On the gap structure of UPt$_3$: phases A and B

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Abstract

We have used thermal conduction and transverse sound attenuation to probe the anisotropy of the gap structure in two superconducting phases of UPt$_3$. For the low-temperature phase B, transverse sound has in the past provided strong evidence for a line node in the basal plane. Now, from the anisotropy of the thermal conductivity we further establish the presence of a node along the c-axis and provide information on its k-dependence. For the largely unexplored high-temperature phase A, our study of the attenuation for two directions of the polarization yields directional information on the quasiparticle spectrum, and the first clear indication of a different gap structure in the two phases.

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1. Introduction

The past decade has seen a tremendous interest in novel superconductors: low dimensional organic compounds, high $T_c$ cuprates and heavy fermion metals [1]. In all of these, the superconducting order parameter is thought to be unconventional, that is not to have the standard s-wave symmetry. A typical consequence of non-s-wave symmetry is a gap structure which goes to zero at certain points on the Fermi surface. A precise determination of the position of such nodes, the topology of the gap in their vicinity and its actual symmetry continue to be one of the central pursuits in the field.

In this paper, we focus on the heavy-fermion compound UPt$_3$, where the case for an unconventional superconducting state is compelling: at ambient pressure and zero magnetic field, the onset of superconductivity at $T_c^+ = 0.5$ K is followed by a second transition at $T_c^- = 0.44$ K, as seen in the specific heat shown in Fig. 1 [2]. The phases above and below $T_c^-$ are called A and B, respectively. Two related questions arise: 1) how do the order parameters in phases A and B differ? 2) which of the several theoretical scenarios proposed for the superconducting phase diagram is correct (if any) [1]?

We have used the propagation of heat and sound to address the first question, and thereby touch on the second. By virtue of their directional nature, these two complementary probes can provide direct information about the anisotropic gap structure in UPt$_3$. Details of the experiments can be found in Refs. [3,4].

2. Results

The crystal structure of UPt$_3$ is hexagonal, and electron transport in the normal state is anisotropic with respect to the c-axis. The electrical resistivity and thermal conductivity below 0.8 K obey respectively $\rho(T)=\rho_0+AT^2$ and $\kappa_N(T)=T[a+bT^2]^{-1}$, with $\rho_0=0.23$ (0.61) $\mu\Omega$ cm, $A=0.59$ (1.60) $\mu\Omega$ cm K$^{-2}$, $a=0.09$ (0.25) m K$^2$ W$^{-1}$ and $b=0.37$ (1.0) m W$^{-1}$, for a current parallel (perpendicular) to the c-axis [3]. This implies that: 1) elastic defect scattering in our crystals is low, 2) the Wiedemann-Franz law is verified ($\rho_0/a=L_0=(\pi k_B/e)^2/3$),
3) inelastic (electron-electron) scattering exceeds elastic scattering just above $T_c$, 4) the anisotropy of $\rho$ and $\kappa$ is independent of temperature, being the same for elastic and inelastic scattering, 5) the anisotropy is the same for transport of heat and charge, with conduction along the c-axis being 2.7 times better. The normal state is seen to have the characteristics of a Fermi liquid with an anisotropy of 2.7 in the average Fermi velocity (or mass).

The thermal conductivity is shown in Fig. 1. With decreasing temperature, the normal state $\kappa/T$ increases and the anisotropy is constant. At $T_c^+$, and with the subsequent growth of the condensate, the number of quasiparticles decreases and $\kappa/T$ goes down dramatically. Therein lies some fruitful information about the structure of the gap in the excitation spectrum which we discuss in the next section. Note that the development of an additional anisotropy in the superconducting state is unambiguous evidence for an anisotropic gap.

The first direct evidence of gap anisotropy in UPt$_3$ came from measurements of the attenuation $\alpha_{q\epsilon}(T)$ of transverse sound propagating in the basal plane ($q//a,b$) where two different temperature dependences were observed for a polarization $\epsilon$ parallel and perpendicular to the c-axis [5]. In these early measurements, a crystal with a single broad transition was used, so that no information was obtained about the A-phase. Recently, we repeated the measurement on a crystal with two well-defined transitions at $T_c^-=435$ mK and $T_c^+=495$ mK [4]. The results are shown in Fig. 1. For phase B, they agree well with the early data. The behaviour characteristic of phase A is now revealed, thanks to the high sensitivity of transverse sound attenuation to the opening of the gap. The main finding is the clear difference in the response of the two phases, which represents the first direct evidence for a change of superconducting order parameter at $T_c^-$.

3. Discussion

A knowledge of the gap structure can lead to the group representation of the order parameter which, in UPt$_3$, would allow one to discriminate between the various phenomenological models for the phase diagram. Depending on the model, the order parameter will belong to
either a one-dimensional ($A_1, A_2, B_1, B_2$) or a two-dimensional representation ($E_1, E_2$) of the hexagonal group, and have either even (g) or odd (u) parity [1].

While there is no consensus at present on the correct theory of transport in unconventional superconductors, a generalization of the standard (s-wave) theory to account for unconventional gap structures which treats impurity scattering in the unitary limit is being actively applied to high $T_c$ cuprates and heavy fermion compounds (see Refs. [6–8], and references therein). Thermal properties such as $\kappa(T)$ and $\alpha(T)$ calculated within any theory will depend on the complex topology of the Fermi surface and the microscopic pairing interaction. However, as argued by Graf et al. [8], there is a ‘diagnostic regime’ at low temperature where only a knowledge of the asymptotic topology of the gap at the nodes is needed. For that regime, it should be reasonable to approximate the Fermi surface by an ellipsoid (however, see Ref. [6]).

Within a simplified picture of a single ellipsoidal Fermi surface with a mass ratio of 2.7 and perfect uniaxial symmetry about the c-axis, the magnitude of the gap can only depend on the polar angle $\theta$. A general gap will be a linear combination of ellipsoidal harmonics $Y_{LM}$ each of which vanishes for one or more values of $\theta$ (except $Y_{00}$). The nodes can therefore be points at the poles ($\theta=0$), a line around the equator ($\theta=90^\circ$), two lines above and below ($\theta=90^\circ \pm \theta_0$) the equator, or a combination of these basic elements (see Ref. [8]). The five lowest harmonics have the following structure: $Y_{00} \sim \text{constant} \quad (\text{‘s-wave’}), \quad Y_{10} \sim \cos \theta \quad (\text{‘polar’}), \quad Y_{11} \sim \sin \theta \quad (\text{‘axial’}), \quad Y_{20} \sim (\cos^2 \theta - 0.15) \quad (\text{‘tropical’, since } \theta_0=23^\circ), \quad Y_{21} \sim \sin \theta \cos \theta \quad (\text{‘hybrid’}).$ The asymptotic behaviour of the axial gap near the poles, for example, is linear ($\sin \theta \sim \theta$ for $\theta < 20^\circ$ or so) and therefore the diagnostic regime corresponds approximately to $k_B T < \Delta(\theta=20^\circ)$, which translates roughly as $T/T_c < 0.3$.

At the lowest temperatures, the theory universally predicts the existence of impurity-induced low-energy quasiparticle excitations giving rise to a ‘gapless regime’, which corresponds approximately to $k_B T < 2\hbar \Gamma_0$ [6–8], where $\Gamma_0$ is the impurity scattering rate. In our crystals, it appears that $\Gamma_0=0.05(k_B/\hbar)T_c^-$ or less [3], so that $T/T_c^- < 0.1$.

At present, the theory is inadequate in treating electron-electron scattering, and a mean-
ingful comparison with experiment should be limited to the ‘elastic regime’. For our UPt3 crystals, this implies $T/T_c < 0.3-0.4$.

**Phase B**

By concentrating on the interval $0 < T < 0.3 T_c$, we can hope for a powerful diagnostic on the nodal structure of phase B, free of the complicating effects of electron interactions and gaplessness.

The rise in $\kappa/T$ and $\alpha$ from T=0 for a heat current and a sound polarization perpendicular to the c-axis is much more rapid than in conventional superconductors. In particular, the linear behaviour of $\alpha(T)$ roughly down to $T/T_c = 0.1$ is strong evidence for a gap vanishing in (or near) the basal plane. For a uniaxial gap structure, this means a line node around (or near) the equator. Note that because transverse sound is mostly attenuated by quasiparticles with wavevectors neither perpendicular to $\mathbf{q}$ nor to $\epsilon$, $\alpha_{ac}$ does not pick out this line node very much. Moreover, neither $\alpha_{ac}$ nor $\alpha_{ab}$ are expected to be very sensitive to possible nodes along the c-axis. As a result, transverse sound in the B-phase of UPt3 has been qualitatively interpreted as evidence for a gap with a line node in the basal plane. This eliminates 2 of the 5 gaps listed above. Indeed, neither the s-wave gap nor the axial gap vanish in (or near) the basal plane. Whether the data can allow one to distinguish between the polar gap and a hybrid gap, for example, requires a model calculation. It is clear, though, that transverse sound is not ideal for probing the gap near $\theta=0$.

In this respect, the conduction of heat is better suited, being dominated by quasiparticles travelling in the forward direction. For example, the presence of a node at $\theta=0$ will enhance the quasiparticle current along the c-axis in a hybrid gap relative to the polar gap. This possibility is best investigated with the anisotropy ratio $\kappa_c/\kappa_b$, plotted in Fig. 2. The striking result is that $\kappa_c/\kappa_b$ extrapolates to a finite value at T=0, about half that of the normal state. By inspection, one can deduce the limiting value of $\kappa_c/\kappa_b$ as $T \to 0$ for 3 of the 5 gaps above: the s-wave with $\Delta_c > \Delta_b$ and the polar gap must go to zero, the s-wave with
$\Delta_c < \Delta_b$ and any axial gap to infinity [3]. Hence, the anisotropy of heat conduction not only confirms that the gap of phase B is most definitely not s-wave or axial, but it also shows quite straightforwardly that it is not polar. Of particular interest are the two lowest hybrid gaps ($\sim \sin^n \theta \cos \theta$, $n=1,2$), because they correspond to two of the states most often postulated for phase B [1]. They belong respectively to the $E_{1g}$ and $E_{2u}$ representation and their overall structures are very similar except near the poles, where the gap opens up linearly in $E_{1g}$ and quadratically in $E_{2u}$ [3][4]. Since the density of states $N(E) \sim E$ for a line node or a quadratic point node, while $N(E) \sim E^2$ for a linear point node, it is natural to expect $\kappa_c/\kappa_b$ to remain finite as $T \to 0$ in $E_{2u}$ and go to zero in $E_{1g}$, as first shown by Fledderjohann and Hirschfeld [7].

In Fig. 2 we compare the data with calculations using resonant impurity scattering with $\Gamma_0 = 0.05T_c^-$, for the two hybrid gaps. The basic gaps $Y_{21}$ and $Y_{32}$ (the lowest harmonics allowed by symmetry) are mixed with a small amount of the next harmonics of the same symmetry to optimize the fit [3]. $\kappa_b/T$ is well reproduced by the calculation for both gaps. It is along the c-axis that the gaps differ and the disparity in the behaviour of the two gaps is dramatically brought out by looking at the ratio of $\kappa_c/\kappa_b$. The data for $\kappa_c/\kappa_b$ is almost flat and extrapolates to a value of 0.4 to 0.5 at $T=0$, as also found by Huxley et al. [4], something which the $E_{2u}$ gap can easily reproduce. On the other hand, the $E_{1g}$ gap above the gapless regime is qualitatively different, being characterized by a smooth extrapolation to zero. If the gapless regime is suppressed by reducing $\Gamma_0$, the calculated ratio does eventually go to zero [3][4], as expected on simple grounds of topology. We conclude that the anisotropy of heat conduction favours a hybrid gap of $E_{2u}$ symmetry over one of $E_{1g}$ symmetry for phase B of UPt$_3$, at least within our ellipsoidal model.

**Phase A**

Let us now turn to phase A, for which very little is known as a result of its limited range in temperature. The most significant information comes from the transverse ultrasound
attenuation data [4], shown in Fig. 1. As may be seen, $\alpha_{ab}$ drops initially with decreasing temperature before becoming roughly constant, while $\alpha_{ac}$ only has a slight "bump" seemingly superimposed on the sharply falling attenuation observed in the B-phase. Qualitatively, this implies that more quasiparticles exist in phase A than would be present if phase B extended up to the same temperature. Furthermore, it appears that these extra excitations preferentially scatter sound when the polarization is in the basal plane. To see this we plot, in Fig. 3, the data of Fig. 1 normalized to the attenuation at either $T_c^+$ or $T_c^-$ as a function of temperature normalized to the appropriate critical temperature. This allows us to compare, say, the B-phase attenuation (for either polarization) with the attenuation in the A-phase over the same reduced temperature range. It is evident that $\alpha_{ab}$ is much enhanced in the A-phase as compared to the B-phase. The data for the c-axis polarization, $\alpha_{ac}$, however, are roughly equal in the two phases.

The data contain precise information on the momentum space distributions of quasiparticles, and thus on the gap structure. Because we are not in the 'diagnostic regime', such information can only be extracted by comparison with complete calculations, analogous to those for the thermal conductivity. It must be stressed, however, that quantitative interpretations of the A-phase data assuming a specific gap must carefully consider the effect of quasiparticle-quasiparticle interactions, since the structure and evolution of the gap at high temperatures affect the quasiparticle density and therefore the magnitude of the inelastic scattering. We emphasize, however, that while changes in inelastic scattering due to superconductivity might affect the size of the observed anisotropy, this anisotropy still derives from that of the gap and thus reflects the symmetry of the order parameter.

We therefore conclude from the observed difference in the anisotropy of the two phases, that the order parameter associated with phase A must change upon going into phase B. This is the first solid evidence for a transition between two distinct superconducting states at $T_c^-$. 
Conclusions

In summary, measurements of the thermal conductivity of UPt$_3$ down to T$_c$/10 have shed light on the nodal structure of the gap function in the low-temperature phase B. The unusual observation of a finite value for the anisotropy ratio $\kappa_c/\kappa_b$ as $T \to 0$ leads to new information: the gap vanishes along the c-axis, and it does so with a special angular dependence compatible with E$_{2u}$ but not with E$_{1g}$ symmetry, within an ellipsoidal model for the Fermi surface, as confirmed by calculations based on resonant impurity scattering [6].

The attenuation of transverse ultrasound in a crystal of UPt$_3$ with two well-defined transitions at $T_c^-$ and $T_c^+$ shows the gap structure of phase A to be qualitatively different to that of phase B, with a significant directionally-dependent enhanced density of quasiparticles. In combination with resonant impurity scattering calculations which take into account the normal state properties and the electron-electron interactions, these data should provide some of the first constraints on the symmetry of the A-phase.

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FIGURES

FIG. 1. Thermal properties of UPt$_3$ in phases A and B of the superconducting state, normalized to their value in the normal state (at 0.53 K). Top panel: specific heat divided by temperature, showing the two distinct transitions at $T_c^-=435$ mK and $T_c^+=495$ mK (vertical dashed lines) [2]. Middle panel: thermal conductivity divided by temperature for a heat current both parallel and perpendicular to the hexagonal axis, showing the appearance of additional anisotropy below $T_c^-$ [3]. Bottom panel: attenuation of transverse ultrasound propagating in the basal plane for a polarization both parallel and perpendicular to the hexagonal axis, showing a distinct change in going from phase A to phase B [4].

FIG. 2. Top panel: low-temperature thermal conductivities along axes c ($\kappa_c$; open circles) and b ($\kappa_b$; solid circles) vs reduced temperature and normalized to 1 at $T_c^-$ [3]. Bottom panel: the anisotropy ratio $\kappa_c/\kappa_b$. The data are compared with calculations [6] for hybrid gaps in $E_{1g}$ (dashed lines) and $E_{2u}$ symmetry (solid lines). The impurity scattering rate $\Gamma_0$ is taken to be 0.05 $T_c^-$. 

FIG. 3. Transverse attenuation data for both polarizations normalized to the value of the attenuation at $T_c^+$ and $T_c^-$ as a function of $T/T_c^{\pm}$. This choice of normalization allows us to compare the attenuation in the A and B phases over the same (reduced) temperature range. The A-phase shows an enhanced in-plane attenuation vs. the B-phase while the out-of-plane polarization data are roughly equal in the two phases. The lines are guides to the eye (after Ref. [4]).
\( \frac{\kappa}{T} \) vs. \( \frac{T}{T_c} \)

- Solid line: \( E_{2u} \)
- Dashed line: \( E_{1g} \)

\( \Gamma_0 = 0.05 \epsilon_T \)
