Specific heat and thermal conductivity in Sr$_2$RuO$_4$ for rotating in-plane magnetic field

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We calculate the density of states $N$ and the thermal conductivity $\kappa$ in layered superconductors for rotating in-plane magnetic field by using approximate analytical expressions for Abrikosov’s vortex lattice state. For a gap with $d_{xy}$-orbital symmetry we find that the differences $\Delta N$ and $\Delta \kappa$ between field directions parallel to the antinodes and parallel to the nodes of the gap are positive for lower fields and change sign for higher fields near $H_{c2}$. For increasing impurity scattering, $\Delta N$ and $\Delta \kappa$ decrease due to a broadening of certain peaks in the angle-resolved density of states. The frequency dependencies of the amplitudes $\Delta N$ and $\Delta \kappa$ exhibit similar crossover behavior at low frequencies which give rise to a sign change of $\Delta \kappa$ at low $T/T_c$. We conclude that variations of the specific heat and thermal conductivity can be observed only in the clean and low temperature limits.

Recently fourfold oscillations of the specific heat have been observed for rotating in-plane magnetic field in pure Sr$_2$RuO$_4$ at very low temperatures. These data have been analyzed on the basis of the Bogoliubov-de Gennes (BdG) equations and the Pesch-approximation for the vortex state with the result that the spin-triplet superconductor Sr$_2$RuO$_4$ has a gap with nodes in the directions of the a and b axes. In an earlier measurement of the thermal conductivity $\kappa$ no appreciable angular variation was observed from which it was concluded that no vertical line nodes exist in Sr$_2$RuO$_4$. However, the amplitude of the oscillation of $\kappa$ for a state with vertical gap nodes was found to be strongly temperature dependent and to change sign for increasing temperature. This explains the failure to observe an angular variation of $\kappa$ because the measuring temperature in the experiment of Ref. 3 was too high.

In the present paper we repeat the calculations of the density of states $N$ and the thermal conductivity $\kappa$ for rotating in-plane field for a superconductor with $d_{xy}$ symmetry of the orbital part of the gap using the analytical expressions of Pesch based on the quasiclassical Green’s functions which are easier to handle than the original expressions based on the Gorkov equations and Abrikosov’s vortex state. Our main purpose is to investigate the effect of impurity scattering. This depends sensitively on the phase shift for impurity scattering as has been shown in a recent paper for $d$-wave pairing in fields parallel to the c-axis. We shall only present results for the unitary limit of impurity scattering with phase shift $\pi/2$ because the relevance of the unitary limit has been strongly suggested by the results for the universal heat transport in Sr$_2$RuO$_4$.

For simplicity we neglect the small c-axis dispersion of the cylindrical Fermi surface and thus the c-axis component of the Fermi velocity. The azimuthal angle of the quasiparticle momentum in the ab-plane with respect to the a-axis is denoted by $\phi$ and we use $\alpha$ for the direction of the magnetic field in the ab-plane. Thus the component of the Fermi velocity in the direction perpendicular to the magnetic field is given by $v \sin(\phi - \alpha)$. For the momentum part of the order parameter we assume $d_{xy}$ symmetry which, together with the field dependence of the spatial average of the modulus of the Abrikosov vortex state, yields the expression

$$|\Delta|^2 = \frac{\Delta_0^2}{1 + h^2} \sin^2(2\phi)$$

where $h = H/H_{c2}$ and $H$ is the spatial average of the field. The Pesch-approximation now yields for the spatial average of the density of states $N(\omega)$, normalized to the normal state density of states $N_0$:

$$N(\omega)/N_0 = \text{Re} \left\{ 1 + 8|\Delta|^2 |\Lambda/v \sin(\phi - \alpha)|^2 [1 + i \sqrt{\pi z w(z)}] \right\}^{-1/2};$$

where

$$z = 2[\omega + i \Sigma_0]/|\Lambda/v \sin(\phi - \alpha)|; \quad \Lambda = (2eH)^{-1/2}.$$ 

Here $\Sigma_0$ is the self energy for impurity scattering which is calculated self-consistently in the t-matrix approximation from the expressions given in Ref. 8. The thermal conductivity $\kappa$ in the BPT-approximation is given in Ref. 4 and in the equivalent Pesch-approximation in Ref. 6. The integrand of the $\omega$-integral in Ref. 6 is proportional to the density...
of states \(\text{[Eq.(2)]}\) times the lifetime of the quasiparticles. This lifetime is equal to the reciprocal of the sum of the scattering rates due to impurity and Andreev scattering which have been discussed at length in Ref. 8.

In Fig.1 we show our results for \(N(\omega = 0)/N_0\) and \(\kappa(T = 0)/\kappa_n\) (\(\kappa_n\) is the normal state thermal conductivity) versus the reduced field \(h = H/H_{c2}\) for fields along the gap node (\(\alpha = 0\), solid curves) and along the antinode (\(\alpha = \pi/4\), dashed curves). The heat current for \(\alpha\) is along the antinode of the gap, \(\phi = \pi/4\). The impurity scattering self energy is calculated self-consistently for the unitary phase shift limit and the reduced scattering rate \(\delta = \Gamma/\Delta_0 = 0.01\) where \(\Gamma = 1/2\tau_n\) is the normal state scattering rate. This is the right order of magnitude for the purest samples of Sr$_2$RuO$_4$ with the highest \(T_c\).\(^3\) One sees that the dashed curve for \(N/N_0\) (antinode) lies above the solid curve (node) for \(h\) from zero to about the crossing field \(h_c = 0.63\) while, above \(h_c\), it lies below the solid curve. The difference \(\Delta N\) between the two curves corresponds to the amplitude of the measured fourfold anisotropy of the specific heat.\(^4\) This amplitude is about 6 percent of \(N(\alpha = 0)\) at \(h = 0.3\). Our results agree approximately with the results obtained in Ref. 2 by solving the BdG equations and by using the Pesch-approximation. For \(\kappa/\kappa_n\) (lower curves in Fig.1) the dashed curve (antinodal direction of the field) lies above the solid curve (nodal direction of the field) for \(h\) between 0 and about \(h_c = 0.95\) where it crosses the solid curve. As with the density of states, the difference \(\Delta \kappa\) between the dashed and solid curve corresponds the amplitude of the fourfold anisotropy and amounts to about 25% of \(\kappa(\alpha = 0)\). It has been shown in Ref. 4 that the amplitude \(\Delta \kappa\) of the fourfold oscillation in rotating field decreases rapidly with increasing temperature and reverses its sign at a very low temperature indicating that the variations with field direction can only be observed at very low temperatures.

In addition to the temperature effect, impurity scattering also diminishes the amplitudes of the fourfold oscillations of the density of states and the thermal conductivity. An example is shown in Fig.2 where we present our results for the unitary phase shift limit and a much larger scattering rate \(\delta = 0.1\) which is of the order of magnitude corresponding to lower \(T_c\)’s in Sr$_2$RuO$_4$.\(^3\) Comparison of Fig.2 with Fig.1 shows that, for the larger scattering rate, the crossing field \(h_c \approx 0.4\) for the curves of \(N\) is much smaller and the relative amplitude \(\Delta N/N(\alpha = 0) \sim 2\%\) is also much smaller. The crossing field for \(\kappa\) and the relative amplitude \(\Delta \kappa/\kappa/(\alpha = 0)\) are of the same orders of magnitude as those for \(N\).

In Ref. 2 the reasons for the crossover behavior of the density of states have been explained in detail by calculating the angle-resolved density of states for low and high fields using the BdG equations and the Pesch-approximation. Similar angle-resolved densities of states \(N(\phi)/N_0\) are shown in Fig.3 for a low field \(h = 0.2\) and nodal field direction (\(\alpha = 0\), solid curves) and antinodal field direction (\(\alpha = \pi/4\), dashed curves). Note that, in the latter case, the angle \(\phi\) is measured from the field direction \(\alpha = \pi/4\). One sees that, for \(\alpha = 0\), a single broad peak occurs at \(\phi = \pi/2\) while, for \(\alpha = \pi/4\), two peaks occur at \(\phi = \pi/4\) and \(\phi = 3\pi/4\). This explains why in this field region the total density of states \(N(\alpha = \pi/4)\) is larger than \(N(\alpha = 0)\) because, for \(\alpha = \pi/4\), all four nodes contribute to \(N\) while, for \(\alpha = 0\), two of the four nodes are parallel to the field and are thus unable to contribute to \(N\). In the high magnetic field region, on the other hand, \(N(\alpha = 0) > N(\alpha = \pi/4)\) because then the behavior is determined by \(N(\phi)\) for \(\phi = 0\) and \(\phi = \pi\).

Comparison of Fig.3(a), calculated for the unitary limit and \(\delta = 0.01\), with Fig.3(b), calculated for \(\delta = 0.1\), shows that the main effect of stronger impurity scattering is to broaden the peaks of the solid curve at \(\phi = 0\) and \(\phi = \pi\) and to enhance the minima at \(\phi = \pi/4\) and \(3\pi/4\). At the same time the minima of the dashed curve \(\phi = 0\) and \(\phi = \pi\) are enhanced. This effect of impurity scattering is similar to the effect of finite c-axis dispersion of the cylindrical Fermi surface which was taken into account in Ref. 2. The total effect of the broadening of the peaks and the enhancement of the minima in the angle-resolved density of states for low fields is the decrease of the amplitudes of variation of \(N\) and \(\kappa\) in rotating in-plane field as shown in Figs.1 and 2.

Finally we consider the frequency dependence of \(N(\omega)/N_0\) for nodal and antinodal field directions and its effect on the frequency and temperature dependence of the thermal conductivity. In Fig.4(a) we have plotted our results for \(N(\omega)/N_0\) versus \(\Omega = \omega/\Delta_0\) for a low field (\(h = 0.2\)) for nodal (\(\alpha = 0\), solid curve) and antinodal (\(\alpha = \pi/4\), dashed curve) field directions. In Fig.4(b) we show the corresponding curves for \(\kappa(\omega)/\kappa_n\) which is the factor multiplying \((\omega/T)^2 \text{sech}^2(\omega/2T)\) in the normalized integral over \(d(\omega/T)\) for \(\kappa/\kappa_n\).\(^6\) This function of \(\Omega = \omega/\Delta_0\) yields approximately the temperature dependence of \(\kappa/\kappa_n\) through the relation \(\Omega \approx 2.4(\Delta_0/T)\) because the integrand is strongly peaked at \(\omega/2T = 2.4\). The expression for \(\kappa(\omega)\) is given by \(N(\omega)\tau(\omega)\) where the quasiparticle scattering rate \(1/2\tau(\omega)\) is equal to the sum of the impurity and Andreev scattering rates.\(^7\) The most interesting results in Figs.4(a) and 4(b) are the crossovers of the dashed and solid curves occuring at very low frequencies which correspond to a sign change of the amplitudes of the variations of fourfold symmetry with rotation angle. For \(\kappa(\omega)\) this first crossover occurs at about \(\Omega_c \approx 0.1\) which means that, at a temperature of about \(T/\Delta_c \approx 0.1\), the amplitude of the variation of the rotation angle vanishes or changes sign. It should be pointed out that for high fields the curves for \(N(\omega)\) and \(\kappa(\omega)\) look quite different. The solid curve for \(N(\omega)\) starts out at a much higher value than the dashed curve and the coherence peak for the solid curve vanishes. This is similar to the results of Ref. 2.

In summary, we have calculated the density of states \(N\) and the thermal conductivity \(\kappa\) for a gap with \(d_{xy}\)-orbital symmetry and magnetic fields in the directions \(\mathbf{H} \parallel \text{gap node (\(\alpha = 0\), solid curves) and \(\mathbf{H} \parallel \text{gap antinode (\(\alpha = \pi/4\), dashed curves). For both calculations we have used the approximate expressions of Pesch}^{6,7}\text{ for Abrikosov’s vortex lattice state which are easier to handle than the original expressions of the BPT-approximation}^{7,4}\text{. Comparison of}
these results with the results of the quasiclassical Eilenberger equations\textsuperscript{10} and the BdG-equations\textsuperscript{2} has shown that these analytical expressions provide very good approximations over the whole field range from $H_{c2}$ down to $H_{c1}$. We have included impurity scattering and used a phase shift of $\pi/2$ because the unitary limit in Sr$_2$RuO$_4$ is strongly suggested by universal heat transport.\textsuperscript{9}

Our main result is that the density of states $N(\omega = 0)$ and the thermal conductivity $\kappa(T = 0)/\kappa_n$ are somewhat larger for the antinodal field direction ($\alpha = \pi/4$) than for the nodal field direction ($\alpha = 0$) in a field region $0 \leq h \leq h_c$ ($h = H/H_{c2}$) where $h_c$ denotes the field where the dashed curves cross the solid curves (see Fig.1). Our results for $N$ agree essentially with the results obtained from the BdG equations and the Pesch-approximation.\textsuperscript{2} These results have led to the conclusion that the observed minima and maxima of the specific heat for rotating in-plane field in Sr$_2$RuO$_4$ are due to vertical line nodes in the directions of the a- and b-axes.\textsuperscript{1} It turns out that the amplitudes $\Delta N = N(\alpha = \pi/4) - N(\alpha = 0)$ and $\Delta \kappa = \kappa(\alpha = \pi/4) - \kappa(\alpha = 0)$ and the crossover field $h_c$ decrease for increasing impurity scattering (see Fig.2). The reason can be seen from a comparison of the angle-resolved density of states $N(\phi)/N_0$ in Figs.3(a) and 3(b). The most important contributions to the density of states [see Eqs.(2) and (3)] are the terms $\Lambda/v |\sin(\phi - \alpha)|$ where $\Lambda = (2eH)^{-1/2}$ is the magnetic length, $v |\sin(\phi - \alpha)|$ is the component of the Fermi velocity perpendicular to $H$, and $\phi$ and $\alpha$ are the azimuthal angles of the quasiparticle momentum and field direction, respectively. Asymptotic expansion of the $w$-function\textsuperscript{7} in Eq.(2) shows that in the limit $\phi \rightarrow \alpha$ the density of states takes on the BCS form for $|\Delta(\phi)|^2$ [see Eq.(1)]. For quasiparticles moving in the directions perpendicular to the field ($\phi - \alpha = \pm \pi/2$) the analytic expression involving the $w$-function yields the full effect of the superfluid flow and the Andreev scattering due to the complex order parameter of Abrikosov’s vortex lattice function. These directional terms, together with the angular dependence $\Delta_\phi^2 \sin^2(2\phi)$ of the gap function, yield quite different angle-resolved densities of states $N(\phi)/N_0$ for $\alpha = 0$ and $\alpha = \pi/4$ shown in Fig.3. Comparison of Figs.3(a) and 3(b) shows that the main effect of stronger impurity scattering is to broaden the peaks of the solid curve at $\phi = 0$ and $\phi = \pi$. It is interesting that this effect is quite similar to the effect of a finite c-axis dispersion of the cylindrical Fermi surface which has been taken into account in the analytic Pesch-expression in Ref. 2. Finally, we have investigated the finite temperature effect on the amplitude $\Delta \kappa$ for the variation with rotating in-plane field by calculating $N(\omega)/N_0$ and $\kappa(\omega)/\kappa_n$ for the field directions $\alpha = 0$ and $\alpha = \pi/4$ (see Figs.4(a) and 4(b) for low field $h = 0.2$ and small impurity scattering $\delta = 0.01$). The large differences between $N(\omega)$ and $\kappa(\omega)$ arise from the quasiparticle lifetime $\tau(\omega)$ in the latter expression which is given by the reciprocal of the sum of scattering rates due to impurity and Andreev scattering. The impurity scattering rate is calculated self-consistently in the unitary limit of the t-matrix approximation, and the Andreev scattering rate arises from the imaginary part of the self energy proportional to $\Delta(r_1)\Delta^*(r_2)G(r_1 - r_2, -\omega)$, where $\Delta(r)$ is Abrikosov’s vortex lattice order parameter\textsuperscript{8} and $G$ is the hole propagator. The crossover of the dashed and solid curves at a low frequency $\omega \simeq 0.1\Delta_0$ in Fig.4(b) leads to a corresponding crossover in the temperature dependencies of $\kappa$ at about $T/T_c \simeq 0.1$ showing that the amplitude of the variation with field rotation vanishes and changes sign at this temperature. Similar results have already been obtained in Ref. 4 using the BPT-approximation.

In conclusion we can say that the amplitudes of the variations of the specific heat and thermal conductivity in rotating in-plane field for a gap with vertical line nodes decrease rapidly with increasing impurity scattering and increasing temperature.
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FIG. 1. 1) Density of states, $N(\omega = 0)/N_0$, and thermal conductivity, $\kappa/\kappa_n(T \to 0)$, versus $h = H/H_{C2}$ for in-plane field direction parallel to the gap node ($\alpha = 0$, solid curves) and parallel to the antinode ($\alpha = \pi/4$, dashed curves). The reduced impurity scattering rate is $\delta = \Gamma/\Delta_0 = 0.01$ with phase shift in the unitary limit.
FIG. 2. 2) The same as Fig. 1 but with $\delta = 0.1$. 
FIG. 3a) Angle-resolved density of states, $N(\phi)/N_0$ for $h = 0.2$. Solid curves are for nodal field direction ($\alpha = 0$) and dashed curves for antinodal direction ($\alpha = \pi/4$). The angle $\phi$ is measured from the field direction. Impurity scattering with $\delta = 0.01$ in the unitary limit.
Fig. 4. 3b) Angle-resolved density of states, $N(\phi)/N_0$ for $h = 0.2$. Solid curves are for nodal field direction ($\alpha = 0$) and dashed curves for antinodal direction ($\alpha = \pi/4$). The angle $\phi$ is measured from the field direction. Impurity scattering with $\delta = 0.1$ in the unitary limit.
Fig. 4a

FIG. 5. 4a) Density of states $N(\omega)/N_0$ versus $\Omega = \omega/\Delta_0$ for $h = 0.2$, $\delta = 0.01$, and field directions $\alpha = 0$ (solid curve) and $\alpha = \pi/4$ (dashed curve).
Fig. 4b

FIG. 6. 4b) Thermal conductivity $\kappa(\omega)/\kappa_n$ versus $\Omega = \omega/\Delta_0$ for $h = 0.2$, $\delta = 0.01$, and field directions $\alpha = 0$ (solid curve) and $\alpha = \pi/4$ (dashed curve). The temperature gradient is in the direction of the antinode.