Anisotropic s-wave superconductivity in MgB$_2$

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Abstract

It has recently been observed that MgB$_2$ is a superconductor with a high transition temperature. Here we propose a model of anisotropic s-wave superconductivity which consistently describes the observed properties of this compound, including the thermodynamic and optical response in sintered MgB$_2$ wires. We also determine the shape of the quasiparticle density of states and the anisotropy of the upper critical field and the superfluid density which should be detectable once single-crystal samples become available.
1. Introduction

The recently discovered superconductor MgB$_2$ has received great attention, mainly because of its high transition temperature of approximately 39K. This relatively high $T_c$ value may not be too surprising since MgB$_2$ involves some of the lightest elements in the periodic table, thus implying a large Debye phonon frequency for this compound. Indeed, data from thermodynamic measurements suggest a Debye frequency $\Theta_D \approx 750$ K as well as a significant isotope effect with $\alpha = 0.26$.

More surprisingly, a rather small zero-temperature energy gap $\Delta_0 = 1.20 k_B T_c$ was deduced from measurements of the specific heat and from the optical conductivity. Presently, we do not know of any other examples for such a small ratio $\Delta_0/k_B T_c$ in conventional s-wave superconductors. This observation naturally suggests an anisotropic s-wave order parameter for this material, where the energy gap detected in the thermodynamic measurements is in fact the minimum of the superconducting gap function. An alternative explanation has been suggested in terms of multi-band models. In many respects the proposed phenomenological model with an anisotropic energy gap is similar to a multi-band model. In fact, the latter may be thought of as a discretized version of the former. More recently, the upper critical critical field for a dense wire of MgB$_2$ was inferred from the field dependence of the critical current. From these measurements it was concluded that MgB$_2$ is an extreme type II superconductor with a Ginzburg-Landau parameter $\kappa \approx 23$.

Drafting an effective model with an anisotropic s-wave order parameter for MgB$_2$, the first important question to address is the direction and the magnitude of the anisotropy over the approximately ellipsoidal Fermi surface. In the distantly related tetragonal systems YNi$_2$B$_2$C and LuNi$_2$B$_2$C, such an anisotropy has been shown to appear in the a-b planes. On the other hand, MgB$_2$ has a hexagonal crystal structure, and thus the anisotropy is most likely to occur along the c-direction similar to other hexagonal crystals, such as UPt$_3$ and UPd$_2$Al$_3$, and tetragonal crystals, such as Sr$_2$RuO$_4$.

We therefore propose a BCS model for MgB$_2$ with a superconducting order parameter given by
$\Delta(k) = \Delta \left( \frac{1 + az^2}{1 + a} \right)$. \hspace{2cm} (1)

where the parameter $a$ determines the anisotropy, $z = \cos \theta$, and $\theta$ is the polar angle. For the calculations outlined in this paper, we impose the experimentally observed gap ratio,

$$\frac{\Delta_{\text{min}}(T = 0)}{k_B T_c} = \frac{\Delta_0}{(1 + a) k_B T_c} = 1.20,$$

which in turn yields $a \simeq 1$. In the following, we will therefore explore the consequences of anisotropic s-wave superconductivity in MgB$_2$ within the framework of weak-coupling BCS theory, setting $a = 1$.

2. Density of States

In Fig. 1(a) the anisotropic s-wave order parameter $\Delta(k) = \Delta(1 + z^2)/2$, is plotted in momentum space. This function is an ellipsoid with a minor axis of length $\Delta/2$ within the a-b plane, and a major axis of length $\Delta$ along the c-direction. The smaller magnitude of the gap function within the a-b plane is consistent with the stronger in-plane Coulomb repulsion that has been suggested in Ref. [15].

![Anisotropic s-wave order parameter](a)

![Quasiparticle density of states](b)

FIG. 1. (a) Anisotropic s-wave order parameter. (b) Quasiparticle density of states.

The corresponding density of states can be calculated from $\Delta(k)$ within weak-coupling theory. It is given by
\[
\frac{N(E)}{N_0} = \int_0^1 dz \Re \left( \frac{|E|}{\sqrt{E^2 - \Delta^2(1 + z^2)^2/4}} \right)
\]
\[= 0 \quad \text{if } 0 < E < \Delta/2, \]
\[= \sqrt{\frac{E}{\Delta}} K \left( \sqrt{\frac{2E - \Delta}{4E}} \right) \quad \text{if } \Delta/2 < E < \Delta, \quad (3)
\]
\[= \sqrt{\frac{E}{\Delta}} F \left( \sin^{-1} \sqrt{\frac{2E\Delta}{(2E - \Delta)(E + \Delta)}}, \sqrt{\frac{2E - \Delta}{4E}} \right) \quad \text{if } E > \Delta,
\]

where \(K(k)\) and \(F(\Phi, k)\) are the complete and incomplete elliptic integrals of the first kind.

This quasiparticle density of states is shown in Fig. 1(b). It is fully gapped with an onset of spectral weight at the minimum gap value \(E = \Delta/2\) and a cusp at \(E = \Delta\).

3. Thermodynamics

![Graphs](image)

**FIG. 2.** (a) Energy gap in an anisotropic s-wave superconductor. (b) Entropy (solid line) and specific heat (dashed line). Above \(T_c\) these quantities are equal (dot-dashed line). (c) Thermodynamic critical field for anisotropic (solid line) and isotropic (dashed line) s-wave superconductors. Inset: deviation of these critical fields from a parabolic temperature dependence.

Following the formalism by Bardeen, Cooper, and Schrieffer [16], we calculate the temperature dependence of the energy gap \(\Delta(T)\), the entropy \(S(T)\), the specific heat \(C(T)\), and the thermodynamic critical field \(H_c(T)\) for the anisotropic s-wave superconductor. Here, the entropy is given by

\[
S(T) = -4 \int_0^\infty dEN(E) \left( f \ln f + (1 - f) \ln (1 - f) \right), \quad (4)
\]
where \( f \equiv (1 + \exp \beta E)^{-1} \). Furthermore, the specific heat and the upper critical field are obtained from

\[
C(T) = T \frac{\partial S(T)}{\partial T} \quad \text{and} \quad \frac{H_c^2(T)}{8\pi} = \int_T^{T_c} dT S(T).
\]

These results are displayed in Fig. 2. As expected, the characteristic jump of the specific heat at \( T_c \), \( \Delta C/C_N = 1.18 \), is small compared with the value 1.43 for an isotropic s-wave superconductor. This is consistent with the experimental picture for MgB\(_2\). \[3\] \[4\] Furthermore, it is seen in Fig. 2(b) that the thermodynamic critical field is also reduced in the anisotropic case. The deviation of the critical field from a parabolic temperature dependence, defined by

\[
D(T/T_c) \equiv \frac{H_c(T)}{H_c(0)} - \left[ 1 - \left( \frac{T}{T_c} \right)^2 \right],
\]

is shown in the inset of Fig. 2(c). The magnitude of this deviation is substantially larger than for the isotropic case, again consistent with the experiments. \[4\]

![Diagram](image)

**FIG. 3.** Superfluid densities of anisotropic and of isotropic s-wave superconductors.

Finally, the superfluid density \( \rho_s(T) \) shown in Fig. 3 is found to be rather anisotropic. Similar to the energy gap and the thermodynamic critical field, upon increasing the tem-
perature its departure from its zero-temperature value is exponentially small in the low-
temperature regime. On the other hand, in the vicinity of $T_c$ the superfluid density for the
isotropic case is linear in temperature, whereas for the anisotropic case $\rho_s(T)$ is observed to
be slightly concave along the c-direction and slightly convex in the a-b plane. Once single
crystals of MgB$_2$ become available, this anisotropy in the superfluid density should serve as
a signature for the order parameter symmetry.

4. Upper Critical Field

Recent measurements of the upper critical field in sintered samples of MgB$_2$ have reported
a somewhat unusual temperature dependence. This is likely related to the apparent
anisotropy of the superconducting order parameter, and should thus become even more
evident in measurements of the upper critical field in single crystals. Therefore we consider
here the two cases of an external magnetic field parallel and perpendicular to the crystal
c-axis of MgB$_2$.

![Diagram of upper critical fields](image_url)

**FIG. 4.** Upper critical fields of anisotropic and isotropic s-wave superconductors.

(a) $H \parallel c$

The upper critical field along the crystal c-direction is determined from

$$\begin{align*}
- \ln \frac{T}{T_c} &= \int_0^\infty \frac{du}{\sinh u} \left( 1 - \frac{15}{28} \int_0^1 dz (1 + z^2)^2 \exp \left( -\rho u^2 (1 - z^2) \right) \right),
\end{align*}$$

(8)
where \( \rho \equiv (v_F^2 e H_{c2}(T))/(2(2\pi T)^2) \) and \( z \equiv \cos \theta \). In Fig. 4, the solution of this integral equation normalized by its derivative at \( T_c \), \( h_{c2}(T) \equiv H_{c2}(T)/(-\partial H_{c2}(T)/\partial T)|_{T_c} \), is plotted along with the \( h_{c2}(T) \)-curves for the a-b-direction and for the isotropic case. In the limit \( T \to 0 \) we obtain \( h_{c2}^0(0) \simeq 0.824 \) which is somewhat larger than the corresponding value for the isotropic s-wave superconductor, \( h_{c2}(0) \simeq 0.728 \). In the opposite limit, \( T \to T_c \), \( h_{c2}^c(T) \) exhibits a rather linear temperature dependence within the weak-coupling BCS model. This behavior is also observed for the isotropic s-wave superconductor.

(b) \( H \parallel a \)

For the upper critical field within the a-b plane a mixing occurs of the zeroth and the second Landau levels, leading to (10,17)

\[
\Delta(k, r) \sim \Delta \left( 1 + C(a^\dagger)^2 \right) |0\rangle, \tag{9}
\]

where \( |0\rangle \) is the Abrikosov state, \( a^\dagger \) is the raising operator, and \( C \) is the mixing coefficient between the Landau levels which has to be determined self-consistently along with the critical field. This leads to a set of coupled integral equations,

\[
-\ln \frac{T}{T_c} = \int_0^\infty \frac{du}{\sinh u} \left( 1 - \frac{15}{28} \int_0^1 dz \left[ (1 + \sin^2 \theta + \frac{3}{8} \sin^4 \theta) + \frac{1}{2} C \rho u^2 \sin^4 \theta(1 + \frac{1}{2} \sin^2 \theta) \right] \exp \left( -\rho u^2 (1 - z^2) \right) \right), \tag{10}
\]

\[
-C \ln \frac{T}{T_c} = \int_0^\infty \frac{du}{\sinh u} \left( C - \frac{15}{28} \int_0^1 dz \left[ \frac{1}{4} \rho u^2 \sin^4 \theta(1 + \frac{1}{2} \sin^2 \theta) + C(1 + \sin^2 \theta + \frac{3}{8} \sin^4 \theta)(1 - 4\rho u^2 \sin^2 \theta + 2\rho^2 u^4 \sin^4 \theta) \right] \exp \left( -\rho u^2 (1 - z^2) \right) \right), \tag{11}
\]

where again \( \rho \equiv (v_F^2 e H_{c2}(T))/(2(2\pi T)^2) \), and \( \sin^2 \theta = 1 - z^2 \). The numerical solution of this set of equations is shown in Fig. 4. The mixing coefficient (not shown) is found to decrease monotonously from 0.069 down to 0.062 as the temperature is increased. This implies a relevant admixture of the second Landau level. In the zero-temperature limit, we obtain \( h_{c2}^0(0) \simeq 0.664 \). By comparing \( h_{c2}^c(0) \) with \( h_{c2}^0(0) \), we can thus conclude from the model calculation that the critical field observed in sintered MgB\(_2\) represents \( H_{c2}^c(T) \) because \( H_{c2}^c(T) > H_{c2}^a(T) \) for all temperatures. We also note that \( H_{c2}^c(T), H_{c2}^a(T) \gg H_c(T) \) since for
sintered MgB$_2$ wires the Ginzburg-Landau parameter was observed to be very large $\kappa \simeq 23$.

5. Conclusions

Based on presently available experimental data on MgB$_2$ we have constructed a model of anisotropic s-wave superconductivity for this compound with $\Delta_{\text{min}}/\Delta_{\text{max}} = 1/2$. This simple theory appears to account rather well for the thermodynamic properties \cite{3,4}, the optical measurements, \cite{1} and for the upper critical field data \cite{2,6,8} on sintered samples of MgB$_2$. Experiments on single crystal samples will clearly be important to further investigate the applicability of this model.

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