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Anisotropic *s*-wave superconductivity in MgB_2

Stephan Haas and Kazumi Maki

Department of Physics and Astronomy, University of Southern California, Los Angeles, California 90089-0484

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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, the tunneling conductance, and the anisotropy of the upper critical field and the superfluid density which should be detectable once single-crystal samples become more generally available.

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I. INTRODUCTION

The recently discovered superconductor MgB_2 has received great attention, mainly because of its high transition temperature of approximately 39 K.[1–6] 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[2,3] suggest a significant isotope effect with $\alpha = 0.26$ as well as a Debye frequency $\Theta_D \approx 750\,\mathrm{K}$, indicating that weak-coupling BCS theory is adequate for this compound.[7] Recently, the upper critical field for a dense wire of MgB_2 was inferred from the field dependence of the critical current.[6] From these measurements it was concluded that MgB_2 is an extreme type-II superconductor with a Ginzburg-Landau parameter $\kappa \simeq 23$.

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[3,4] and from the optical conductivity.[5] 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 two-band models.[8,9] Multigap scenarios have a long history, starting from Ref. 10, but have never been realized in superconducting materials so far. On a qualitative level, two-gap models can have similar properties to the anisotropic *s*-wave model we are proposing, and therefore experimental tests to distinguish between these theories are highly desirable.

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_2B_2C and $LuNi_2B_2C$, such an anisotropy has been shown to appear in the *a-b* planes.[11,12] 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 (Ref. 13) and UPd_2Al_3 (Ref. 14), and tetragonal crystals, such as Sr_2RuO_4 (Refs. 15 and 16).

We therefore propose a BCS model for MgB_2 with a superconducting order parameter given by

$$\Delta(\mathbf{k}) = \Delta\left(\frac{1+az^2}{1+a}\right), \tag{1}$$

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

$$\frac{\Delta_{\min}(T=0)}{k_B T_c} = \frac{\Delta_0}{(1+a)k_B T_c} = 1.20, \tag{2}$$

which in turn yields $a \approx 1$. 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 $a = 1$.

II. DENSITY OF STATES AND TUNNELING CONDUCTANCE

In Fig. 1(a) the anisotropic *s*-wave order parameter $\Delta(\mathbf{k}) = \Delta(1+z^2)/2$, 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 Δ along the

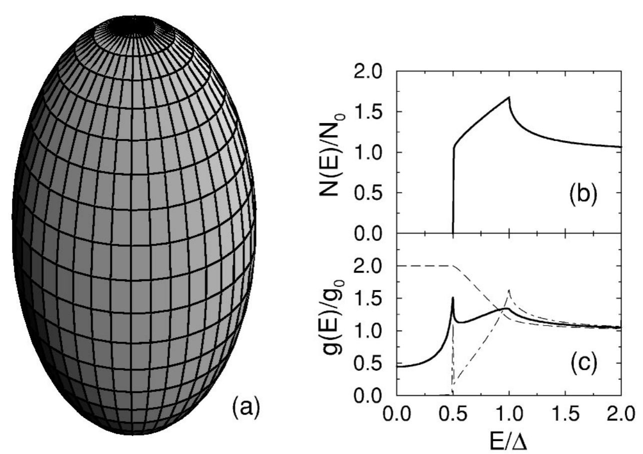

FIG. 1. (a) Anisotropic *s*-wave order parameter, (b) quasiparticle density of states, (c) tunneling conductance. Dashed line: Andreev limit, dot-dashed line: Giaever limit, solid line: intermediate tunneling matrix element.

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. 17.

The corresponding density of states can be calculated from $\Delta(\mathbf{k})$ within weak-coupling theory. It is given by

$$N(E)/N_0=0 \quad \text{if } 0<E<\Delta/2,$$
$$=\sqrt{\frac{E}{\Delta}}K\left(\sqrt{\frac{2E-\Delta}{4E}}\right) \quad \text{if } \Delta/2<E<\Delta, \tag{3}$$
$$=\sqrt{\frac{E}{\Delta}}F\left(\sin^{-1}\sqrt{\frac{2E\Delta}{(2E-\Delta)(E+\Delta)}},\sqrt{\frac{2E-\Delta}{4E}}\right) \quad \text{if } E>\Delta\ ,$$

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 $E=\Delta$. Recent scanning tunneling microscope measurements report a density of states in good agreement with $N(E)$.[18]

More generally, the tunneling conductance between a normal metal point contact and a superconductor depends on the tunneling matrix element Z, as described by the Blonder, Tinkham, and Klapwijk formalism.[19] For unconventional superconductors the order parameter can be written as a product of the amplitude Δ and a momentum-dependent factor f, i.e., $\Delta(\mathbf{k})=\Delta f$, where $f=(1+z^2)/2$ in our case. The zero-temperature tunneling conductance normalized by its normal-state value is then given by

$$g(E)/g_0=\int_0^1 dz\,\frac{2(1+Z^2)f^2}{x^2+(f^2-x^2)(1+2Z^2)^2} \quad \text{if } |x|<1/2,$$
$$=2(1+Z^2)[I_1(x)+I_2(x)] \quad \text{if } 1/2<|x|<1, \tag{4}$$
$$=\int_0^1 dz\,\frac{2(1+Z^2)|x|}{|x|+\sqrt{x^2-f^2}(1+2Z^2)} \quad \text{if } 1<|x|,$$

where

$$I_1(x)=\int_{\lim}^1 dz\,\frac{f^2}{x^2+(f^2-x^2)(1+2Z^2)^2},$$
$$I_2(x)=\int_0^{\lim} dz\,\frac{|x|}{|x|+\sqrt{x^2-f^2}(1+2Z^2)}, \tag{5}$$

and $\lim=(2x-1)$.

In Fig. 1(c) the tunneling conductance is shown for tunneling matrix elements $Z=0$, 1.0, and 10.0. In the Andreev limit ($Z=0$), the conductance is at its maximum, $g(E)/g_N=2$, for energies below the gap minimum $\Delta_0=1/(1+a)$. Above Δ_0, it decays rapidly, approaching the normal-state value at high energies, $g(E\to\infty)\to g_N$. For finite values of the tunneling matrix element Z, the tunneling conductance exhibits two features at the minimum and at the maximum of the superconducting gap energy. While for small Z the conductance is dominated by the Andreev peak at Δ_0, at larger Z the cusp at $E=\Delta$ emerges into a peak, and for $Z\to\infty$ (Giaver limit) the tunneling spectrum resembles the quasiparticle density of states. From Fig. 1(c) it appears that the two-peak structure observed in the point contact measurements of Ref. 20 can be well described within the anisotropic s-wave model with a tunneling matrix element in the range $0.5<Z<1.5$. We conclude from this calculation that the tunneling conductance is quite sensitive to the detailed structure of the point contact which is a likely reason for the different observed spectra of Refs. 18 and 20.

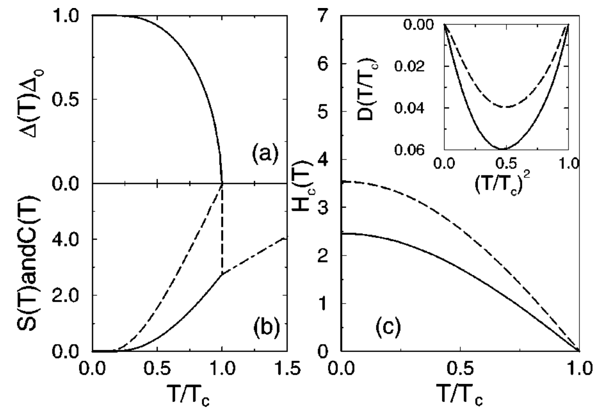

FIG. 2. (a) Energy gap in an anisotropic s-wave superconductor. (b) Entropy (solid line) and specific heat (dashed line). Above T_c these quantities are equal (dot-dashed line). (c) Thermodynamic critical field for anisotropic (solid line) and isotropic (dashed line) s-wave superconductors. Inset: deviation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

III. THERMODYNAMICS

Following the formalism by Bardeen, Cooper, and Schrieffer,[21] 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

$$S(T)=-4\int_0^\infty dE N(E)[f\ln f+(1-f)\ln(1-f)], \tag{6}$$

where $f\equiv(1+\exp\beta E)^{-1}$. Furthermore, the specific heat and the upper critical field are obtained from

$$C(T)=T\frac{\partial S(T)}{\partial T} \quad \text{and} \quad \frac{H_c^2(T)}{8\pi}=\int_T^{T_c} dT S(T). \tag{7}$$

These results are displayed in Fig. 2, where the vertical scale of $S(T)$ and $C(T)$ is given in units of N_0T_c, and $H_c(T)$ is normalized by $(N_0)^{1/2}T_c$. As expected, the characteristic

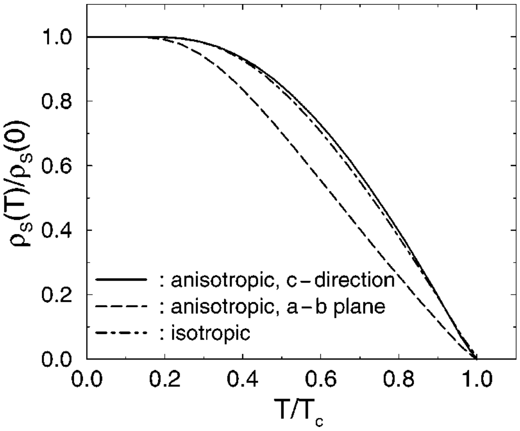

FIG. 3. Superfluid densities of anisotropic and of isotropic *s*-wave superconductors.

jump of the specific heat at T_c, $\Delta C/C_N = 1.18$, is rather small compared with the value 1.43 for an isotropic *s*-wave superconductor. This is consistent with the experimental picture for MgB_2 of Ref. 3, although larger than the value $\Delta C/C_N = 0.82$ quoted in Ref. 4. Furthermore, it is seen in Fig. 2(b) that the thermodynamic critical field is also reduced in the anisotropic case. Converting $H_c(T)$ into physical units, we find $H_c(0) = 0.27$ T, consistent with 0.26 T observed in Ref. 4. The deviation of the critical field from a parabolic temperature dependence, defined by

$$D(T/T_c) \equiv \frac{H_c(T)}{H_c(0)} - \left[1 - \left(\frac{T}{T_c}\right)^2\right], \tag{8}$$

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]

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 temperature 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 anisotropy of the order parameter.

IV. UPPER CRITICAL FIELD

Recent measurements of the upper critical field in sintered and *c*-axis oriented samples of MgB_2 have reported a somewhat unusual temperature dependence.[6,9,22] 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.[23]

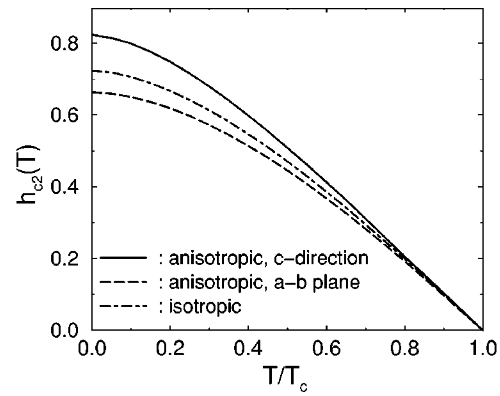

FIG. 4. Upper critical fields of anisotropic and isotropic *s*-wave superconductors.

A. H∥c

The upper critical field along the crystal *c* direction is determined from[12,24]

$$-\ln\frac{T}{T_c} = \int_0^\infty \frac{du}{\sinh u}\left(1 - \frac{15}{28}\int_0^1 dz(1+z^2)^2 \times \exp[-\rho u^2(1-z^2)]\right), \tag{9}$$

where $\rho \equiv [v_F^2 e H_{c2}(T)]/[2(2\pi T)^2]$, $z \equiv \cos\theta$, and v_F is the Fermi velocity within the *a*-*b* plane. 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 $h_{c2}^c(0) \simeq 0.824$ 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, strongly resembling recent observations in *c*-axis oriented samples of MgB_2.[22]

B. H∥a

For the upper critical field within the *a*-*b* plane a mixing occurs of the zeroth and the second Landau levels, leading to[12,24] $\Delta(\mathbf{k},\mathbf{r}) \sim \Delta(1 + C(a^\dagger)^2)|0\rangle$, 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 yields a set of coupled integral equations,

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

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

where again $\rho\equiv[v_F^2 eH_{c2}(T)]/[2(2\pi T)^2]$, $\sin^2\theta=1-z^2$, and $v_F=(v_F^b v_F^c)^{1/2}$. 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 $h_{c2}^a(0)\simeq 0.664$.

In general, the upper critical field depends on the anisotropy of the Fermi surface (i.e., different Fermi velocities in different directions) as well as on the anisotropy of the superconducting order parameter.[23] In order to separate these two effects, in Fig. 4 the reduced upper critical field is shown. The temperature dependence of h_{c2} reflects only the anisotropy in $\Delta(\mathbf{k})$, because the effect of the anisotropy in the Fermi surface has been eliminated in this *reduced* quantity by rescaling of the Fermi velocity.[25]

V. CONCLUSIONS

Based on presently available experimental data on MgB_2 we have constructed a model of anisotropic *s*-wave superconductivity for this compound with $\Delta_{min}/\Delta_{max}=\frac{1}{2}$. This simple theory appears to account rather well for the thermodynamic properties,[3,4] the optical measurements,[5] and for the upper critical field data[2,6,9,22] on sintered and *c*-axis oriented 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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[23] In general, the upper critical field depends both on the anisotropy of the Fermi surface and on the anisotropy of the superconducting order parameter. Recent experiments on *c*-axis oriented samples of MgB_2 suggest $H_{c2}^a(T)>H_{c2}^c(T)$ (Ref. 22), which can be interpreted consistently within the anisotropic *s*-wave model, assuming $v_F^c/v_F^a\simeq 0.45$ (Ref. 25).

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