

$$\gamma^2 = \sum_i \nu_i \Omega_i^2 (\nu_i^2) \bar{\nu_i} \beta_i^{-3}, \quad i = 1, 2, \quad (37)$$

where $\beta_i = \sqrt{\hbar^2 \omega_i^2 + \psi^2(T) \Omega_i^2}$. Based on the band structure calculations, the relative densities of states $\nu_1$ and $\nu_2$ of our model are $\approx 0.56$ and $0.44$ [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 [36] yields $\Omega_1 = 0.36$ and $\Omega_2 = 1.45$.

Now, we have all parameters needed to solve the self-consistency equation (10) for $\psi(T)$ with $f = \Delta/\beta$ (the clean case). This is done numerically and the result is shown in Fig. 1 along with $\Delta_i(T)$. 

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FIG. 1. Temperature dependence of the two gaps calculated as $\Delta_i = \psi(T)\Omega_i$ 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.

To evaluate $\gamma(T)$ of Eq. \((37)\) we use the averages over separate Fermi sheets calculated in Ref. 26: $\langle v_1^2 \rangle_1 = 33.2$, $\langle v_1^2 \rangle_1 = 42.2$, $\langle v_2^2 \rangle_2 = 23$, and $\langle v_2^2 \rangle_2 = 0.5 \times 10^{14}$ cm$^2$/s$^2$. The result of numerical evaluation of $\gamma(T)$ is shown in Fig. 2.

The ratio of $\lambda$'s can be obtained, e.g., from the angular dependence of the reversible torque on single crystals in intermediate magnetic fields tilted relative to the principal crystal directions. Some torque data for MgB$_2$ were reported by M. Andst et al.\(^5\) but the $T$ dependence was not examined in detail. The ratio $H_{c2,ab}/H_{c2,c}$ was shown to drop with increasing $T$ from about 6 at 15 K to 2.8 at 35 K (see also Refs. 27,28). The authors estimate this ratio as $\approx 2.3 - 2.7$ at $T_c$. Near $T_c$, the ratios of $H_{c2}$'s should coincide with the ratio of $\lambda$'s. In this work we estimate the latter as $\approx 2.4$, see Fig. 3. Given this agreement and the prediction made here that the $T$ dependence of $\gamma = \lambda_c/\lambda_{ab}$ should be opposite to that of the observed behavior of $H_{c2,ab}/H_{c2,c}$, the detailed studies of $\gamma$ by torque or other methods are desirable.

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