Thermal conductivity in the Vortex State of the Superconductor UPd$_2$Al$_3$

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The magneto-thermal conductivity $\kappa$ is calculated for the vortex state of UPd$_2$Al$_3$ by assuming horizontal gap nodes. The Green’s function method we employed takes into account the effects of supercurrent flow and Andreev scattering on the quasiparticles due to Abrikosov’s vortex lattice order parameter. The calculated angular dependence of $\kappa_{yy}$ for field rotation $\theta_0$ in the ac-plane depends strongly on field strength $H$, impurity scattering, anisotropy of the Fermi velocity, and temperature. For finite temperatures and the clean unitary scattering limit we get qualitative agreement with recent experiments for all four proposed gap functions having horizontal line nodes at $c k_z = 0$, $\pm \pi/4$, and $\pm \pi/2$.

Angle-dependent magneto-thermal conductivity is a powerful tool for determining the nodal structure of the gap in unconventional superconductors. Recently, the thermal conductivity has been measured in the heavy-Fermion superconductor UPd$_2$Al$_3$ for a variety of magnetic field orientations.$^1$ The thermal conductivity $\kappa_{yy}$ displays two-fold oscillations when the magnetic field $H$ is rotated in the ac-plane, while no oscillations are observed when $H$ is rotated within the basal ab-plane. These results provide strong evidence that the gap function $\Delta(k)$ has horizontal line nodes orthogonal to the c-axis. Four gap models have been proposed and denoted in Ref. 1 as types I - IV, respectively: $\Delta(k) \propto \sin \chi$, $\cos \chi$, $\sin 2\chi$, and $\cos 2\chi$ (with $\chi = c k_z$). Cooper pairing mediated by magnetic excitons yields the highest $T_c$ for the model $\cos \chi$. The magneto-thermal conductivity for these models has been calculated by the method of the Doppler shift of the energy of quasiparticles due to the circulating supercurrent flow of the vortices.$^3,4$ This effect depends sensitively on the angle between $H$ and the direction of the nodes of the gap. Comparison of these Doppler shift results with the data indicates that the model type IV, $\Delta(k) = \Delta \cos 2\chi$, gives the most consistent description of the experiments of Ref. 1.$^3$ A new Doppler shift approximation however yields the opposite result, i.e., that the models of types I - III are in better agreement with experiment.$^4$

The purpose of the present paper is to calculate the magneto-thermal conductivity for horizontal gap nodes by another method which takes into account, beside the effect of the supercurrent flow, the Andreev scattering off the vortex cores.$^5$ These effects are calculated from the real and imaginary parts of the Andreev scattering self energy for the quasiparticle Green’s function in the presence of Abrikosov’s vortex lattice order parameter. This method was applied to Sr$_2$RuO$_4$ by assuming vertical and horizontal nodes of the superconducting gap.$^6$ An equivalent method based on the quasiclassical equations and linear response theory$^7$ provides much more compact expressions for the density of states and thermal conductivity.$^8$ We have shown that the latter expressions yield very nearly the same results as the original expressions derived in Refs. 5 and 6 (see Ref. 9).

The Pesch-approximation$^7$ yields for the spatial average of the normalized density of states:

$$N(\omega, k) = \text{Re} g(\omega, k); \quad g(\omega, k) = \left\{ 1 + 8|\Delta(k)|^2 [\Lambda/v_\perp(k)]^2 \left[ 1 + i\sqrt{\pi} z w(z) \right] \right\}^{-1/2} \quad (1)$$

where

$$z = 2[\omega + i \Sigma_1(\omega)][\Lambda/v_\perp(k)]; \quad \Lambda = (2eH)^{-1/2}. \quad (2)$$

Here $v_\perp(k)$ is the component of the Fermi velocity perpendicular to the magnetic field $H$, and $\Sigma_1(\omega)$ is the self energy for impurity scattering which is calculated self-consistently in the t-matrix approximation.$^9$ The integrand of the $\omega$-integral for the thermal conductivity is proportional to $v_\perp^2$ times the transport scattering time $\tau(\omega, k)$ where$^8$

$$\frac{1}{2 \tau(\omega, \phi)} = \text{Re} \Sigma_1(\omega) + 2\sqrt{\pi} [\Lambda/v_\perp(k)]|\Delta(k)|^2 \frac{\text{Re}[g(\omega, k) w(z)]}{\text{Re} g(\omega, k)}. \quad (3)$$

The first term in Eq.[3] is the scattering rate due to impurities which reduces in the normal state to $\Gamma = 1/2\tau_n$. The second term is the Andreev scattering rate due to the vortex cores.

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For the heavy-Fermion superconductor UPd$_2$Al$_3$ we consider only the cylindrical Fermi surface and approximate the Fermi velocity by

$$v_F = v_a [\cos \phi \, e_a + \sin \phi \, e_b + \varepsilon \sin 2\chi \, e_c], \quad (\chi = c k_z, \quad -\pi/2 < \chi < +\pi/2),$$

where $\varepsilon = v_c/v_a$. Furthermore we assume the following gap function with horizontal nodes:

$$\Delta(k) = \Delta \cos \chi; \quad (\chi = c k_z); \quad \Delta = \Delta_0[1 - h^2]^{1/2}; \quad (h = H/H_c).$$

For a field direction given by polar and azimuthal angles $\theta_0$ and $\phi_0$, i.e.,

$$H = H [\sin \theta_0 \cos \phi_0 \, e_a + \sin \theta_0 \sin \phi_0 \, e_b + \cos \theta_0 \, e_c],$$

the component of $v_F$ perpendicular to $H$ becomes:

$$v_\perp(k) = v_F \left\{1 - \frac{\sin \theta_0 \cos(\phi - \phi_0) + \varepsilon \cos \theta_0 \sin 2\chi^2}{[1 + \varepsilon^2 \sin^2 2\chi]} \right\}^{1/2}.$$  

From this expression it is obvious that the combination $\Delta(k)/v_\perp(k)$ occurring in Eqs. (1) and (3) depends sensitively on the direction of $H$ relative to $k$ and thus relative to the gap nodes. For this model we have calculated $\kappa_{yy}/\kappa_n$ for field orientations $H$ in the xz-plane ($\phi_0 = 0$; $0 \leq \theta_0 \leq \pi$). For the anisotropy parameter $\varepsilon = v_c/v_a$ in Eq. (4) we take the value $\varepsilon = 0.6$. We first consider an impurity scattering rate $\delta = \Gamma/\Delta_0 = 0.024$ and a scattering phase shift $\rho = 0.9(\pi/2)$. In Fig. 1a we show $\kappa_{yy}/\kappa_n$ versus the reduced field $h$ for $\theta_0 = 0$ (solid curve) and $\theta_0 = \pi/2$ (dashed curve) for $T = 0$ ($\omega = 0$). We have also plotted the relative amplitude of the oscillation, $\Delta(\kappa) = [\kappa_{yy}(\theta_0 = 0) - \kappa_{yy}(\theta_0 = \pi/2)]/\kappa_{yy}(\theta_0 = 0)$. In Fig. 1b we show two examples of the oscillation as functions of the polar angle $\theta_0$ for the fixed field strengths $h = 0.05$ and $h = 0.3$. Our results for the unitary limit (phase shift $\rho = \pi/2$) are nearly the same as those shown in Fig. 1. Different results are obtained in Ref. 4 for phase shift $\rho = 0.9(\pi/2)$ where a small region (denoted by I in Ref. 1) exists in which $\kappa_{yy}$ decreases with increasing $h$ and the amplitude of the oscillation $\Delta(\kappa)$ becomes negative. This would be in agreement with the data of Ref. 1.

The measured angular variation of $\kappa_{yy}(\theta_0)$ is decomposed into a constant and a term with twofold symmetry with respect to the $\theta_0$ rotation, i.e., $C_{yy} \cos 2\theta_0$.$^1$ In the region denoted by II in Ref. 1, where $\kappa_{yy}$ depends linearly on $H$, $C_{yy}$ is positive. In the small region I near $H = 0$, where $\kappa_{yy}$ decreases with increasing $H$, the measured amplitude $C_{yy}$ becomes negative.

We have not been able to confirm the results of Ref. 4 where the origin of the sign change of $\Delta(\kappa)$ at low fields is the tiny deviation of the impurity scattering phase shift $0.9(\pi/2)$ from the unitary limit $\pi/2$. We show now that this sign change is actually due to the finite temperature. We estimate the finite temperature effect by considering finite values of $\Omega = \omega/\Delta_0$ where $\omega$ occurs in Eqs. (2) and (3) and is the integration variable for the $\omega$-integral yielding $\kappa$. Since this integrand is strongly peaked at $\omega/T \approx 2.4$, the temperature corresponding to $\Omega$ is approximately given by $\Omega \approx 2.4(T/\Delta_0) \sim T/T_c$. We have verified that this is a good approximation by numerical computation of the $\omega$-integral at finite $T$. As an example, in Fig. 2a we show $\kappa_{yy}/\kappa_n$ versus $h$ for $\Omega = 0.3$ for the impurity scattering rate $\delta = 0.024$ and phase shift $\pi/2$. The solid curve refers to the angle $\theta_0 = 0$ and the dashed curve to $\theta_0 = \pi/2$. One observes now a small range from $h = 0$ to about $h = 0.1$ where the amplitude $\Delta(\kappa)$ of the oscillation is negative. In the enlarged scale of Fig. 2b it is seen more clearly that in this region $\kappa_{yy}/\kappa_n$ bends upwards for decreasing $h$, which also occurs in region I in the experiments. In Fig. 2c we have plotted the oscillation of $\kappa_{yy}$ as a function of the polar angle $\theta_0$ for fixed field strengths $h = 0.05, 0.3$, and =0.5. One sees that oscillations of approximately twofold symmetry in $\theta_0$ occur. In the region of approximately linear field dependence of $\kappa_{yy}$ (see Fig. 2a), which corresponds to region II in the experiments, the amplitude $\Delta(\kappa)$ corresponding to $C_{yy}$ in Ref. 1 is positive. In the region of low fields, corresponding to region I of Ref. 1, $\Delta(\kappa)$ is in fact negative for this finite temperature. It is important to note that the experiments are carried out at a finite temperature of about 0.4 K.$^1$

We discuss now the dependence of our results on the various parameters. First we consider the effect of impurity scattering. For a larger scattering rate, for example, $\delta = \Gamma/\Delta_0 = 0.1$, and the unitary limit, we obtain for $\Omega = 0.3$ the functions $\kappa_{yy}(h)$ and $\Delta(\kappa)$ shown in Fig. 3a. Comparison with the results shown in Fig. 2a for $\delta = 0.024$, and all other parameters the same, shows that the slope of $\kappa_{yy}$ in the linear range of region II is larger, while it is smaller in the region, denoted by III in Ref. 1, where $\kappa_{yy}/\kappa_n$ rises steeply to one. This field dependence in Fig. 3a is in better agreement with experiment. However, no region I occurs where $\kappa_{yy}$ decreases with $h$ and $\Delta(\kappa)$ becomes negative. The function $\kappa_{yy}(\theta_0)$ exhibits an approximate twofold symmetry in $\theta_0$ for all values of $h$. For $\delta = 0.1$ we have to go to higher values of $\Omega$ to obtain a sign change in $\Delta(\kappa)$ near $h = 0$. This is shown in Fig. 3b where $\Delta(\kappa)$ and $\kappa_{yy}$ are plotted vs $h$ in an enlarged scale for $\Omega = 0.3, 0.4$, and 0.5. One sees that for $\Omega = 0.4 (0.5)$, $\Delta(\kappa)$ becomes negative below $h \approx 0.06 (0.18)$. These regions of negative $\Delta(\kappa)$ correspond to region I because $\kappa_{yy}$ bends upwards for decreasing $h$.
Another important parameter is the phase shift for impurity scattering. We have already pointed out that, contrary to the results of Ref. 4, we obtain practically no difference between the results for the unitary phase shift limit $\pi/2$ and $0.9(\pi/2)$. However, for the Born limit, phase shift zero, the curve for $\kappa_{yy}(h)$ is much flatter in the lower $h$-range than the curves for the unitary limit in Figs. 2a and 3. Also, the amplitude $\Delta \kappa$ is negative and $|\Delta \kappa|$ is much larger over the entire range of $h$. These results in the Born limit are in agreement with those obtained in Ref. 4.

We come now to the most crucial parameter, $\varepsilon = v_c/v_a$ in Eq.(4), which determines the anisotropy of the Fermi velocity for the corrugated cylindrical Fermi surface sheet. For the range of $\varepsilon$-values between about $\varepsilon = 0.5$ and 0.7 we obtain nearly the same results as those shown for $\varepsilon = 0.6$. These values agree approximately with the $\varepsilon$ value which is obtained according to Ref. 4 if we take for $v_c^2$ and $v_a^2$ the average values over the corrugated cylindrical Fermi surface where $(v_c/v_a)^2 = (1/2)(v_c/v_a)^2$ and $\alpha = (v_a/v_o)^2 \approx 0.69$ is the appropriate value for UPd$_2$Al$_3$. In addition to the order parameter $\Delta \propto \cos \chi$ (type II), we also obtain, for $\varepsilon$ between 0.5 and 0.7, nearly the same results for the other order parameters proposed in Ref. 1, namely, $\Delta \propto \sin \chi$ (type I), $\sin 2\chi$ (type III), and $\cos 2\chi$ (type IV). In all cases $\chi = c k_z$. However, for $\Omega$ small, as $\varepsilon$ increases from 0.7 to about 0.84, the minimum of $\kappa_{yy}(\theta_0)$ at the field angle $\theta_0 = (\pi/2)$ changes to a smaller maximum and two minima develop at the intermediate angles of about $\theta_0 \approx \pm 1.3(\pi/4)$. It should be pointed out that, for the type IV gap, the minima already start to form just above $\varepsilon = 0.6$ and become more pronounced than for the type I - III gaps. For increasing $\Omega$, the small peak at $\pi/2$ is reduced and becomes a flat, broad minimum at about $\Omega = 0.3$. Furthermore, for $\Omega$ above 0.26, the amplitude $\Delta \kappa$ of the variation of $\kappa_{yy}(\theta_0)$ becomes negative in a small range near $h = 0$. This behavior is similar to that of $\Delta \kappa$ shown in Fig. 2 for $\varepsilon = 0.6$ and $\Omega = 0.3$ and again we see the importance of finite $\Omega$ (temperature) in reproducing the experimental results. We remark that, for $\Omega = 0.3$ and $\varepsilon = 0.6$, $\Delta \kappa$ is negative below $h = 0.05$ for the type IV gap while it is negative below $h = 0.1$ for the type II gap.

We also find that, for $\Omega$ larger than 0.4, a sign change of $\Delta \kappa$ occurs in a small range of $h$ just below $h = 1$. In this connection we remark that experiments yield a negative sign of the amplitude $C_{yy}$ in a region denoted by III in Ref. 1 where $\kappa_{yy}$ rises steeply with $h$. This negative sign has however been attributed to the anisotropies of the Fermi velocity and the upper critical field $H_{c2}$. Since we have neglected here the anisotropy of $H_{c2}$ it may be that our calculated values of $|\Delta \kappa|$ in region III are much smaller than the measured values.

Let us compare our results with those obtained by the Doppler shift method. For the clean unitary scattering limit and intermediate field strengths we obtain for the angular variation of $\kappa_{yy}(\theta_0)$ a positive amplitude $\Delta \kappa = [\kappa_{yy}(\theta_0 = 0) - \kappa_{yy}(\theta_0 = \pi/2)]/\kappa_{yy}(\theta_0 = 0)$ for all four of the gap models of types I - IV proposed in Ref. 1. The first Doppler shift calculation $^4$ yielded a positive $\Delta \kappa$ for the gaps $\cos 2\chi$ and $\sin \chi$ and a negative $\Delta \kappa$ for $\cos \chi$. Another, more recent, Doppler calculation $^4$ finds a positive $\Delta \kappa$ for $\sin \chi$, $\cos \chi$, and $\sin 2\chi$ whereas the variation for the gap $\cos 2\chi$ is completely different from the form $\cos 2\theta_0$ and exhibits pronounced minima at the angles $\theta_0 = \pm 51^\circ$. It is interesting that we obtain similar structure in $\kappa_{yy}(\theta_0)$ with minima at intermediate angles $\theta_0 \approx \pm 1.3(\pi/4)$ for all four gap models I - IV if the anisotropy parameter $\varepsilon = v_c/v_a$ is increased from 0.6 to 0.84. It is not surprising that our analytical expressions yield different results than the Doppler shift method because we take the Andreev scattering of the quasiparticles by the vortex cores into account. It has been shown by comparison with the exact results of the quasiclassical Eilenberger equations (see Fig. 7 in Ref. 10) that the analytical expressions $^5,^7$ provide good approximations over the whole field range from $H_{c2}$ to $H_d$ whereas the Doppler shift method is a good approximation only at low fields. However we want to caution that in the low field regime the higher Fourier components of the Green's function with respect to the vortex lattice vectors $^9$ might lead to important corrections. Therefore a fully self-consistent numerical calculation, in particular for the internal field, would be necessary $^{11}$ in order to obtain more reliable results. This means that the method of Ref. 11 for the density of states should be extended to the calculation of the Andreev scattering from the superfluid flow in the single vortex regime which is important for the thermal conductivity $\kappa$. The large effect of this Andreev scattering can be seen from the fact that, at $T = 0$ and impurity scattering phase shift $= 0.9 (\pi/2)$, $\kappa$ increases for small fields while the Doppler shift method together with a scattering lifetime due to impurity scattering only yields an initial drop of $\kappa$ for small fields. $^4$ We stress again that only at finite temperature ($\Omega$) do we obtain an initial drop of $\kappa$ together with a sign reversal of the oscillation amplitude $\Delta \kappa$ as shown in Figs. 2b and 3b.

In summary, in the clean unitary scattering limit, and for not too large anisotropy $\varepsilon$ of the Fermi velocity, we obtain angular variations of $\kappa_{yy}(\theta_0)$ of approximately twofold symmetry in the field rotation angle $\theta_0$ for all of the four proposed gap models having horizontal line nodes at $c k_z = \chi = 0, \pm \pi/4, \pm \pi/2$. The amplitude $\Delta \kappa$ is positive in the range of field values $H$ where $\kappa_{yy}$ is nearly linear in $H$. At finite temperature $\Delta \kappa$ becomes negative at small fields which is in agreement with experiment. The range of field values with negative $\Delta \kappa$ is smaller for the gap of type IV ($\cos 2\chi$) than for types I - III. Our results depend crucially on the anisotropy parameter $\varepsilon = v_c/v_a$ for the corrugated cylindrical Fermi surface. For values of $\varepsilon$ above about 0.7 we find a small maximum at $\theta_0 = \pi/2$ and two minima at about $\theta_0 \approx \pm 1.3(\pi/4)$ in the curve of $\kappa_{yy}(\theta_0)$ for the gap models I - III. For the gap model IV this critical value of $\varepsilon$ is smaller, about $\varepsilon = 0.6$. It should be pointed out that even for a constant gap the density of states depends strongly on the shape of the Fermi surface and the field orientation. $^{12}$ Thus we can say that the angular variations of $\kappa_{yy}(\theta_0)$
are determined by two competing effects: the positions of the gap nodes and the amount of anisotropy of the Fermi velocity given by the shape of the Fermi surface. Here the latter effect appears to predominate.

In conclusion, our calculations indicate that at present one cannot determine which one of the proposed gap models with horizontal line nodes is most consistent with the measured magneto-thermal conductivity of UPd$_2$Al$_3$. The gap model $\cos \chi$ however seems to be somewhat more favorable than $\cos 2\chi$. Our calculations also indicate the importance of accounting for finite temperature and lead us to expect that the value of the field at which the amplitude of the oscillation $\Delta \kappa$ changes sign should decrease with decreasing temperature. It is thus desirable to have measurements available at lower temperatures in very clean samples. It will also be interesting to see whether additional structure, minima, for example, occur in the form of $\kappa_{yy}(\theta_0)$. 

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Fig. 1a

FIG. 1. 1a) Thermal conductivity $\kappa_{yy}$ for the gap model I vs reduced field $h = H/H_{c2}$ for field direction $\theta_0 = 0$ (solid curve) and $\theta_0 = \pi/2$ (dashed curve). Also shown is the relative amplitude of the oscillation $\Delta \kappa = [\kappa_{yy}(\theta_0 = 0) - \kappa_{yy}(\theta_0 = \pi/2)]/\kappa_{yy}(\theta_0 = 0)$. The impurity scattering rate is $\delta = \Gamma/\Delta_0 = 0.024$, the phase shift is $0.9(\pi/2)$, and the anisotropy parameter $\varepsilon = v_c/v_a = 0.6$. 
Fig. 2. 1b) Angular variation of $\kappa_{yy}$ vs polar angle $\theta_0$ for field strengths $h = 0.05$ and $h = 0.3$. 
FIG. 3. 2a) $\kappa_{yy}$ vs $h$ for $\theta_0 = 0$ (solid curve) and $\theta_0 = \pi/2$ (dashed curve), and $\Delta \kappa$ vs $h$, for impurity scattering rate $\delta = 0.024$, phase shift $\pi/2$ (unitary limit), and $\varepsilon = 0.6$. The reduced frequency is $\Omega = \omega/\Delta_0 = 0.3$ which corresponds to a finite temperature of order $T/T_c \sim \Omega$. 
Fig. 2b

FIG. 4. 2b) the same as in a) for an enlarged scale.
Fig. 2c

FIG. 5. 2c) Angular variation of $\kappa_{y y}(\theta_0)$ for field strengths $h = 0.05$, 0.3, and 0.5.
FIG. 6. 3a) $\kappa_{yy}$ and $\Delta \kappa$ vs $h$ (see notations in Fig. 1a) for impurity scattering rate $\delta = 0.1$, phase shift $\pi/2$, and finite frequency (temperature) $\Omega = 0.3$. 
Fig. 3b

FIG. 7. 3b) $\kappa_{yy}$ vs $h$ for $\Omega = 0.3$, 0.4 and 0.5 (upper curves from bottom to top) and $\Delta \kappa$ vs $h$ for $\Omega = 0.3$, 0.4 and 0.5 (lower curves from top to bottom).