Thermal conductivity in B- and C- phase of UPt$_3$

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Although the superconductivity in UPt$_3$ is one of the most well studied, there are still lingering questions about the nodal directions in the B and C phase in the presence of a magnetic field. Limiting ourselves to the low temperature regime ($T \ll \Delta(0)$), we study the magnetothermal conductivity with in semiclassical approximation using Volovik’s approach. The angular dependence of the magnetothermal conductivity for an arbitrary field direction is calculated for both phases. We show that cusps in the polar angle dependence appear in B and C phases which are due to the polar point nodes.

PACS numbers: 74.20.Rp, 74.25.Fy, 74.70.Tx

I. INTRODUCTION

Perhaps due to the exceptional appearance of two superconducting (sc) transitions with two associated critical field curves, UPt$_3$ is one of the most well studied Heavy Fermion superconductors. The history of this subject was described in Ref.$^1$. The T linear dependence of the low temperature thermal conductivity both parallel to the c axis and the a axis was in favor of the $E_{2u}$ rather than $E_{1g}$ type sc order parameter.$^2$ Further Pt- NMR experiments confirmed the triplet nature of the superconductivity and the details of the triplet gap function $d\; (k)$ n A, B, and C- phases were determined.$^3$ This assignment of the spin configuration is consistent with the weak spin-orbit coupling limit also assumed here. $H_{c2}$ along the c axis requires a strong Pauli limiting effect. This favors strong spin orbit coupling but then $H_{c2}$ results are inconsistent with the NMR data. We assume that $d\; (k)$=$\Delta(k)z$ to be weakly pinned along c. Then the $E_{2u}$ gap functions of for the low temperature B and C phases of UPt$_3$ are given by

\[
B : \Delta(\vartheta, \varphi) = \frac{3}{2} \sqrt{3} \Delta \cos \vartheta \sin^2 \vartheta \exp(\pm 2i\varphi) \\
C : \Delta(\vartheta, \varphi) = \frac{3}{2} \sqrt{3} \Delta \cos \vartheta \sin^2 \vartheta \cos(2\varphi)
\]  

(1)

Here $\vartheta$, $\varphi$ are the polar and azimuthal angles of $k$. The angular dependence of $\Delta(\vartheta, \varphi)$ is shown in Fig.$^1$. In the B- phase the poles are second order node points and the equator is a node line. In the C- phase two additional vertical nodal lines appear at 45 degrees away from the vertical plane containing $H$. The thermal conductivity in the vortex phase for field along the symmetry axis also decided in favor of the $E_{2u}$ state and against the $E_{1g}$-state.$^4$ This is reviewed in.$^5$ The angular dependent thermal conductivity has been measured in.$^6$ and analyzed in.$^7$. Unfortunately the experiment was done for $T$>0.3 K which is not sufficiently low to determine node structures. Recently we have been studying the thermal conductivity in nodal superconductors (B and C). In particular we shall restrict to the low temperature limit $T \ll \tilde{\nu} \sqrt{\epsilon H} \ll \Delta(0)$ and the superclean limit $(\Gamma \Delta)^{\frac{1}{2}} \ll \tilde{\nu} \sqrt{\epsilon H}$, where $\tilde{\nu}$ =$(v_{u}.v_{c})^{\frac{1}{2}}$, $\Gamma$ is the scattering rate and $v_{u,c}$ are the anisotropic Fermi velocities. The condition $\tilde{\nu} \sqrt{\epsilon H} \ll \Delta(0)$ can be satisfied in the B- phase while $\tilde{\nu} \sqrt{\epsilon H} \leq \Delta(0)$ in the C- phase since the latter appears only for $H \geq 0.6$ T and $H \geq 1.2$ T for field along a and c respectively. Our results in the C- phase may therefore only have qualitative significance. Restriction to the superclean limit does not influence the main conclusions on the connection between node topology and magnetothermal conductivity. We first examine the quasiparticle DOS and the thermodynamic properties of the B and C phase of UPt$_3$ in the presence of a magnetic field with arbitrary orientation at low temperatures. Then we study the thermal conductivity in the B and C phase in the low temperature regime which provides clear evidence for the nodal positions in $\Delta(k)$. In this regime the influence of the AF order in UPt$_3$ may be neglected contrary to the A- phase regime.

II. DENSITY OF STATES AND THERMODYNAMICS

The quasiparticle DOS in the vortex state of UPt$_3$ is given by

\[
g(0) = \text{Re}\left(\frac{C_0 - ix}{\sqrt{(C_0 - ix)^2 + f^2}}\right)
\]

(2)

Where the brackets denote both Fermi surface and vortex lattice average. With the form factor $f_B(x)=\frac{2}{\sqrt{2}}(1-x^2)z$ and $f_C(x,z')=(2z'^2-1)f_B(z)$ ($z'=\cos \vartheta, z'=\cos \varphi$) for B and C- phase respectively the average may be computed and one obtains

\[
g_B(0) = \frac{1}{\sqrt{3}} \left(\frac{\pi}{2} x + C_0(\ln(\frac{C_0}{x}) - 1)\right)
\]

\[
g_C(0) = \frac{1}{\sqrt{3}} \left(\frac{\pi}{2} x \ln\left(\frac{2}{x}\right) + \frac{2}{\pi} C_0(\ln^2\frac{2}{x})\right)
\]

(3)
where \( x = \frac{\nu c}{v a} \) is the normalized Doppler shift of quasiparticle energies, \( C_0 = \lim_{\omega \to 0} \text{Im}(\omega/\Delta) \) and \( \bar{w} \) is the renormalized quasiparticle energy in the presence of impurity scattering. Furthermore \( v \) is the quasiparticle velocity and \( 2q \) is the pair momentum around the vortex. Following Volovik we obtain

\[
\langle x \rangle_B = \frac{2}{\pi} \sqrt{\frac{eH}{\Delta}} I_B(\theta)
\]

\[
\langle x \ln(x) \rangle_C = \frac{2}{\pi} \sqrt{\frac{eH}{\Delta}} I_C(\theta) \ln\left(\frac{\Delta}{\sqrt{eH}}\right)
\]

\[
I_B(\theta) = \alpha \sin \theta + \frac{2}{\pi} E(\sin \theta)
\]

\[
I_C(\theta) = I_B(\theta) + I(\theta)
\]

where \( E(\sin \theta) \) is the complete elliptic integral of the second kind. Furthermore we used the definition

\[
I(\theta) = \frac{1}{\sqrt{1 - \alpha^2 \sin^2 \theta}} + 2 \alpha \sin \theta
\]

where \( \alpha = v_c/v_a \) is the anisotropy of Fermi velocities and \( \theta \) is the polar angle of \( \mathbf{H} \) with respect to \( c \) axis. The averages in Eq. (4) are evaluated by replacing the \( k \) space integration by a summation over nodal positions and then integrating out the superfluid velocity field. We assume a square vortex lattice for simplicity, a hexagonal lattice would lead to an additional numerical factor 0.93.

Substituting Eq. (3) into Eq. (3) we obtain

\[
g_B = \frac{1}{\sqrt{3}} \frac{\bar{\nu} \sqrt{eH}}{\Delta} I_B(\theta)
\]

\[
g_C = \frac{2}{\pi \sqrt{3}} \frac{\bar{\nu} \sqrt{eH}}{\Delta} I_C(\theta) \ln\left(\frac{\Delta}{\sqrt{eH}}\right)
\]

In addition we have \( C_0 = \frac{\bar{\nu}}{\gamma} |g(0)|^{-1} \). The low temperature specific heat, the spin susceptibility etc. are given by

\[
\frac{C_s}{\gamma_N T} = \frac{\chi_s}{\chi_N} = 1 - \frac{\rho_s(H)}{\rho_s(0)} = g(0)
\]

where \( \rho_s \) is the superfluid density. The \( \theta \)-dependence of \( g(0) \) for B- and C- phases is shown in Figs. 2 and 3 respectively.

III. THERMAL CONDUCTIVITY IN THE VORTEX PHASE

The thermal conductivity tensor in the vortex phase depends on the angles \( (\theta, \phi) \) of \( \mathbf{H} \) due to the angle dependence of the Doppler shift energy \( \Delta x \). Here \( \phi \) is the azimuthal angle between \( \mathbf{H} \) and the direction of the heat current \( I_0 \) in the \( ab \) plane. Following Carter we obtain for the B- phase

\[
\begin{align*}
\kappa_{zz} &= \frac{2}{3} \frac{\nu_c \nu_a}{\Delta^2} (eH) I_B(\theta) F_{zz}^B(\theta)
\kappa_{xx} &= \frac{1}{3} \frac{\nu_c^2}{\Delta^2} (eH) I_B(\theta) F_{xx}^B(\theta)
\kappa_{xy} &= \frac{1}{3} \frac{\nu_c^2}{\Delta^2} (eH) I_B(\theta) F_{xy}^B(\theta)
\end{align*}
\]

\[
F_{zz}^B(\theta, \phi) = \sin \theta
\]

\[
F_{xx}^B(\theta, \phi) = \left[ \sin^2 \phi E(\sin \theta) + \cos(2\phi) \right] \frac{1}{3 \sin^2 \theta} \left[ \cos^2 \phi K(\sin \theta) - \cos(2\phi) E(\sin \theta) \right]
\]

FIG. 2. Polar field angle dependence of \( I_B(\theta) \) and \( I_B(\theta) F_{ij}^B(\theta, 45) \) \((ij = xx, zz, xy)\) which determine the \( \theta \)-dependence of DOS \( g(0) \), thermal conductivities \((\kappa_{xx}, \kappa_{zz})\) and thermal Hall coefficient \((\kappa_{xy})\) respectively.

The thermal Hall coefficient in the B- phase is obtained as

FIG. 1. Spherical plots of \( |\Delta(\theta, \varphi)| \) for B phase (left) and C phase (right). For the C- phase two additional vertical nodal planes appear an angle \( \frac{\pi}{2} \) away from the vertical plane which contains \( \mathbf{H} \) assumed at \( \phi = \frac{\pi}{4} \).
\[ \frac{\kappa_{xy} \phi}{\kappa_n} = -\frac{v_0^2(eH)}{3\Delta^2} I_B(\theta) F_{B}^{xy}(\theta, \phi) \]

\[ F_{B}^{xy}(\theta, \phi) = \frac{2 \sin(2\phi)}{3 \sin^2 \theta} \left[ (2 - \sin^2 \theta)E(\sin \theta) - 2 \cos^2 \theta K(\sin \theta) \right] \]

The \( \theta \)- and \( \phi \)- angle dependences of \( \kappa_{ij} \) (\( ij=xx,zz,xy \)) in the B-phase are shown in Fig. 2 and Fig. 4. For heat current along \( c \) (\( \kappa_{zz} \)) no \( \phi \)-dependence appears.

In the limit \( \theta = \frac{\pi}{2} \), \( I_B(\frac{\pi}{2}) = \alpha + \frac{2}{\pi} \) and then

\[ \kappa_{xx} \sim \frac{1}{(1 - \frac{2}{3} \cos(2\phi))}; \quad \kappa_{xy} \sim \frac{2}{3\pi} \sin(2\phi) \]  

The maximum in \( \kappa_{xx}(90, \phi) \) at \( \phi = \pm 90 \) occurs for heat current \( \perp \mathbf{H} \) when the Doppler shift gives rise to the largest quasiparticle DOS parallel to the heat current and we have \( \kappa_{xx}(\phi = 90)/\kappa_{xx}(\phi = 0) = 2 \).

Now we consider the C-phase. Again \( \kappa_{zz} \) does not exhibit a \( \phi \)-dependence. The C-phase according to Eq. 11 has two additional perpendicular node lines. Rotating the field at a given \( \theta \) around \( c \) (i.e. changing \( \phi \)) will lead to a co-rotation of these node lines such that the vertical plane containing \( H \) always stays at half angle between the two perpendicular planes of the node lines parallel to \( \mathbf{H} \) (see inset of Fig. 3). Consequently \( \kappa_{zz}(\theta) \) will again be independent of \( \phi \) while \( \kappa_{xx}(\theta, \phi) \) depends on both field angles. We find for heat current along \( c \):

\[ \frac{\kappa_{zz}}{\kappa_n} = \frac{1}{\kappa_n} \left( \frac{v_0^2(eH)}{6\Delta^2} I_C(\theta) F_C^{zz}(\theta, \phi) \right) \ln^2 \left( \frac{\Delta}{\sqrt{v_0 eH}} \right) \]

\[ F_C^{zz}(\theta, \phi) = \frac{2 \sin(2\phi)}{\sin^2 \theta} \int_{-1}^{1} dz |z| \left( 1 + \cos^2 \theta \right) (1 - z^2) + \frac{3}{2} \sin^2 \theta \frac{1}{2} \left( 1 + \cos^2 \theta \right) (1 - z^2) \]  

On the other hand we obtain for heat current along \( a \):

\[ \frac{\kappa_{xx}}{\kappa_n} = \frac{1}{\kappa_n} \left( \frac{v_0^2(eH)}{3\Delta^2} I_C(\theta) F_C^{xx}(\theta, \phi) \right) \ln^2 \left( \frac{\Delta}{\sqrt{v_0 eH}} \right) \]

\[ F_C^{xx}(\theta, \phi) = F_{B}^{xx}(\theta, \phi) + \frac{\sqrt{2(1 + \cos^2 \theta)}}{\kappa_n} \]  

As is readily seen \( \kappa_{zz} \) depends only on \( \theta \), while \( \kappa_{xx} \) depends both on \( \theta \) and \( \phi \). Both angular dependences are shown in Fig. 3 and Fig. 4 respectively.

FIG. 3. Polar field dependence of \( I_C(\theta) \) and \( I_C(\theta) F_C^{xx}(\theta, 45) \) (\( ij=xx,zz,xy \))

FIG. 4. Azimuthal field dependence of \( I_C(\theta) F_C^{yy}(\theta, \phi) \) for various \( \theta \). For \( \theta \to 0 \) the \( \phi \)-dependence is suppressed completely. The \( xx \)-component is always \( \phi \)-independent.

In both B and C phase \( \kappa_{ij} \) (\( ij=xx,zz \)) and also the specific heat which is determined by \( I_{B,C} \) exhibit clear cusps at the poles \( \theta = 0 \) (and \( \theta = \pi \)) caused by the contributions from the respective second order node points which are present in both B and C phase. This is very similar to what has been recently observed and analyzed in YNi_2B_2C [1]. There the second order node points lie along the equator and hence the cusps appear as function of \( \phi \). The most significant difference in the B- and C-phase results can be seen in the behaviour of \( \kappa_{zz} \) for small polar angle \( \theta \). While in the B-phase it approaches zero it remains finite in the C-phase. Furthermore the \( \kappa_{xx} - \kappa_{zz} \) anisotropy for \( \theta = \frac{\pi}{2} \) is considerably smaller in the C-phase as compared to the B-phase. In both B- and C-phase the \( xx \)-component exhibits nonmonotonic behaviour as function of \( \theta \).

The thermal Hall coefficient in the C-phase reads

\[ \frac{\kappa_{xy}}{\kappa_n} = \frac{1}{\kappa_n} \left( \frac{v_0^2(eH)}{3\Delta^2} I_C(\theta) F_C^{xy}(\theta, \phi) \right) \ln^2 \left( \frac{\Delta}{\sqrt{v_0 eH}} \right) \]

where \( F_C^{xy}(\theta, \phi) \) holds because the contributions from perpendicular node lines with \( H \) lying at half angle in between cancel and so as in the B-phase one is left with polar and equatorial contributions to the thermal Hall constant. For numerical calculations we used the anisotropy ratio \( \alpha = \frac{\kappa_{xx}}{\kappa_{yy}} = 1.643 \). It can be directly obtained from experimental anisotropies of thermal and electrical conductivities \( \frac{\sigma_{xx}}{\sigma_{yy}} = 2.7 \) which are equal to \( \alpha^2 \).
anisotropy for \( H \) occurs even for \( \theta \) along the nodal direction (both B- and C- phase). ii) in the C- phase for heat current \( j_Q \) the contribution vanishes. iii) the \( v \) dependence which will help to identify the nodal directions in \( \Delta(k) \) to verify the predictions of the commonly discussed \( E_{2u} \) model for the gap function in B and C phases. Most significantly we predict that i) cusps appear in the thermal conductivity and specific heat for \( \theta = 0 \) (and \( \theta = \pi \)) due to the polar point nodes of UPt\(_3\) in both B- and C- phase. ii) in the C- phase for heat current along the nodal direction (\( \phi = \frac{\pi}{2} \)) a finite \( \kappa_{zz}(\theta, \frac{\pi}{2}) \) occurs even for \( \theta \rightarrow 0 \) which is caused by the contribution from the additional perpendicular node regions. For the B-phase this contribution vanishes. iii) the \( \kappa_{xx} - \kappa_{zz} \) anisotropy for \( H \) in the ab-plane (\( \theta = \frac{\pi}{2} \)) is considerably larger in the B-phase as compared to C-phase. This is again caused by the perpendicular node lines which contribute and enhance \( \kappa_{xx} \) only for the C-phase. We hope that these different features in the field-angle dependent thermal conductivity tensor above and below the critical field of the B-C transition will resolve a part of the remaining controversy surrounding \( \Delta(k) \) in UPt\(_3\). We recall that thermal conductivity experiments have been very useful to identify \( \Delta(k) \) in unconventional superconductors. For example Izawa et al have succeeded in identifying \( \Delta(k) \) in Sr\(_2\)RuO\(_4\), \( \text{CeCoIn}_5 \), organic salts\(^\text{11}\) and more recently YNi\(_2\)B\(_2\)C\(^\text{22}\). Indeed the thermal conductivity appears to provide a unique window to access the nodal structure in unconventional superconductors.

**IV. CONCLUDING REMARKS**

We have found that in UPt\(_3\) at low temperatures (i.e. \( T \ll \sqrt{cH} \)) and in the superclean limit ((\( \Gamma \Delta \)) \( \ll \sqrt{cH} \)), the thermal conductivity exhibits clear angular dependence which will help to identify the nodal directions in \( \Delta(k) \) and to verify the predictions of the commonly discussed \( E_{2u} \) model for the gap function in B and C phases. Most significantly we predict that i) cusps appear in the thermal conductivity and specific heat for \( \theta = 0 \) (and \( \theta = \pi \)) due to the polar point nodes of UPt\(_3\) in both B- and C-phase. ii) in the C-phase for heat current along the nodal direction (\( \phi = \frac{\pi}{2} \)) a finite \( \kappa_{zz}(\theta, \frac{\pi}{2}) \) occurs even for \( \theta \rightarrow 0 \) which is caused by the contribution from the additional perpendicular node regions. For the B-phase this contribution vanishes. iii) the \( \kappa_{xx} - \kappa_{zz} \) anisotropy for \( H \) in the ab-plane (\( \theta = \frac{\pi}{2} \)) is considerably larger in the B-phase as compared to C-phase. This is again caused by the perpendicular node lines which contribute and enhance \( \kappa_{xx} \) only for the C-phase. We hope that these different features in the field-angle dependent thermal conductivity tensor above and below the critical field of the B-C transition will resolve a part of the remaining controversy surrounding \( \Delta(k) \) in UPt\(_3\). We recall that thermal conductivity experiments have been very useful to identify \( \Delta(k) \) in unconventional superconductors. For example Izawa et al have succeeded in identifying \( \Delta(k) \) in Sr\(_2\)RuO\(_4\), \( \text{CeCoIn}_5 \), organic salts\(^\text{11}\) and more recently YNi\(_2\)B\(_2\)C\(^\text{22}\). Indeed the thermal conductivity appears to provide a unique window to access

**Acknowledgement**

We would like to thank Koichi Izawa and Yuji Matsuda for useful discussions.

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