

## 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 a 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,  $\lambda_c/\lambda_{ab}$ , is evaluated for all  $T$ 's. Within the two-gap model of  $\text{MgB}_2$ ,  $\gamma(T)$  is an increasing function of  $T$ .

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### INTRODUCTION

A remarkable confirmation for the observed two-gap structure<sup>1-5</sup> of superconducting  $\text{MgB}_2$  came from solving the Eliashberg equations for the gap distribution on the Fermi surface.<sup>6,7</sup> According to this, the gap on the four Fermi-surface sheets of this material has two sharp maxima:  $\Delta_1 \approx 1.7$  meV at the two  $\pi$  bands and  $\Delta_2 \approx 7$  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  $T$  independent. In this situation, a weak-coupling model with two gaps on two parts of the Fermi surface may prove useful in relating various macroscopic properties of  $\text{MgB}_2$ . 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  $\text{MgB}_2$  done with different techniques yield widely varying values for  $\gamma$ .<sup>10-16</sup>

The anisotropic Ginzburg-Landau (GL) equations, derived for clean superconductors with an arbitrary gap anisotropy in the seminal work by Gor'kov and Melik-Barkhudarov,<sup>17</sup> led to the commonly used concept of a single parameter  $\gamma$  defined as  $\xi_a/\xi_c \equiv \lambda_c/\lambda_a$  ( $\xi$  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 that 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 shown by Choi and Muzikar<sup>18</sup> and later by Pokrovsky and Pokrovsky<sup>19</sup> 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 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. 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.

In the following the near- $T_c$  result of Ref. 19 is reproduced using the Eilenberger formalism. Moreover, the ratio  $\lambda_c/\lambda_a$  for arbitrary temperatures  $T$  is derived for the clean

case. It is shown that for  $\text{MgB}_2$ ,  $\lambda_c/\lambda_a$  should increase with increasing  $T$ , the result that calls for experimental verification.

We begin with the quasiclassical version of the BCS theory for a general anisotropic Fermi surface,<sup>20</sup>

$$\mathbf{v}\mathbf{\Pi}f = 2\Delta g/\hbar - 2\omega f + (g\langle f \rangle - f\langle g \rangle)/\tau, \quad (1)$$

$$-\mathbf{v}\mathbf{\Pi}^*f^+ = 2\Delta^*g/\hbar - 2\omega f^+ + (g\langle f^+ \rangle - f^+\langle g \rangle)/\tau, \quad (2)$$

$$g^2 = 1 - ff^+, \quad (3)$$

$$\Delta(\mathbf{r}, \mathbf{v}) = 2\pi TN(0) \sum_{\omega>0}^{\omega_D} \langle V(\mathbf{v}, \mathbf{v}') f(\mathbf{v}', \mathbf{r}, \omega) \rangle_{\mathbf{v}'}. \quad (4)$$

$$\mathbf{j} = -4\pi|e|N(0)T \text{Im} \sum_{\omega>0} \langle \mathbf{v}g \rangle. \quad (5)$$

Here  $\mathbf{v}$  is the Fermi velocity,  $\mathbf{\Pi} = \nabla + 2\pi i\mathbf{A}/\phi_0$ ;  $\Delta$  is the gap function,  $f(\mathbf{r}, \mathbf{v}, \omega)$ ,  $f^+$ , and  $g$  are Eilenberger Green's functions,  $N(0)$  is the total density of states at the Fermi level per one spin;  $\hbar\omega = \pi T(2n+1)$  with an integer  $n$ . Further,  $\tau$  is the scattering time on nonmagnetic 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

$$\langle X \rangle = \int \frac{d^2\mathbf{k}_F}{(2\pi)^3 \hbar N(0) |\mathbf{v}|} X. \quad (6)$$

Commonly, the interaction  $V$  is assumed factorizable,<sup>21</sup>  $V(\mathbf{v}, \mathbf{v}') = V_0 \Omega(\mathbf{v}) \Omega(\mathbf{v}')$ , and one looks for  $\Delta(\mathbf{r}, T; \mathbf{v}) = \Psi(\mathbf{r}, T) \Omega(\mathbf{v})$ . Then, the self-consistency Eq. (4) takes the form

$$\Psi(\mathbf{r}, T) = 2\pi TN(0) V_0 \sum_{\omega>0}^{\omega_D} \langle \Omega(\mathbf{v}) f(\mathbf{v}, \mathbf{r}, \omega) \rangle. \quad (7)$$

The function  $\Omega(\mathbf{v})$  can be normalized by requiring that the critical temperature  $T_{c0}$  for the *clean* material ( $\tau \rightarrow \infty$ ) is given by the standard isotropic weak-coupling model with the effective interaction  $V_0$ ,<sup>22</sup>

$$\langle \Omega^2 \rangle = 1. \quad (8)$$

As usual, we incorporate  $T_{c0}$  in the Eilenberger system using the identity

$$\frac{1}{N(0)V_0} = \ln \frac{T}{T_{c0}} + 2\pi T \sum_{\omega>0}^{\omega_D} \frac{1}{\hbar\omega}. \quad (9)$$

We substitute this in Eq. (7) and replace  $\omega_D$  with infinity due to the fast convergence,

$$\frac{\Psi}{2\pi T} \ln \frac{T_{c0}}{T} = \sum_{\omega>0}^{\infty} \left( \frac{\Psi}{\hbar\omega} - \langle \Omega f \rangle \right). \quad (10)$$

### EFFECT OF NONMAGNETIC IMPURITIES ON $T_c$

It is long known that scattering by nonmagnetic impurities suppress  $T_c$  provided the gap is weakly anisotropic.<sup>21,23</sup> The suppression is readily obtained from Eilenberger equations without assuming that the anisotropy is weak. In zero field, all quantities are coordinate independent; besides, as  $T \rightarrow T_c$ ,  $g \rightarrow 1$ . Then, Eq. (1) gives

$$f = \frac{1}{\hbar\omega'} \left( \Delta + \frac{\langle \Delta \rangle}{2\omega\tau} \right) \equiv \frac{D}{\hbar\omega'}, \quad (11)$$

where  $\omega' = \omega + 1/2\tau$ . Substitute this in Eq. (10) to obtain

$$\ln \frac{T_{c0}}{T_c} = \frac{\pi T_c}{\hbar\tau} (1 - \langle \Omega \rangle^2) \sum_{\omega>0} \frac{1}{\omega\omega'}. \quad (12)$$

Hence  $T_c = T_{c0}$  for  $\tau \rightarrow \infty$  and any gap anisotropy; the same is true for the isotropic gap ( $\Omega = 1$ ) and any  $\tau$ . This equation can be written as

$$\ln \frac{T_{c0}}{T_c} = (1 - \langle \Omega \rangle^2) \left[ \psi \left( \frac{1 + \mu}{2} \right) - \psi \left( \frac{1}{2} \right) \right], \quad (13)$$

where  $\mu = \hbar/2\pi T_c \tau$  and  $\psi$  is the digamma function. For a weak anisotropy  $\langle \Omega \rangle^2 = 1 - \chi$  with  $\chi \ll 1$ , this reduces to Hohenberg's result.<sup>23</sup> Although Eq. (13) is reminiscent of the case of magnetic impurities, the factor  $1 - \langle \Omega \rangle^2$  makes a difference. For  $\mu \ll 1$ , one has

$$T_c = T_{c0} - \frac{\pi\hbar}{8\tau} (1 - \langle \Omega \rangle^2). \quad (14)$$

For large  $\mu$ 's, unlike the case of the magnetic pair breaking, we obtain

$$T_c = T_{c0} [\Delta_0(0)\tau/\hbar]^{(\Omega)^{-2}-1}, \quad (15)$$

where  $\Delta_0(0) = 1.76 T_{c0}$ . Therefore,  $T_c$  does not turn zero at a finite  $\tau$ , unless  $\langle \Omega \rangle = 0$  as, e.g., for the  $d$ -wave superconductors.<sup>19</sup>

### ANISOTROPY NEAR $T_c$

As is seen from Eq. (11), impurities cause isotropization of  $f$ , 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<sup>17</sup> 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.<sup>24</sup> Within Eilenberger formalism this is done in the clean case by expanding  $f$  near  $T_c$  in two small parameters:  $\Delta/\hbar\omega \sim \sqrt{\delta t}$  and  $\mathbf{v}\mathbf{\Pi}\Delta/\hbar\omega^2 \sim \xi_0\Delta/\xi T_c \sim \delta t$  (here  $\delta t = (T_c - T)/T_c$  and  $\xi_0$  is zero- $T$  coherence length),

$$f = \frac{\Delta}{\hbar\omega} + a \frac{\mathbf{v}\mathbf{\Pi}\Delta}{\hbar\omega^2} + O(\delta t^{3/2}). \quad (16)$$

Substituting this in Eq. (1) one obtains  $a = -1/2$ . The second GL equation follows by using Eq. (5) in which we substitute  $g \approx 1 - ff^+/2$  with  $f$ 's of Eq. (16),

$$j_i = - \frac{7\zeta(3)|e|\hbar N(0)}{4\pi^2 T_{c0}^2} \langle \Omega^2 v_i v_k \rangle \text{Im} \Psi^* \Pi_k \Psi. \quad (17)$$

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

$$j_i = - \frac{c\phi_0}{4\pi^2} (\lambda^2)_{ik}^{-1} \left( \nabla\theta + \frac{2\pi}{\phi_0} \mathbf{A} \right)_k, \quad (18)$$

with

$$(\lambda^2)_{ik}^{-1} = \frac{14\zeta(3)e^2 N(0)}{\pi c^2 T_{c0}} \Psi_0^2 \langle \Omega^2 v_i v_k \rangle. \quad (19)$$

The anisotropy parameter follows,

$$\gamma^2(T_c) = \frac{\lambda_{cc}^2}{\lambda_{aa}^2} = \frac{\langle \Omega^2 v_a^2 \rangle}{\langle \Omega^2 v_c^2 \rangle}. \quad (20)$$

In fact, this is the result of Ref. 17.

In the presence of impurities, the first-order term in the expansion (16) should have the form (11). With  $D$  defined in Eq. (11), we verify readily that

$$f = \frac{D}{\hbar\omega'} - \frac{\mathbf{v}\mathbf{\Pi}D}{2\hbar\omega'^2} + O(\delta t^{3/2}) \quad (21)$$

satisfies Eq. (1). Writing  $D$  in the form,

$$D = \Psi \left( \Omega + \frac{\langle \Omega \rangle}{2\omega\tau} \right) \equiv \Psi \Omega', \quad (22)$$

we obtain, with the help of Eqs. (5) and (21),

$$j_i = - \frac{2\pi|e|N(0)T}{\hbar^2} \sum_{\omega} \frac{\langle \Omega'^2 v_i v_k \rangle}{\omega'^3} \text{Im} \Psi^* \Pi_k \Psi. \quad (23)$$

In the London limit, we have

$$(\lambda^2)_{ik}^{-1} = \frac{16\pi^2 e^2 N(0) T_c}{c^2 \hbar^3} \Psi_0^2 \sum_{\omega} \frac{\langle \Omega'^2 v_i v_k \rangle}{\omega'^3}, \quad (24)$$

and

$$\gamma^2(T_c) = \frac{\lambda_{cc}^2}{\lambda_{aa}^2} = \frac{\sum_{\omega} \langle \Omega'^2 v_a^2 \rangle / \omega'^3}{\sum_{\omega} \langle \Omega'^2 v_c^2 \rangle / \omega'^3}. \quad (25)$$

This is the result of Refs. 18 and 19. In the clean limit it reduces to Eq. (20), whereas the effect of impurities on  $\gamma$  depends on the order-parameter symmetry.

For the  $d$ -wave symmetry  $\langle \Delta \rangle = 0$  and  $\Omega' = \Omega$ . In other words, the strong  $T_c$  suppression notwithstanding, nonmagnetic impurities do not affect  $\gamma$ . For order parameters with a nonzero  $\langle \Delta \rangle$ , the strong scattering erases the effect of gap anisotropy on  $\gamma$  altogether,

$$\gamma_{\text{dirty}}^2 = \frac{\langle v_a^2 \rangle}{\langle v_c^2 \rangle}. \quad (26)$$

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. (5). We consider only the clean case for which  $f_0, g_0$  in the absence of currents are

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

in general, both  $\Delta_0$  and  $\beta$  depend on  $\mathbf{k}_F$ . A weak supercurrent causes the order parameter  $\Delta$  and the amplitudes  $f$  to acquire an overall phase  $\theta(\mathbf{r})$ . We look for the perturbed solutions in the form

$$\Delta = \Delta_0 e^{i\theta}, \quad f = (f_0 + f_1) e^{i\theta},$$

$$f^+ = (f_0 + f_1^+) e^{-i\theta}, \quad g = g_0 + g_1, \quad (28)$$

where the subscript 1 denotes corrections. In the London limit, the only coordinate dependence is that of the phase  $\theta$ , i.e.,  $f_1, g_1$  can be taken as  $\mathbf{r}$  independent.<sup>25</sup> Equations (1)–(3) then give,

$$\Delta_0 g_1 - \hbar\omega f_1 = i\hbar f_0 \mathbf{v} \mathbf{P} / 2,$$

$$\Delta_0 g_1 - \hbar\omega f_1^+ = i\hbar f_0 \mathbf{v} \mathbf{P} / 2, \quad (29)$$

$$2g_0 g_1 = -f_0 (f_1 + f_1^+).$$

Here,  $\mathbf{P} = \nabla\theta + 2\pi\mathbf{A}/\phi_0 \equiv 2\pi\mathbf{a}/\phi_0$  with the ‘‘gauge-invariant vector potential’’  $\mathbf{a}$ . To evaluate the current (5), one solves the system (29) for  $g_1$ ,

$$g_1 = i\hbar \frac{\Delta_0^2}{2\beta^3} \mathbf{v} \mathbf{P}. \quad (30)$$

Then one obtains the London relation between the current and the vector potential,  $4\pi j_i/c = -(\lambda^2)_{ik}^{-1} a_k$ , with

$$(\lambda^2)_{ik}^{-1} = \frac{16\pi^2 e^2 T}{c^2} N(0) \sum_{\omega} \left\langle \frac{\Delta_0^2 v_i v_k}{\beta^3} \right\rangle. \quad (31)$$

The anisotropy parameter now reads

$$\gamma^2 = \frac{\lambda_{cc}^2}{\lambda_{aa}^2} = \frac{\left\langle v_a^2 \Delta_0^2 \sum_{\omega} \beta^{-3} \right\rangle}{\left\langle v_c^2 \Delta_0^2 \sum_{\omega} \beta^{-3} \right\rangle}. \quad (32)$$

As  $T \rightarrow 0$ , we have  $2\pi T \Delta_0^2 \sum_{\omega} \beta^{-3} \rightarrow 1$ , and

$$\gamma^2(0) = \frac{\langle v_a^2 \rangle}{\langle v_c^2 \rangle}. \quad (33)$$

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.<sup>26</sup>

Near  $T_c$ ,  $\sum_{\omega} \beta^{-3} \rightarrow 7\zeta(3)/8\pi^3 T_c^3$ , and we obtain the GL result (20) that 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.

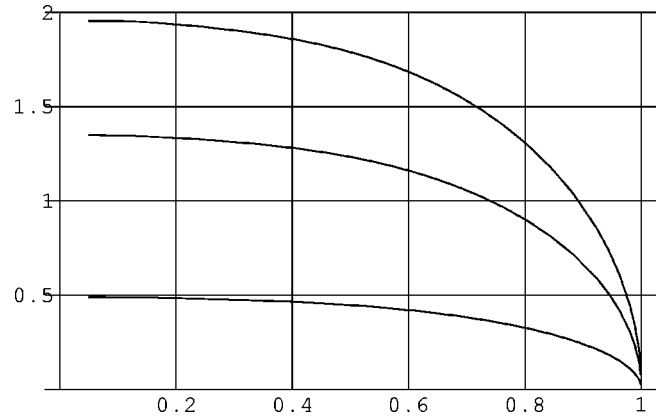


FIG. 1. The gaps  $\Delta_{1,2} = \Psi(T) \Omega_{1,2}$  versus  $T/T_c$ . The upper curve is  $\Delta_2/T_c$ , the lower one is  $\Delta_1/T_c$ , and the middle curve is  $\Psi(T)/T_c$  evaluated as described in the text.

It is of interest to examine the consequences of our results for  $\text{MgB}_2$ . The reported  $\gamma$ 's vary from 1.7 to 8,<sup>10–13</sup> or even higher as in Ref. 16. 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

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

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 (8)

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

where we introduce normalized densities of state  $\nu_{1,2} = N_{1,2}/N(0)$  for brevity. We have then instead of Eq. (8),

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

We also assume that the two parts of the Fermi surface have the symmetries of the total, e.g.,  $\langle \mathbf{v} \rangle_1 = 0$  where the average is performed only over the first Fermi sheet. Within this model, Eq. (32) reads

$$\gamma^2 = \frac{\sum_i \nu_i \Omega_i^2 \langle v_a^2 \rangle_i \sum_{\omega} \beta_i^{-3}}{\sum_i \nu_i \Omega_i^2 \langle v_c^2 \rangle_i \sum_{\omega} \beta_i^{-3}}, \quad i = 1, 2, \quad (37)$$

where  $\beta_i = \sqrt{\hbar^2 \omega^2 + \psi^2(T) \Omega_i^2}$ .

Based on the band-structure calculations, the relative densities of states  $\nu_1$  and  $\nu_2$  of our model are  $\approx 0.56$  and  $0.44$ .<sup>27,6</sup> 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. 6, 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 two gaps  $\Delta_i(T)$ .

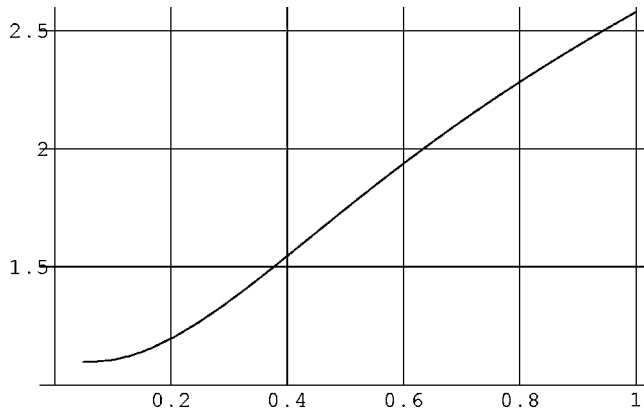


FIG. 2. The anisotropy parameter  $\gamma = \lambda_c / \lambda_a$  versus  $T/T_c$  for clean  $\text{MgB}_2$  calculated using parameters given in the text.

To evaluate  $\gamma(T)$  of Eq. (37) we use the averages over separate Fermi sheets calculated in Ref. 27:  $\langle v_a^2 \rangle_1 = 33.2$ ,  $\langle v_c^2 \rangle_1 = 42.2$ ,  $\langle v_a^2 \rangle_2 = 23$ , and  $\langle v_c^2 \rangle_2 = 0.5 \times 10^{14} \text{ cm}^2/\text{s}^2$ . The numerical result for  $\gamma(T)$  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 in-

termediate magnetic fields tilted relative to the principal crystal directions.<sup>28</sup> Some torque data for  $\text{MgB}_2$  were reported by Angst *et al.*<sup>14</sup> (and recently in Refs. 29 and 30), 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. 31 and 32). At  $T_c$ , this ratio is estimated to be  $\approx 2.3$ – $2.7$ .<sup>14</sup> Near  $T_c$ , the ratio of  $H_{c2}$ 's should coincide with the ratio of  $\lambda$ 's. In this work we estimate the latter as  $\approx 2.6$ , see Fig. 2. Given this agreement and the prediction made here that  $\lambda_c/\lambda_{ab}$  should drop with decreasing  $T$  whereas the experiment shows increase of  $H_{c2,ab}/H_{c2,c}$ , the detailed studies of  $\gamma = \lambda_c/\lambda_{ab}$  are desirable.

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