Quasiparticle spectrum of the hybrid s+g-wave superconductors

YNi$_2$B$_2$C and LuNi$_2$B$_2$C

Kazumi Maki,$^1$ Hyekyung Won,$^2$ and Stephan Haas$^1$

$^1$Department of Physics and Astronomy, University of Southern California, Los Angeles, CA 90089-0484

$^2$Department of Physics, Hallym University, Chunchon 200-702, South Korea

(Dated: January 9, 2022)

Abstract

Recent experiments on single crystals of YNi$_2$B$_2$C have revealed the presence of point nodes in the superconducting energy gap $\Delta(k)$ at $\hat{k} = (1,0,0)$, $(0,1,0)$, $(-1,0,0)$, and $(0,-1,0)$. In this paper we investigate the effects of impurity scattering on the quasiparticle spectrum in the vortex state of s+g-wave superconductors, which is found to be strongly modified in the presence of disorder. In particular, a gap in the quasiparticle energy spectrum is found to open even for infinitesimal impurity scattering, giving rise to exponentially activated thermodynamic response functions, such as the specific heat, the spin susceptibility, the superfluid density, and the nuclear spin lattice relaxation. Predictions derived from this study can be verified by measurements of the angular dependent magnetospecific heat and the magnetothermal conductivity.

PACS numbers: 74.25.Op, 74.25.Fy, 74.70.Dd
1. Introduction

The recently discovered superconductivity in the borocarbides YNi$_2$B$_2$C and LuNi$_2$B$_2$C has attracted much attention due to the rather unusual apparent structure of their gap function $\Delta(k)$. [1, 2] On the one hand, the presence of a substantial s-wave component has been observed by thermodynamic measurements of samples in which Ni was substituted by small amounts of Pt, causing the opening of an energy gap. [3, 4] On the other hand, there is also mounting experimental evidence for the presence of nodes in the superconducting order parameter. [5, 6, 7] A consistent way to account for these seemingly contradictory observations is to consider the hybrid s+g-wave order parameter [8, 9], given by

$$\Delta(k) = \Delta \left(1 - \sin^4(\theta) \cos(4\phi)\right)/2,$$

where the angles $\theta$ and $\phi$ indicate the direction of the quasiparticle wave vector $k$. A graphical representation of $\Delta(k)$ is given in Fig. 1(a). This order parameter has recently been shown to account for the Raman spectra measured in YNi$_2$B$_2$C and LuNi$_2$B$_2$C. [10, 11] Furthermore, it was observed that the corresponding quasiparticle spectrum is very sensitive to impurity scattering. In particular, the thermal conductivity of Y(Ni$_{1-x}$Pt$_x$)$_2$B$_2$C for $x=0.05$ in the vortex state at $T=0.8K$ does not exhibit any angular dependence, contrary to the clear cusp structure observed in the pure system. [12]

![FIG. 1: (a) s+g-wave order parameter with four point nodes, (b) quasiparticle density of states for various impurity scattering rates.](image-url)
Theoretical studies of nonmagnetic impurity scattering in anisotropic superconductors indicate that this type of disorder has much more profound effects on the hybrid s+g-wave superconductors with point nodes than on other unconventional superconductors with line nodes. In particular, it was observed that the unitary limit and the weak-scattering Born limit give practically the same results over a wide range of parameters. Also, contrary to superconductors with line nodes, no low-frequency resonance is found for the strong-scattering case. Even more surprisingly, a disorder-induced quasiparticle energy gap $\omega_g$ opens up even for infinitesimal scattering rates $\Gamma$. This dependence is well approximated by $\omega_g = \Gamma / (1 + 2\Gamma/\Delta)$. Typical quasiparticle densities of states for the pure s+g-wave system and in the presence of impurity scattering are shown in Fig. 1(b).

The opening of a disorder-induced quasiparticle energy gap offers a natural explanation for the reported exponentially activated temperature dependence of the thermal conductivity and the specific heat,

$$\frac{C_S}{T}, \frac{\kappa_{zz}}{T} \propto \left( \frac{\omega_g}{T} \right)^{3/2} \exp(-\omega_g/T).$$

For the same reason, no universal heat conduction is expected for these systems as opposed to superconductors with line nodes. Because these effects of impurity scattering are rather singular compared with other nodal superconductors, it is necessary to reexamine how transport properties are affected by disorder. One finds that in the superclean limit, i.e. $\Gamma \ll \sqrt{v_a v_c eH}$ where $v_a$ and $v_c$ are the Fermi velocities along the crystallographic a- and c-directions, the thermal conductivity $\kappa_{zz}$ has a similar angular dependence as in the pure system. However, the opening of the energy gap due to the impurity scattering drastically reduces nodal excitations. For $\Gamma/\sqrt{v_a v_c eH} > \pi/\sqrt{2}$ practically all of the nodal excitations are eliminated, and therefore the angular dependence of the thermal conductivity is suppressed, as it was recently observed by Kamata et al. The impurity scattering rate $\Gamma$ can be accurately estimated in terms of its effect on the superconducting transition temperature,

$$-\ln \left( \frac{T_c}{T_{c0}} \right) = \frac{\langle f^2 \rangle}{1 + \langle f^2 \rangle} \left[ \psi \left( \frac{1}{2} + \frac{\Gamma}{2\pi T} \right) - \psi \left( \frac{1}{2} \right) \right],$$

where $\psi(z)$ is the di-gamma function, $f \equiv \sin^4(\theta) \cos(4\phi)$ denotes the angular dependence of the s+g-wave gap function, $\langle f^2 \rangle \simeq 0.203$ results from angular averaging, and $T_{c0}$ is the critical superconducting transition temperature of the pure system. For the 5% Pt doped
YNi₂B₂C, the reduced critical temperature $T_c = 13.5$K therefore indicates a scattering rate $\Gamma = 28.3$K, where $T_{c0}= 15.5$ K was used. This implies that for the doping level $x \sim 0.05$ the corresponding disorder induced energy gap is $\omega_g \sim 10$K. Since this is already a rather strong effect, it may be necessary to measure single crystals with $x < 0.01$, in order to observe the associated disappearance of the angular dependence in the thermal conductivity.

2. Quasiparticle Density of States in the Vortex State

The quasiparticle density of states and the quasiparticle scattering rate are obtained from the integral\[^{[18]}\]

$$I = \langle (x + iC_0)^2 - ((\Gamma / \Delta) + (1 - f)/2)^2 \rangle^{-1/2},$$

(4)

where $x \equiv \langle |v \cdot q|/\Delta \rangle$, and $v \cdot q$ is the Doppler shift due to the supercurrents circulating around the vortices.\[^{[17, 18]}\] The terms $(\Gamma / \Delta)$ and $C_0$ in Eq. 4 arise from the renormalization of the order parameter and of the frequency due to the presence of impurity scattering,

$$\tilde{\Delta}_{\omega=0} = \Gamma,$$

(5)

$$\tilde{\omega}_{\omega=0} = iC_0\Delta.$$  

(6)

For the gap symmetry of $\Delta(k)$ given in Eq. 1, and in a magnetic field $\mathbf{H}$ directed along $(\theta, \phi)$ with the polar axis along the crystal c-direction, one obtains

$$x \simeq \sqrt{\frac{v_a v_e e H}{2 \Delta}} \left( \sqrt{1 - \sin^2 \theta \cos^2 \phi} + \sqrt{1 - \sin^2 \theta \sin^2 \phi} \right).$$

(7)

For small impurity scattering $\Gamma/\Delta \ll 1$, the angular averages Eq. 4 can be performed analytically, giving

$$I \simeq \frac{1}{2} (x + iC_0) \left( \cosh^{-1} \left( \frac{1}{x} \right) + \cos^{-1} y - \frac{iC_0}{x} \left( 1 - \frac{y}{\sqrt{1 - y^2}} \right) \right),$$

(8)

where $y \equiv \Gamma/x\Delta$. Within this limit, one obtains closed expressions for the quasiparticle density of states $g(\mathbf{H}, \Gamma)$ and for the quasiparticle damping constant $C_0\Delta$:

$$g(\mathbf{H}, \Gamma) \equiv \frac{N(E)}{N_0} = \frac{x}{2} \cos^{-1} y \theta (1 - y) + O(C_0),$$

(9)

$$C_0\Delta = \frac{\Gamma x}{2} \left[ \ln \left( \frac{2}{x} \right) + O(C_0) \right].$$

(10)
Consequently, the low-temperature specific heat, the spin susceptibility, the superfluid density in the a-b plane, and the nuclear spin lattice relaxation rate are given by

\[
\frac{C_S}{\gamma N T} = \frac{\chi_S}{\chi_N} = g(H, \Gamma),
\]

(11)

\[
\frac{\rho_{Sab}(H)}{\rho_{Sab}(0)} = 1 - \frac{3}{2} g(H, \Gamma),
\]

(12)

\[
\frac{T_{1N}^{-1}}{T_{1N}^{-1}} = g^2(H, \Gamma).
\]

(13)

Note that in contrast to \(\rho_{Sab}(H)\) the superfluid density along the c-direction \(\rho_{Sc}(H)\) is not linear in \(g(H, \Gamma)\).

FIG. 2: Dependence of the quasiparticle density of states on the azimuthal angle \(\phi\) for various impurity scattering strengths. The polar angle is fixed to \(\theta = \pi/2\).

In Fig. 2, the dependence of the quasiparticle density of states \(g(H, \Gamma)\) on the azimuthal angle \(\phi\) is shown for a fixed polar angle \(\theta = \pi/2\), and for \(y_0 = 0.0, 0.4, 1.0,\) and \(1.2\), where \(y_0 \equiv (2\Gamma)/(\pi \sqrt{v_a v_c e H})\) is a measure of the impurity scattering strength. From Eq. 9 it follows that \(g(H, \Gamma) = 0\) for \(y_0 > \sqrt{2}\). Furthermore, it is observed in Fig. 2 that the \(\phi\)-independent part of \(g(H, \Gamma)\) gets cut off for increasing \(\Gamma\). For \(y_0 > 1\) the constant part is completely eliminated, and only small islands survive for \(1 < y_0 < \sqrt{2}\). This is a signature of a \(k\)-independent energy gap \(\omega_g\) that opens up due to impurity scattering.

Thermodynamic response functions, such as the specific heat, the spin susceptibility, the
superfluid density, and the nuclear spin lattice relaxation rate provide a direct way to study this disorder-induced phenomenon.

3. Angular Dependent Thermal Conductivity

Following the procedure given in Ref. [18], the diagonal components of the thermal conductivity tensor are given by

\[
\frac{\kappa_{zz}}{\kappa_n} = \frac{x}{2 \ln(2/x)} \left( (1 - y^2)^{3/2} - \frac{3y}{2} \left( \cos^{-1} y - y \sqrt{1 - y^2} \right) \right) \theta(1 - y),
\]

\[
\frac{\kappa_{xx}}{\kappa_n} = \frac{3}{2 \ln(2/x)} \left( \frac{x'}{x} \right)^2 \left( \cos^{-1} y' - y' \sqrt{1 - y'^2} \right) \theta(1 - y'),
\]

where \( x' \equiv \sqrt{v_a v_c e H / \sqrt{1 - \sin^2 \theta \cos^2 \phi / 2 \Delta}} \) and \( y' \equiv y_0 / | \sin \phi | \).

FIG. 3: Angular dependent thermal conductivity of a s+g-wave superconductor in a magnetic field. (a) zz-component, and (b) xx-component of the thermal conductivity tensor for various impurity scattering strengths. The polar angle is fixed to \( \theta = \pi / 2 \).

The angular dependence of \( \kappa_{zz} \) and \( \kappa_{xx} \) is shown in Figs. 3(a) and (b). In the limit \( y_0 \to 0 \) Eq. 14 has a similar angular dependence as given in Ref. [9], with the exception of a weak \( \ln x \) correction in the denominator. Moreover the dependence on the impurity scattering strength \( \Gamma \) is similar to the one for the quasiparticle density of states described in the previous section. On the other hand, the structure of the angular dependence of \( \kappa_{xx} \)
described in Eq. 15 is dominated by an inverted cusp centered at $\phi = \pi/2$. Furthermore, we note that for small applied magnetic fields $\kappa_{zz}$ increases like $\sqrt{H}$, whereas $\kappa_{xx}$ remains independent of $H$. The reason for this is that the current operator $\hat{Q}_z$ vanishes at the nodal points in the $k_x - k_y$ plane, whereas $\hat{Q}_x$ is non-zero in the nodal plane. This peculiar effect should be explored experimentally.

We observe that there are a number of similarities of the order parameter of these hybrid s+g-wave compounds with the newly discovered heavy fermion superconductor PrOs$_4$Sb$_{12}$. In particular, the singlet s+g-wave gap function can describe consistently the angular dependent thermal conductivity data for this compound. [20, 21] However, the presence of remnant magnetization observed in muon spin rotation measurements is suggestive of spin triplet pairing. [22] More recently, Chia et al. have reported a surprisingly isotropic superfluid density in the B-phase of PrOs$_4$Sb$_{12}$. [23] It appears that none of the currently proposed models for superconductivity in this material match this experimental data. [24, 25, 26] Clearly, more experimental measurements on this compound are necessary to settle this issue.

4. Concluding Remarks

We have seen that impurity scattering has surprisingly profound effects on s+g-wave superconductors such as YNi$_2$B$_2$C and LuNi$_2$B$_2$C. In particular measurements of the magnetothermal conductivity provide a unique window to observe the disorder induced opening of a gap in the quasiparticle energy through their angular dependence. Furthermore, there is evidence that the skuttertide PrOs$_4$Sb$_{12}$ may also have a hybrid s+g-wave superconducting order parameter. The discovery of these point-node compounds opens up new opportunities to explore unconventional superconductivity.

We thank P. Thalmeier, K. Kamata, K. Izawa, and Y. Matsuda for useful discussions on borocarbide superconductors, and acknowledge financial support by the National Science Foundation, Grant No. DMR-0089882.

[1] K. Izawa et al., Phys. Rev. Lett. 89 137006 (2002).
[2] T. Park et al., Phys. Rev. Lett. 90, 177001 (2003).
[3] M. Nohara et al., J. Phys. Soc. Jpn. 68, 1078 (1999).
[4] L.S. Borkowski and P.J. Hirschfeld, Phys. Rev. B 49, 15404 (1994).
[5] M. Nohara et al., J. Phys. Soc. Jpn. 66, 1888 (1997).
[6] G.-Q. Zhang et al., J. Phys. Chem. Solid 59, 2167 (1998).
[7] K. Izawa et al., Phys. Rev. Lett. 86, 1327 (2001).
[8] K. Maki, P. Thalmeier, and H. Won, Phys. Rev. B 65, 140502 (2002).
[9] P. Thalmeier and K. Maki, Acta Physica Polonica B 34, 557 (2003).
[10] H. Jang, H. Won, and K. Maki, cond-mat/0302103.
[11] I.-S. Yang et al., Phys. Rev. B 62, 1291 (2000).
[12] K. Kamata, Master Thesis, University of Tokyo (2003).
[13] H. Won et al., Brazilian Journal of Physics 33, (2003).
[14] Q. Yuan et al., Phys. Rev. B (in press).
[15] P.A. Lee, Phys. Rev. Lett. 71, 1887 (1993).
[16] Y. Sun and K. Maki, Europhys. Lett. 32, 355 (1995).
[17] G.E. Volovik, JETP Lett. 58, 469 (1993).
[18] H. Won and K. Maki, cond-mat/004105.
[19] H. Won and K. Maki, Europhys. Lett. 56, 729 (2001).
[20] K. Izawa et al., Phys. Rev. Lett. 90, 11701 (2003).
[21] K. Maki et al., Europhys. Lett. (in press).
[22] Y. Aoki et al., Phys. Rev. Lett. 91, 67003 (2003).
[23] E.E. Chia et al., cond-mat/0308454.
[24] M. Ichioka, N. Nakai, and K. Machida, J. Phys. Soc. Jpn. 72, 1322 (2003).
[25] K. Miyake et al., J. Condens. Matter 15, L275 (2003).
[26] J. Goryo, Phys. Rev. B 67, 184511 (2003).