Unconventional superconductivity in YNi$_2$B$_2$C

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Abstract

We use the semiclassical (Doppler shift) approximation to calculate magnetic field angle-dependent density of states and thermal conductivity $\kappa_\Theta$ for a superconductor with a quasi-two-dimensional Fermi surface and line nodes along $k_x = 0$ and $k_y = 0$. The results are shown to be in good quantitative agreement with experimental results obtained for YNi$_2$B$_2$C (Izawa K et al 2002 Phys. Rev. Lett. 89 137006).

1. Introduction

YNi$_2$B$_2$C is a type II superconductor with a relatively high transition temperature $T_c = 15.6$ K [2]. Although initially thought to be a conventional s-wave superconductor, accumulated evidence soon suggested otherwise. Power law behaviour in the heat capacity $C_p/T \propto T^2$ was the first indication that YNi$_2$B$_2$C is an unconventional superconductor with point nodes in the gap function [3, 4]. However, the field dependence of the heat capacity and thermal conductivity was found to be $C_p \propto \sqrt{T}$, indicative of line nodes [1, 4, 5]. The NMR spin relaxation rate $1/T_1$ was measured to be $\propto T^3$ with no Hebel–Slichter peak [6], again consistent with line nodes in the gap function. Finally, Raman scattering showed a peak in the electronic $A_{1g}$ and $B_{2g}$ response [7], possibly indicative of a $B_{2g}$ symmetry gap function. Such a gap function takes the form $\Delta(k) \propto k_x k_y$, and thus has symmetry-required line nodes along $k_x = 0$ and $k_y = 0$ [8, 9]. In contrast to these findings, field-angle-dependent measurements of thermal conductivity and specific heat were claimed to be indicative of point nodes in the gap function [1, 10, 11]. The reconciliation of these results, and hence the symmetry of the gap function, remains an important unresolved issue.

YNi$_2$B$_2$C belongs to the crystallographic space group $I4/mmm$ (No. 139, $D_{4h}^4$) [12]. The lattice is body-centred tetragonal (bct) with $a = 3.526$ Å and $c = 10.543$ Å [3]. According to symmetry analysis for $D_{4h}$ crystals [8, 9], gap functions with line nodes are found only for singlet pairing, while point nodes are found only for triplet pairing. Various nodal configurations can occur, depending on the irreducible representation of $D_{4h}$ by which the superconducting order parameter transforms. Nodes in the gap function are normally detected via quasiparticles (qps) which appear in the vicinity of gap nodes in $k$-space as a result of either finite temperature, impurities or Doppler shift in the presence of an applied magnetic field. In these kinds of measurements, the nodes will be invisible if there is no Fermi surface in the direction of the nodes; thus the shape and connectivity of the Fermi surface plays an important role.

The Fermi level crosses the 17th, 18th and 19th bands. The topology of the Fermi surface is highly sensitive to the precise position of the Fermi level due to a dispersionless band between the $\Gamma$ and $X$ points. Thus different band structure calculations share common features but the resulting Fermi surfaces have significant differences [13–15]. Yamaguchi et al [15] correlated their results with de Haas–van Alphen (dHvA) measurements in order to fix the Fermi energy. The 18th and 19th bands were found to produce closed Fermi surfaces around various points in the Brillouin zone. However, the 17th band produces a large electron Fermi surface multiply connected by necks. Part of this surface appears as dHvA oscillations perpendicular to the $c$ axis. The orbits do not appear to be closed in the $c$ direction; instead, they seem to possess a two-dimensional character that extends in the $c$ direction, as shown by the upward curvature of the dHvA frequencies about the [001] direction, shown in figure 3 of [15].

In the vortex phase of a type II superconductor qps may be either localized about vortex cores or delocalized. It was shown some time ago that the contribution to the low-energy density of states in a superconductor with line nodes comes from delocalized qps in the vicinity of the nodes [16]. The delocalized qps can be treated with a semiclassical (Doppler shift) approximation; this approach provided a good description of field-angle-dependent specific heat and thermal conductivity of the line node.

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superconductors YBa$_2$Cu$_3$O$_{17}$, CeCoIn$_5$, and YNi$_2$B$_2$C. However, Volovik’s argument does not extend to typical point node superconductors for which the gap function vanishes linearly in $k$. For these point node superconductors, the semiclassical calculation may still be performed [20] but, as may be expected, these results are not in agreement with any experiment involving putative point node superconductors so far.

In this paper, we use the semiclassical approximation to calculate the field-angle-dependent density of states and thermal conductivity for a superconductor with line nodes and a quasi-2D Fermi surface, for the purpose of demonstrating that the results of such measurements on YNi$_2$B$_2$C are, in fact, consistent with this scenario, in contrast to what has been claimed [1].

For simplicity, we assume that the Fermi surface has the shape shown in figure 1, for which the qp energy spectrum takes the form

$$\epsilon(k) = \frac{k_z^2 + k_y^2}{2m} + \varepsilon_F \cos ck_z - \varepsilon_F$$  \hspace{1cm} (1)

where $\varepsilon_F' \equiv \frac{k_F^2}{2m} \ll \varepsilon_F$. A gap function with B$_2g$ symmetry has line nodes along $k_y = 0$ and $k_z = 0$. The Fermi momenta along these nodes (parametrized by $k_z$) are

$$k_{F1,3} = (0, \pm (2m(\varepsilon_F - \varepsilon_F' \cos ck_z))^{1/2}, k_F' \sin ck_z)$$
$$\approx (0, \pm k_F, k_F' \sin ck_z)$$  \hspace{1cm} (2)

$$k_{F2,4} = (\pm (2m(\varepsilon_F - \varepsilon_F' \cos ck_z))^{1/2}, 0, k_F' \sin ck_z)$$
$$\approx (\pm k_F, 0, k_F' \sin ck_z).$$  \hspace{1cm} (3)

The magnetic field rotates in the $xy$ plane with an angle $\beta$ with respect to the $x$ axis:

$$H = H(\cos \epsilon, \sin \epsilon, 0).$$  \hspace{1cm} (4)

The supercurrent circulates perpendicular to the field as a function of the distance $r$ from the vortex core and winding angle $\beta$:

$$v_s(r) = \frac{1}{2mr}( - \sin \epsilon \cos \beta, \cos \epsilon \cos \beta, \sin \beta).$$  \hspace{1cm} (5)

The Doppler shifts associated with each line node are $\alpha_i(r) = k_{Fj} \cdot v_s$:

$$\alpha_{1,3}(r) = \frac{1}{2mr}[\pm k_F \cos \epsilon \cos \beta + k_F' \sin \beta \sin ck_z]$$  \hspace{1cm} (6)

$$\alpha_{2,4}(r) = \frac{1}{2mr}[\mp k_F \sin \epsilon \cos \beta + k_F' \sin \beta \sin ck_z].$$  \hspace{1cm} (7)

2. Density of states

In the semiclassical treatment, the argument of Green’s function $i\omega_n$ is replaced by $i\omega_n + \alpha$, where $\alpha$ is the Doppler shift. The quasiparticle energy is $E(k) = \sqrt{\varepsilon^2(k) + \Delta^2(k)}$, which is $\approx \sqrt{\varepsilon_{k1}^2 + \varepsilon_{k2}^2}$ in the vicinity of a node [23]. Here $k_1$ points in the direction of the node, $k_2$ is perpendicular to $k_1$ in the $xy$ plane and the gap velocity is $v_g = \partial \Delta / \partial k_2$. In the vicinity of the $j$th node, Green’s function takes the form

$$G(k, i\omega_n, r) = \frac{i\omega_n + \alpha_j(r) + v_g k_1}{(i\omega_n + \alpha_j(r))^2 + v_g^2 k_1^2 + v_g^2 k_2^2}$$  \hspace{1cm} (8)

where $\omega_n = \pm i\gamma_n$ and $\gamma_n$ is the scattering rate at zero energy. The density of states is

$$N(\omega, r) = -\frac{1}{\pi} \sum_k \text{Im} G(k, \omega, r).$$  \hspace{1cm} (9)

We divide the volume of integration into four curved cylinder-shaped volumes, each centred around a line node on the Fermi surface [23], and perform the integration across the disc spanned by $k_1$ and $k_2$:

$$N(0, r) = \frac{\Gamma_0}{4\pi^3 v_g} \int_{-\beta/2}^{\beta/2} dk_z \int_{-\pi/c}^{\pi/c} dk_y \int_{-\pi/c}^{\pi/c} dk_x$$

$$\times \left[ \ln \frac{p_0}{\sqrt{\alpha_j^2(r) + \Gamma_0^2}} + \alpha_j(r) \tan^{-1} \frac{\alpha_j(r)}{\Gamma_0} \right]$$  \hspace{1cm} (10)

where $p_0$ is the integration cutoff. In the clean limit $|\alpha_j / \Gamma_0| \gg 1$ the density of states is

$$N(0, r) = \frac{1}{4\pi^3 v_g} \int_{-\pi/c}^{\pi/c} dk_z \int_{-\pi/c}^{\pi/c} dk_y \int_{-\pi/c}^{\pi/c} \frac{1}{\alpha_j(r) + |\alpha_j(r)|}$$
$$\times (|\alpha_j(r)| + |\alpha_j(r)|).$$  \hspace{1cm} (11)

Averaging over the vortex cross section, we obtain

$$\langle N(0, r) \rangle_H = \frac{8}{\pi^3 v_g} \frac{1}{\pi R^2} \int_0^2 \frac{2\pi}{r} \frac{d\beta}{\pi} \int_{-\pi/c}^{\pi/c} dk_z \int_{-\pi/c}^{\pi/c} dk_y$$
$$\times (|\alpha_1(r)| + |\alpha_2(r)| + |\alpha_3(r)| + |\alpha_4(r)|).$$  \hspace{1cm} (12)

This leads to the result

$$\langle N(0, r) \rangle_H \approx \frac{8}{\pi^3 v_g} \frac{1}{\pi R} \left[ \sqrt{b^2 + C^2 E \left( \frac{b^2}{b^2 + C^2} \right)} + \sqrt{b^2 + S^2 E \left( \frac{b^2}{b^2 + S^2} \right)} \right]$$  \hspace{1cm} (13)

where $b = v_g / v_g$, $c$ is the lattice constant in the $c$ direction, $C = \cos \epsilon$, $S = \sin \epsilon$ and $E$ is the complete elliptic integral of
the cusp features shown in figure 2 do not appear in \[21\]. Slightly different due to different considerations; in particular, in terms of elliptic integrals. However, their final results are different. Won and Maki \[21\] performed a similar calculation and seen that deviations from the perfectly 2D cylindrical Fermi field.

3. Thermal conductivity

The thermal conductivity tensor is given by the Kubo formula, which is expressed in terms of the imaginary part of Green’s function as

\[
\tilde{\kappa}(0, r) = \frac{k_B^2}{3} \sum_k v_k v_k \text{Tr}[\Im \hat{G}_{\text{rel}}(0, r) \Im \hat{G}_{\text{rel}}(0, r)],
\]

where \(k_B\) is the Boltzmann constant and \(v_F\) is the Fermi velocity in the direction of \(k\). By again dividing the volume of integration into four regions and introducing the integration variable \(p = \sqrt{v_F^2 k_z^2 + v_F^2 k_z^2}\) we find

\[
\tilde{\kappa}(0, r) = \frac{k_B^2}{3} \frac{1}{(2\pi^2 v_F)\sqrt{b^2 + C^2}} \int_0^2 \frac{2\pi}{\Gamma_0^2} \int_0^\pi/c \int_{-\pi/c}^{\pi/c} dk_z \times \sum_{j=1}^4 (v_F v_F)_{j} \left[ (\alpha_j(r) + p)^2 + \Gamma_0^2 \right]^{1/2}
\]

\[
= \frac{k_B^2}{6\pi^2 v_F v_F} \int_{-\pi/c}^{\pi/c} dk_z \times \sum_{j=1}^4 (v_F v_F)_j \times \left( 1 + \alpha_j(r) \left( \tan^{-1} \frac{\alpha_j(r)}{\Gamma_0} - \frac{\pi}{2} \right) \right).
\]

Using (2) and (3), in zero magnetic field we get

\[
\frac{\tilde{\kappa}(0, 0)}{T} = \frac{2k_B^2 v_F}{3\pi^2 v_F} \left( \begin{array}{ccc} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \frac{1}{2} \end{array} \right).
\]

In a finite magnetic field, terms linear in the Doppler shift will vanish upon integration. So the magnetic part of the thermal conductivity is

\[
\frac{\delta\tilde{\kappa}(0, r)}{T} = \frac{k_B^2}{12\pi^2 v_F v_F} \int_{-\pi/c}^{\pi/c} dk_z \times \sum_{j=1}^4 (v_F v_F)_j \frac{|\alpha_j(r)|}{\Gamma_0}.
\]

The integrand is

\[
\frac{v_F}{\Gamma_0} \left( \begin{array}{ccc} |\alpha_1| + |\alpha_2| & |\alpha_3| \\ |\alpha_1| + |\alpha_3| & 0 \\ 0 & 0 \end{array} \right) \frac{\frac{\sqrt{b^2 + C^2}}{b^2 + C^2}}{b^2 + C^2} \left( |\alpha_1| + |\alpha_2| + |\alpha_3| \right)^2 \sin^2 c k_z.
\]

The off-diagonal components vanish in the vortex average and the diagonal components are

\[
\frac{\delta\kappa_{xy}}{T} = \frac{4 k_B^2}{3\pi^2 R\Gamma_0 v_F} \frac{v_F}{\Gamma_0} \left( \begin{array}{ccc} b^2 & b^2 + C^2 \\ b^2 & b^2 + C^2 \end{array} \right)
\]

\[
+ (2b^2 + 2C^2) \left( \begin{array}{ccc} b^2 & b^2 + C^2 \\ b^2 + C^2 & b^2 + C^2 \end{array} \right)
\]

\[
+ \sqrt{b^2 + C^2} \left( \begin{array}{ccc} -2C^2 & b^2 \\ b^2 & C^2 \end{array} \right)
\]

\[
+ \left( b^2 + C^2 \right) \left( \begin{array}{ccc} b^2 & b^2 \\ b^2 & b^2 \end{array} \right).
\]
rotating-field-dependent oscillations in the dirty limit of $\kappa$. Similar to the dirty limit density of states (15), there are no cusps; however, the oscillation amplitude goes to zero. The oscillation amplitude increases rapidly with the average and the diagonal elements are

$$\frac{\delta k(0, r)}{T} = \frac{k_B^2}{6\pi^2 v_F v_g} \int_{-\pi/c}^{\pi/c} dk_z \sum_{j=1}^{4} (v_F v_j) \frac{\alpha_j^2(r)}{\Gamma_0^2}. \quad (26)$$

Again, the off-diagonal components vanish in the vortex average and the diagonal elements are

$$\left\{ \frac{\delta k_{xx}(0, r)}{T} \right\}_H = \frac{k_B^2 v_F^3}{12\pi v_g} \log(R/\xi_0)(2C^2 + b^2) \quad (27)$$

$$\left\{ \frac{\delta k_{yy}(0, r)}{T} \right\}_H = \frac{k_B^2 v_F^3}{12\pi v_g} \log(R/\xi_0)(2S^2 + b^2) \quad (28)$$

$$\left\{ \frac{\delta k_{zz}(0, r)}{T} \right\}_H = \frac{k_B^2 v_F^3}{12\pi v_g} \log(R/\xi_0)(1 + 3b^2/2). \quad (29)$$

Similar to the dirty limit density of states (15), there are no rotating-field-dependent oscillations in the dirty limit of $\kappa_{zz}$.

4. Discussion and conclusions

The topology of the true Fermi surface of YNi$_2$B$_2$C shown in [15] is difficult to discern: however, the validity of our calculation only requires that the Fermi surface exists at the positions of the nodes and spans all or most of the Brillouin zone in the $c$ direction with a slight curvature characterized by the parameter $b$. The main point is that the cusps features observed in the field angle-dependent heat capacity [10] are a feature of line nodes and the cusp features observed in the field angle-dependent thermal conductivity are a feature of line nodes on a quasi-2D Fermi surface.

Alternatively, a scenario involving point nodes that vanish quadratically in $k$, such as that proposed by Maki et al [22], will display the same qualitative features as line nodes on a cylindrical Fermi surface. The thermodynamics are the same and a non-zero Fermi velocity in the $c$ direction in the vicinity of the node is required. A semiclassical treatment of quasiparticles originating from quadratic point nodes does not depend on the shape of the Fermi surface outside the vicinity of nodes. While this scenario does satisfactorily account for experimental observations, it must be noted that, among all possible symmetry-allowed order parameters for a superconductor with $D_{4h}$ symmetry, there are none with symmetry-required quadratic point nodes [8, 9].

In the wake of the Maki et al proposed gap function, several improvements to the semiclassical (Doppler shift) treatment of point node superconductors have been implemented, all of which include realistic anisotropy of the Fermi velocity in the $a$-$b$ plane [24–26]. However, as we now show, our semiclassical results are in reasonable quantitative agreement with experimental results. Using $R \approx 4 \times 10^{-8}$ m (for a 1 T field), $T = 0.56$ K, $E_F = 9$ Ryd [15], $v_F \approx 3 \times 10^5$ m s$^{-1}$, gap maximum $\Delta_0 = v_g k_F = 30$ K and scattering rate $\Gamma_0 = 1$ K leads to an estimate of the prefactor in (25) of $4\pi \frac{\delta k}{\Gamma_0} \approx 10^4$ W K$^{-1}$ m$^{-1}$. The experimentally observed oscillation amplitude is $\approx 2 \times 10^{-2}$ W K$^{-1}$ m$^{-1}$. Comparing with the oscillation amplitudes shown in figure 3, one may deduce that the value of $b$ is approximately 0.02. Such a small value of $b$ produces sharp cusps in the field angle-dependent $\kappa_{zz}$ oscillations and is therefore fully consistent with experiment.

Finally, we comment on the uniqueness of the proposed order parameter, $\Delta \sim k_x k_y$. As we discussed in section 1, and as shown by our calculations of angle-dependent thermal conductivity, most experiments (with the possible exception of early heat capacity measurements) are best explained by a superconducting gap function with line nodes and not point nodes. Moreover, the angular dependence of the thermal conductivity indicates that the nodes are in the directions $k_x = 0$ and $k_y = 0$. Among all possible superconducting order parameters for a crystal with $D_{4h}$ symmetry classified in [8] and [9], the gap function $\Delta \sim k_x k_y$, which belongs to the irreducible representation $B_{2g}$ of the point group $D_{4h}$, is the only one with line nodes in the directions $k_x = 0$ and $k_y = 0$ only.

Thus the most straightforward model that best describes accumulated observations on YNi$_2$B$_2$C is that the superconducting gap function is $\Delta \sim k_x k_y$, which belongs to the irreducible representation $B_{2g}$ of the point group $D_{4h}$, with associated line nodes along $k_x = 0$ and $k_y = 0$. 

![Figure 3](image-url)
References

[1] Izawa K, Kamata K, Nakajima Y, Matsuda Y, Watanabe T, Nohara M, Takagi H, Thalmeier P and Maki K 2002 Phys. Rev. Lett. 89 137006

[2] Cava R J, Takagi H, Zandbergen H W, Krajewski J J, Peck W F Jr, Sigrist T, Batlogg B, van Dover R B, Felder R J, Mizuhashi K, Lee J O, Eisaki H and Uchida S 1994 Nature 367 252

[3] Godart C, Gupta L C, Nagarajan R, Dhar S K, Noel H, Potel M, Mazumdar C, Hossain Z, Levy-Clement C, Schiffmacher G, Padalia B D and Vijayaraghavan R 1995 Phys. Rev. B 51 489

[4] Nohara M, Isshiki M, Sakai F and Takagi H 1999 J. Phys. Soc. Japan 68 1078

[5] Izawa K, Shibata A, Matsuda Y, Kato Y, Takeya H, Hirata K, van der Beek C J and Konczykowski M 2001 Phys. Rev. Lett. 86 1327

[6] Zheng G-Q, Wada Y, Hashimoto K, Kitaoka Y, Asayama K, Takeya H and Kadowaki M 1998 J. Phys. Chem. Solids 59 2169

[7] Yang I-S, Klein M V, Cooper S L, Canfield P C, Cho B K and Lee S-I 2000 Phys. Rev. B 62 1291

[8] Volovik G E and Gor’kov L P 1985 Sov. Phys.—JETP 61 843

[9] Sigrist M and Ueda K 1991 Rev. Mod. Phys. 63 239

[10] Park T, Salammon M B, Choi E M, Kim H J and Lee S-I 2003 Phys. Rev. Lett. 90 177001

[11] Matsuda Y, Izawa K and Vekhter I 2006 J. Phys.: Condens. Matter 18 R705

[12] Siegrist T 1994 Nature 367 254

[13] Lee J I, Zhao T S, Kim I G, Min B I and Youn S J 1994 Phys. Rev. B 50 4030

[14] Singh D J 1996 Solid State Commun. 98 899

[15] Yamaguchi K, Katayama-Yoshida H, Yanase A and Harima H 2004 Physica C 412–414 225

[16] Volovik G E 1993 JETP Lett. 58 471

[17] Aubin H, Behnia K, Ribault M, Gagnon R and Taillefer L 1997 Phys. Rev. Lett. 78 2624

[18] Vekhter I, Hirschfeld P J, Carbotte J P and Nicol E J 1999 Phys. Rev. B 59 R9023

[19] Izawa K, Yamaguchi H, Matsuda Y, Shishido H, Settai R and Onuki Y 2001 Phys. Rev. Lett. 87 057002

[20] Abu Alrub T R and Curnoe S H 2008 Phys. Rev. B 78 104521

[21] Won H and Maki K 2001 Europhys. Lett. 56 729

[22] Maki K, Thalmeier P and Won H 2002 Phys. Rev. B 65 140502

[23] Thalmeier P and Maki K 2003 Acta Phys. Pol. B 34 557

[24] Miranovic P, Ichioka M, Machida K and Nakai N 2005 Phys. Rev. B 71 024511

[25] Udagawa M, Yanase Y and Ogata M 2005 Phys. Rev. B 71 024511

[26] Nagai Y, Kato Y, Hayashi N, Yamauchi K and Harima H 2007 Phys. Rev. B 76 214514

[27] Nagai Y and Hayashi N 2008 Phys. Rev. Lett. 101 097001

[28] Nagai Y, Hayashi N, Kato Y, Yamauchi K and Harima H 2009 J. Phys.: Conf. Ser. 150 052177