What Does the Field Dependence of the Thermal Conductivity of the Heavy Fermion Superconductor UPt_3 Tell Us about the Symmetry of the Order Parameter?

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We investigate the field dependence of the thermal conductivity κ of UPt_3 single crystals for magnetic fields applied along the basal (*ab*) plane and along the *c* axis, respectively. The effect of heat carrying electrons scattered by quasiparticle excitations in the vortex cores is calculated for an anisotropic superconducting gap parameter of either E_{1g} or E_{2u} symmetry. It is shown that the anisotropy of the field dependence of κ allows one to probe the symmetry of the superconducting order parameter and favors the E_{2u} gap parameter, i.e., with quadratic point nodes along the *c* axis. [S0031-9007(97)04248-8]

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It is now widely accepted that heavy fermion materials like UPt_3 and related compounds are unconventional superconductors [1,2]. The low temperature power law behavior of their thermodynamic and transport properties [3–5], the coexistence of superconductivity and antiferromagnetic long range order [1], and the complex $(H\text{-}T)$ phase diagram observed in these materials [1,2] are signatures of unconventional (anisotropic) superconducting pairing mechanism. However, it was recently pointed out that the symmetry of the superconducting order parameter of heavy fermions is still undetermined and controversial [6]. Knowing the extreme importance of such a physical property for the understanding of the superconductivity mechanism(s), as in the case of high-T_c superconductors [7], it is of interest to tackle the problem in a convincing way.

In this Letter, we analyze the experimental data of Suderow *et al.* [8] on the effect of a magnetic field H on the thermal conductivity κ of UPt_3 single crystals for fields applied either along the basal plane or along the *c* axis in the low temperature and low magnetic field region, i.e., in the so-called "*B* phase" of UPt_3. We show for the first time (to our knowledge) that the anisotropy of the field dependence of κ is *consistent* with a gap parameter of E_{2u} type [9], in contrast to the alternative E_{1g} form [10]. We recall here that the E_{1g} gap parameter has linear lines of nodes along the basal plane and linear point nodes along the *c* axis while the E_{2u} gap parameter possesses linear lines of nodes along the basal plane and quadratic point nodes along the *c* axis.

Let us first recall that Behnia *et al.* [11] have shown that the temperature dependence of the thermal conductivity of UPt_3 below T_c is almost entirely due to electrons. Besides, Lussier *et al.* [12,13] and Fledderjohann and Hirschfeld [14] have pointed out that the *anisotropy* of the temperature dependence of κ along the *ab* plane and *c* axis should probe the symmetry of the superconducting order parameter of heavy fermions superconductor; see also Huxley *et al.* [15]. As a matter of fact, the *temperature* behavior of the thermal conductivity is related to the *energy E* dependence of the density of states (DOS). Since the DOS depends linearly on E both along the *ab* plane and the *c* axis for an E_{2u} gap parameter, $\kappa_e(T)$ is found to be isotropic in that case [14]. On the other hand, the energy dependence of the DOS is anisotropic for an E_{1g} gap parameter, leading to an anisotropic *temperature* dependence of the electronic thermal conductivity in the E_{1g} model [14]. However, the complex structure of the Fermi surface and inelastic scattering effects complicate the analysis of experimental results; see, e.g., Ref. [16]. Consequently, the E_{1g} and E_{2u} symmetry for the order parameter of heavy fermions cannot be definitively distinguished through the field free temperature dependence of κ.

The *anisotropy of the field dependence* of the thermal conductivity seems, however, to discriminate between these two gap parameter symmetries. Behnia *et al.* [17] previously reported the field dependence of the thermal conductivity of UPt_3 single crystals. These authors argued that the anisotropy of $\kappa(H)$ could probe the symmetry of the order parameter of UPt_3, but failed to explain their experimental results from a quantitative point of view. Besides, their analysis was mainly restricted to the data in the close vicinity of the upper critical field H_{c2}, thus considering the so-called "*C* phase" of the $H\text{-}T$ phase diagram of UPt_3. In the present Letter, we are concerned about the low temperature and low magnetic field region (the so-called "*B* phase"), i.e., $T \in [0.1\ \text{K}, 0.3\ \text{K}]$ and $B \in [0\ \text{kOe}, 1.2\ \text{kOe}]$.

The field dependence of the thermal conductivity of a superconductor can be calculated using the expression of Kadanoff and Martin [18], derived within the linear response method

$$\kappa_\mu^{e\text{-}v}(H,T) = \frac{\hbar^3}{2k_BT^2m_\mu^*} \int d\vec{k}\, \frac{k_\mu^2\,\varepsilon(\vec{k})^2}{\Gamma_{e\text{-}v}(\vec{k},H,T)} \times \operatorname{sech}^2\!\left(\frac{E(\vec{k})}{2k_BT}\right), \tag{1}$$

where m_μ^* is the anisotropic effective mass with $\mu = (x,y,z)$, $\Gamma_{e\text{-}v}$ the electron-vortex scattering rate, and $E(k) = \sqrt{\varepsilon(\vec{k})^2 + |\Delta(\vec{k})|^2}$ the quasiparticle energy spectrum in which $\varepsilon(\vec{k})$ is the normal state band structure and $\Delta(\vec{k})$ the $\vec{k}$-dependent superconducting energy gap parameter.

We point out that Eq. (1) has been recently used by Yu *et al.* [19] and Aubin *et al.* [20] in order to analyze the field dependence of the thermal conductivity of $YBa_2Cu_3O_{7-x}$. These authors [19,20] found that their data in the low field and low temperature region could be quite well reproduced by considering an anisotropic *d*-wave gap parameter. The same approach should also be valid in the case of UPt_3, and the more so in the low field and low temperature region investigated in this paper.

An ellipsoidal Fermi surface with $m^*_{ab}/m^*_c = 2.8$ [12,13] is considered in order to model the anisotropic *normal* state electronic structure of UPt_3. Below T_c, we consider either an anisotropic E_{1g} hybrid gap parameter

$$\Delta(\vec{k}, T)_{E_{1g}} = \Delta(0)\,[\hat{k}_z(\hat{k}_x + i\hat{k}_y)]\tanh\left(1.74\sqrt{\frac{T_c}{T} - 1}\right) \tag{2}$$

or an anisotropic E_{2u} hybrid gap parameter

$$\Delta(\vec{k}, T)_{E_{2u}} = \Delta(0)\,[\hat{k}_z(\hat{k}_x + i\hat{k}_y)^2]\tanh\left(1.74\sqrt{\frac{T_c}{T} - 1}\right), \tag{3}$$

where $\hat{k}_\mu$ are normalized wave vectors along the μ direction. These latter expressions for the k dependence of the gap parameter have been previously considered by Sauls [2] within the anisotropic Ginzburg-Landau theory of superconductivity—expressions which come from developments of the order parameter on the basis function of the D_{6h} group.

Equations (2) and (3) should be compared to the ones used by Graf *et al.* [21], for instance. These authors used restricted developments of Eqs. (2) and (3) in the vicinity of the gap nodes in order to perform analytic calculations in the very low temperature regime. We consider that such different choices for the form of the order parameter should not alter the main conclusions of our investigations.

The electron-vortex scattering rate $\Gamma_{e\text{-}v}$ is calculated here in the Born approximation, considering the Coulomb scattering between heat carrying electrons and the bound quasiparticles in the vortex cores as in Refs. [22], i.e.,

$$\Gamma_{e\text{-}v}(\vec{k}, H, T) = \frac{V}{2\pi^3}\int d\vec{k}'\,(1 - \cos\theta)P_{e\text{-}v}(k, k'), \tag{4}$$

where $P_{e\text{-}v}(\vec{k}, \vec{k}')$ is the scattering probability given by

$$P_{e\text{-}v}(\vec{k}, \vec{k}') = \frac{2\pi}{\hbar}\,|\langle\vec{k}, \psi|\,(e^2/\varepsilon_0 r)\,|\vec{k}', \psi'\rangle|^2 f^0(E) \times [1 - f^0(E')]f^0(\varepsilon_n)\delta(E' - E), \tag{5}$$

where ψ is the wave function of the bound states in the vortex cores and $\varepsilon_n = n\hbar^2/m^*\xi^2$ $(n = 1, 2, \ldots)$ the bound energy levels [23], with ξ the superconducting coherence length. We point out that we have considered a quite simple form for the scattering by the bound states in the vortex cores. Let us recall that Volovik [24] has emphasized that the vortex structure of unconventional superconductors should contain all the basis functions of the symmetry point group of the material, and more specifically an *s*-wave component. Like in our previous work [22], we have then used wave functions ψ in Eq. (5) that are linear combinations of spherical harmonics. Since all the orbitals of the hydrogen atom can be generated using such linear combinations, our simple modelization of the vortex structure of UPt_3 seems to be reasonable and is supported by symmetry arguments indeed.

On the other hand, in the low field region investigated in this paper, the assumption that the electron-vortex scattering strength lies in the weak coupling limit seems reasonable. Hence, the Born approximation should be valid here. Notice that the situation is different for electron-impurity scattering in the field free case. As a matter of fact, impurity scattering is pair breaking in an unconventional superconductor, which in turn leads to the better validity of the unitarity (strong scattering) limit [16].

In the low field and low temperature region, the order parameter of a superconductor with lines of nodes in the gap parameter has been shown by Won and Maki [25] to behave like

$$\Delta(\vec{k}, T, H) = \Delta(\vec{k}, T)\sqrt{1 - [H/H_{c2}(T)]}, \tag{6}$$

where $H_{c2}(T)$ is the temperature dependent upper critical field. The temperature dependence of the upper critical field in UPt_3 presents an anomalous anisotropic behavior for fields applied along the basal plane and along the c axis, respectively [26]. In order to account for this latter anisotropy, we have fitted the experimental results of Shivaram *et al.* [26] by using the phenomenological expression

$$H^\mu_{c2}(T) = H^\mu_{c2}(0)\,[1 - (T/T_c)^\alpha], \tag{7}$$

where $H_{c2}(0) = 27.2$ kOe and $\alpha = 1.2$ for $\mu = a, b$ and $H_{c2}(0) = 21.2$ kOe and $\alpha = 2$ for $\mu = c$, respectively.

The field dependence of the normalized thermal conductivities $\kappa_\mu/\kappa_\mu(B = 0)$ of UPt_3 single crystals has been measured in Grenoble [8], for thermal gradients ∇T and magnetic fields H applied, respectively, along the *ab* plane and the c axis $(H \parallel \nabla T)$ at $T = 0.1$ K and $T = 0.3$ K (Fig. 1). The thermal conductivity is seen to decrease rapidly at low magnetic fields and to saturate at higher fields, i.e., for $H \geq 0.8$ kOe. The decrease is faster at low temperature, where the anisotropy of the thermal conductivity between the *ab* plane and c axis is more important.

The solid lines in Fig. 1 result from direct fits to the thermal conductivity data obtained with an E_{2u} gap parameter. We fixed the following values of the physical parameter for UPt_3 [27]: $T_c = 0.5$ K, $\Delta(0) = 1.76k_BT_c = 7.6 \times 10^{-2}$ meV, $m^*_{ab}/m_0 = 130$, and $m^*_{ab}/m^*_c = 2.8$. In contrast, for the E_{1g} model, the field dependence of

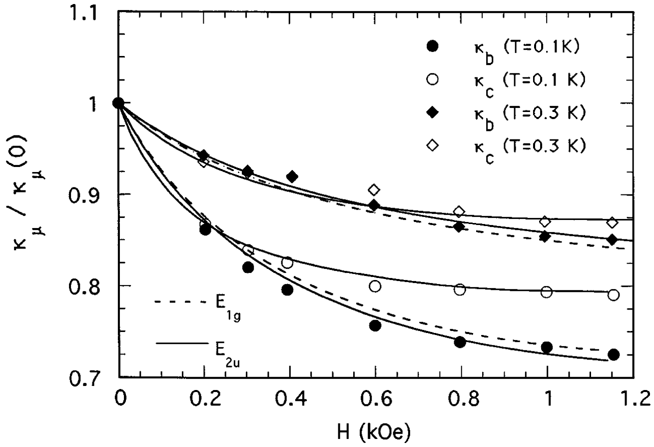

FIG. 1. Field dependence H of the normalized thermal conductivity $\kappa_\mu/\kappa_\mu(0)$ of UPt_3 single crystals [8] for fields applied, respectively, along the *ab* plane (dark symbols) and along the *c* axis (open symbols) at $T = 0.1$ K (circles) and $T = 0.3$ K (diamonds). The solid and dashed lines are theoretical curves obtained, respectively, for an E_{2u} [Eq. (3)] and an E_{1g} [Eq. (2)] gap parameter symmetry.

the thermal conductivity is found to be *isotropic* (see below), and the best fits to the *ab*-plane thermal conductivity correspond to the dashed lines in Fig. 1.

The experimental results of Suderow *et al.* [8] are thus quite well recovered by our theoretical calculations for an E_{2u} energy gap parameter. A further quantitative test resides in the values of the anisotropic in-plane and out-of-plane upper critical fields $H_{c2}(0)$ obtained from these fits, i.e., $H_{c2}^{ab}(0) = 26.7$ kOe and $H_{c2}^{c}(0) = 20.5$ kOe, in fair agreement indeed with the values found from the data of Shivaram *et al.* [26]; see above.

The *anisotropy* value of the field dependence of the normalized $\kappa_b(H)/\kappa_c(H)$ ratio is next shown in Fig. 2 at, respectively, $T = 0.1$ K and $T = 0.3$ K. The theoretical curves resulting from the above theory are shown as well. One can see that $\kappa(H)$ is predicted to be completely *isotropic* for the E_{1g} symmetry. One can also observe that the experimental data of Suderow *et al.* [8] can be *quantitatively* reproduced by considering an E_{2u} gap parameter.

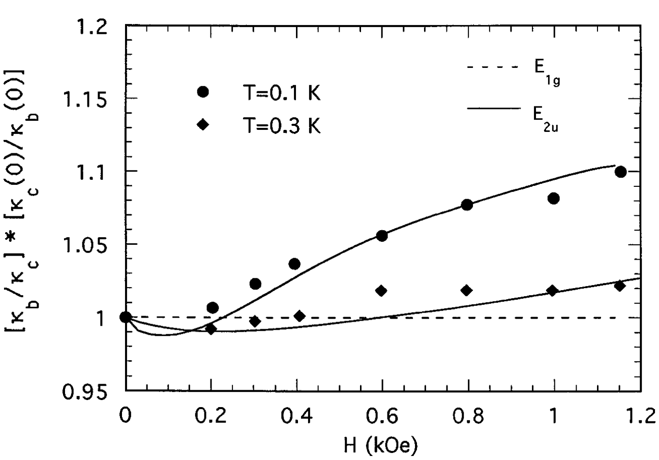

FIG. 2. Anisotropy of the normalized field dependence of the thermal conductivity κ_b/κ_c of UPt_3 single crystals from Ref. [8] at $T = 0.1$ K and $T = 0.3$ K. The solid and dashed lines are fits obtained with our calculations for, respectively, an E_{2u} and an E_{1g} gap parameter.

We recall that Volovik [24] has predicted that the main contribution to the *field dependence of the quasiparticle density of states* in an unconventional superconductor arises mainly from the excitations in the vicinity of the gap nodes below T_c. Since the E_{1g} gap parameter Eq. (2) vanishes *linearly* along the basal plane lines of nodes as well as along the *c*-axis point nodes, the *field dependence* of the quasiparticle DOS [hidden in the kernel of the integral of Eq. (1)] is quite similar along these two directions. This leads to the same *field dependence* of the thermal conductivity in both directions, as shown in Fig. 2 for the E_{1g} case indeed. On the other hand, $\kappa(H)$ is markedly *anisotropic* for the E_{2u} symmetry. This allows us to conclude that a different *field* dependence of the DOS exits when the field is along the basal plane *linear* lines of nodes or along the *c*-axis *quadratic* point nodes.

Finally, we should comment on the thermal conductivity in UPd_2Al_3 single crystals which increases with the magnetic field in the whole field range at $T/T_c \approx 0.2$ [28]. This is due to the fact that the size of the vortex cores in UPd_2Al_3, of the order of 150 Å [29], is small compared to the electron wave length $\lambda_e \approx 350$ Å. Consequently, the electron-vortex scattering rate should be quasinoneffective in UPd_2Al_3, leading to an increase of $\kappa(H)$ due to the increase of the quasiparticle DOS with the magnetic field. The behavior is quite different in UPt_3 since $\lambda_e \approx 400$ Å is of the same order of magnitude as the vortex core size $2\xi(0) \approx 300$ Å [27]. Hence, the electron-vortex scattering rate is important in UPt_3 and $\kappa(H)$ decreases at low fields; see Fig. 1.

In conclusion, the field dependence of the thermal conductivity of UPt_3 can be explained by considering the scattering of heat carrying electrons by the bound quasiparticles in the vortex cores of an unconventional superconductor. Besides, the anisotropy of the field dependence of the thermal conductivity for fields applied along the *ab* plane and the *c* axis has been shown to be mostly sensitive to the field dependence of the DOS in the vicinity of the gap nodes, whatever the form of the Fermi surface and the occurrence of inelastic scattering processes. Besides, this anisotropic behavior is not compatible with an E_{1g} gap parameter symmetry but can be quite satisfactorily reproduced by considering a gap parameter with linear point nodes along the basal plane and quadratic point nodes along the *c* axis, i.e., as in a E_{2u} superconducting gap parameter.

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