Possible $f$-wave superconductivity in Sr$_2$RuO$_4$?

H. Won$^{1,2}$ and K. Maki$^2$

$^1$Department of Physics, Hallym University, Chunchon 200-702, South Korea
$^2$Department of Physics and Astronomy, University of Southern California, Los Angeles, CA 90089-0484, USA

(received ; accepted )

PACS. 74.20.Fg – BCS theory and its development.
PACS. 74.25.Bt – Thermodynamic Properties.
PACS. 74.25.Fy – Transport properties.

Abstract. – Until recently it has been believed that the superconductivity in Sr$_2$RuO$_4$ is described by $p$-wave pairing. However, both the recent specific heat and the magnetic penetration depth measurements on the purest single crystals of Sr$_2$RuO$_4$ appear to be explained more consistently in terms of $f$-wave superconductivity. In order to further this hypothesis, we study theoretically the thermodynamics and thermal conductivity of $f$-wave superconductors in a planar magnetic field. We find the simple expressions for these quantities when $H \ll H_{c2}$ and $T \ll T_c$, which should be readily accessible experimentally.

Introduction. – The recently discovered superconductivity in Sr$_2$RuO$_4$ has been believed to be described in terms of $p$-wave superconductor with the full energy gap. For example, the spontaneous spin polarization seen by muon spin rotation experiment and the flat Knight shift seen by NMR, are consistent with the triplet pairing. However, the recent specific heat, $T_1^{-1}$ in NMR and the superfluid density of the purest Sr$_2$RuO$_4$ single crystals with $T_c = 1.5$ K are inconsistent with the $p$-wave superconductivity.

The $T^2$-dependence of the specific heat, the $T^3$-dependence of $T_1^{-1}$, and the $T$-dependence of the superfluid density indicate clearly the presence of the nodal structure in the superconducting order parameter. One possible interpretation is that the superconducting order parameter in the $\gamma$-band has the full gap as assumed earlier, while the ones in the $\alpha$- and $\beta$-band have the nodal structure.

Alternatively, we may consider the possibility that the superconducting order parameters in these 3 bands are the same and described by $f$-wave superconductor with the order parameter

$$ d(\mathbf{k}) = \frac{3\sqrt{3}}{2} \Delta \hat{d} k_3 (\hat{k}_1 \pm i\hat{k}_2)^2 $$

with $\hat{d} \parallel \hat{c}$ which is believed to describe the superconductivity in UPt$_3$. Indeed the overall temperature dependence of the specific heat and the superfluid density are described...
Fig. 1. – The specific heat data $[5]$ divided by $\gamma T$ where $\gamma$ is Sommerfeld constant is compared with the theoretical results for the isotropic $p$-wave $[7]$ and $f$-wave $[8]$ superconductors.

Fig. 2. – The superfluid density data of single crystal $\text{Sr}_2\text{RuO}_4$ $[6]$ is compared with the theoretical results of $p$-wave $[7]$ and $f$-wave $[8]$ superconductors.

much more consistently by $f$-wave superconductor. We compare the experimental data of the specific heat $[7]$ and the superfluid density $[8]$ of $\text{Sr}_2\text{RuO}_4$ crystals with the theoretical results for the weak coupling $p$-wave and $f$-wave superconductors in Fig.1 and Fig.2, respectively. Of course, there are still obvious discrepancies in this identification. For example, the data for $C_s(T)/\gamma T$ exhibits weakly convex behavior while the theory predicts weakly concave behavior, though the discrepancy is not so striking. Also the theory cannot account for the $T^3$-dependence of the superfluid density observed in the less pure samples. But this may be due to the non-locality effect suggested by Kosztin and Leggett $[10]$.

In a recent series of papers $[11, 12]$, we have proposed that the thermal conductivity tensor in a planar magnetic field near $H_{c2}$ provide the crucial test of the symmetry of the underlying superconductivity. We recall also ingenious thermal conductivity experiments $[3, 4]$ have been carried out to elucidate the nodal structure of $d$-wave superconductivity in YBCO.

In the following we take the superconducting order parameter given by Eq.(1), and first study the quasi-particle density of states in the presence of both magnetic field and impurities. Starting from the pioneering work by Volovik $[15]$, we have fully developed technology for this purpose, at least, for $H \ll H_{c2}$ and $T \ll T_c$ $[14, 17, 18, 19]$. The central idea is to introduce the effect of the magnetic field or the supercurrent in the quasi-particle spectrum through the Doppler shift $[20]$. When computing the effect of the magnetic field to the quasi-particle density of states, for example, we take the average of terms containing the Doppler shift over both the quasi-particle momentum and over the Wigner-Seitz cell containing a single vortex in a real space. Further impurity scattering is treated in the unitarity limit as in most of unconventional superconductors $[8]$.

Perhaps the most important result is that the thermal conductivity tensors exhibit significant $\tilde{\theta}$-dependence, where $\tilde{\theta}$ is the angle between the magnetic field and the heat current both lying in the $a$-$b$ plane. Recently the thermal conductivity of $\text{Sr}_2\text{RuO}_4$ in a planar magnetic field has been measured, which does not exhibit clear $\theta$-dependence $[21, 22]$. Of course the $\theta$-dependence we found for $f$-wave superconductor is much smaller than the one found for $p$-wave superconductor $[23]$, but should be still visible. Therefore it appears that the thermal conductivity data exclude both $p$- and $f$-wave superconductors from the candidate for superconductivity in $\text{Sr}_2\text{RuO}_4$. Clearly we have to look for another candidate.

On the other hand, the present result should apply to $\text{UPt}_3$ in a low magnetic field with a heat current within the $a$-$b$ plane. We have already studied the thermal conductivity of $f$-wave superconductor in the vicinity of $H_{c2}$ $[12]$. Indeed this calculation reproduces the $\tilde{\theta}$-dependence of the thermal conductivity of $\text{UPt}_3$ observed by Suderow et al $[24]$.

Quasi-particle density of states, the specific heat, and superfluid density. – In the following we shall use the approach given in $[16]$. The residual density of states in $f$-wave superconductors is given by

$$\frac{N(\omega = 0)}{N_0} = \text{Re} \left( \frac{\tilde{\omega} - \mathbf{v} \cdot \mathbf{q}}{\sqrt{(\tilde{\omega} - \mathbf{v} \cdot \mathbf{q})^2 - \Delta^2 |f|^2}} \right) \bigg|_{\omega = 0}$$
where \( f = \frac{3\sqrt{3}}{2} \cos \theta (1 - \cos^2 \theta) \), \( x = |\mathbf{v} \cdot \mathbf{q}|/\Delta \) with \( \mathbf{v} \) the Fermi velocity, \( \mathbf{q} \) the superfluid momentum, and \( C_0 = -i\tilde{\omega}|_{\omega=0} \) with \( \tilde{\omega} \) the renormalized frequency \([13]\). In deriving Eq. (2), we have assumed \( C_0, x \ll 1 \). Now in the unitarity limit of the impurity limit we obtain \([8]\)

\[
C_0 = \frac{\Gamma}{\Delta} \left( \frac{N(\omega = 0)}{N_0} \right)
\]

and \( \Gamma \) and \( \Delta \) are the impurity scattering rate and the superconducting order parameter, respectively.

We can solve Eq. (2) and (3) analytically in the two limiting cases:

a) superclean limit (\( C_0 \ll \langle x \rangle \ll 1 \), i.e. \( \frac{\Gamma}{\Delta} \ll \frac{H}{H_{c2}} \ll 1 \))

\[
\frac{N(H)}{N_0} \approx \frac{\pi}{2\sqrt{3}} \langle x \rangle + \frac{2}{\pi} \frac{\Gamma}{\Delta} \langle x \rangle \langle \ln(\frac{2}{x}) - 1 \rangle
\]  

and

\[
C_0 \approx \frac{2\sqrt{3}}{\pi} \frac{\Gamma}{\Delta} \langle x \rangle
\]

Finally, following \([17]\) the spatial average gives

\[
\frac{N(H)}{N_0} \approx \frac{1}{\sqrt{3}} \frac{\sqrt{vv'eH}}{\Delta} + \frac{\Gamma}{\sqrt{vv'eH}} \ln\left( \frac{4\Delta}{\sqrt{3} \Gamma \langle x \rangle} \right)
\]

where \( \langle x \rangle \approx \frac{2\sqrt{vv'eH}}{\pi} \Delta \) and \( \langle \ln x \rangle \approx \ln(\frac{\sqrt{vv'eH}}{2\Delta}) \) after the spatial average. Here \( v \) and \( v' \) are the Fermi velocity in the \( a-b \) plane and parallel to the \( c \)-axis, respectively. As shown by Volovik \([15]\) already the density of states increases like \( \sqrt{H} \) for \( H \ll H_{c2} \).

b) clean limit (\( \langle x \rangle \ll C_0 \ll 1 \), i.e. \( \frac{H}{H_{c2}} \ll \frac{\Gamma}{\Delta} \ll 1 \))

\[
\frac{N(H)}{N_0} \approx \frac{N_{\text{imp}}}{N_0} (1 + \frac{\Delta}{2\sqrt{3} \Gamma} \langle x^2 \rangle)
\]

\[
= \frac{N_{\text{imp}}}{N_0} (1 + \frac{vv'eH}{8\sqrt{3} \Gamma \Delta} \ln(\frac{2\Delta}{\sqrt{vv'eH}}))
\]

and

\[
C_0^2 \ln(\frac{2}{C_0}) \approx \sqrt{3} \frac{\Gamma}{\Delta} - \frac{1}{2} \langle x^2 \rangle
\]

where

\[
\frac{N_{\text{imp}}}{N_0} \approx \sqrt{\frac{\Gamma}{2\sqrt{3} \Delta \ln(\frac{4\Delta}{\sqrt{3} \Gamma})}}
\]

Here \( \frac{N_{\text{imp}}}{N_0} \) is the density of states in the \( H = 0 \) case with the unitarity impurity scatterer.
Also, unlike in $d$-wave superconductors \cite{18, 19}, the specific heat is independent of the direction of the planar magnetic field. Making use of $N/N_0$ given in Eqs. (5) and (8) the low temperature specific heat and the superfluid density are expressed as in \cite{25}

$$C_s(T, H) = \frac{2\pi^2}{3}TN(H)$$  \hspace{1cm} (10)

and

$$\rho_s(H, T=0) = 1 - N(H)/N_0$$  \hspace{1cm} (11)

The thermal conductivity tensor. – As already discussed, the angular independence of the thermal conductivity tensor in a planar magnetic field appears to offer the test of $f$-wave superconductivity. Following the formalism developed by Ambegaokar-Griffin \cite{26}, the thermal conductivity tensor for $T \ll \Delta_0$ is given by

$$\kappa_\parallel/\kappa_n = 3 \frac{\Gamma}{\Delta} \left< (1 - \cos^2 \theta) \cos^2 \phi \frac{1}{2} \left( 1 + \frac{C_0^2 + x^2 - |f|^2}{[(C_0 + ix)^2 + |f|^2]^2} \right) \right>$$  \hspace{1cm} (12)

and

$$\kappa_\perp/\kappa_n = 3 \frac{\Gamma}{2\Delta} \left< (1 - \cos^2 \theta) \sin(2\phi) \frac{1}{2} \left( 1 + \frac{C_0^2 + x^2 - |f|^2}{[(C_0 + ix)^2 + |f|^2]^2} \right) \right>$$  \hspace{1cm} (13)

and $\kappa_n = \frac{\pi^2 T n}{6\Gamma m}$, the thermal conductivity in the normal state.

a) superclean limit($C_0 \ll \langle x \rangle \ll 1$, i.e. $\frac{H}{H_c2} \ll \frac{\Gamma}{\Delta} \ll 1$)

Making use of $C_0$ obtained in Eq.(5) and integrating over $\cos \theta$ and $\phi$, we obtain

$$\kappa_\parallel/\kappa_n \simeq \frac{1}{6} \frac{vv'eH}{\Delta^2} (1 - \frac{1}{3} \cos(2\tilde{\theta}))$$  \hspace{1cm} (14)

and

$$\kappa_\perp/\kappa_n \simeq -\frac{1}{18} \frac{vv'eH}{\Delta^2} \sin(2\tilde{\theta})$$  \hspace{1cm} (15)

where $\tilde{\theta}$ is the angle between $\mathbf{H}$ and $\mathbf{q}$ the heat current within the $a$-$b$ plane. The above expressions may be contrasted with those in $d$-wave superconductors which is given by \cite{19}

$$\kappa_\parallel/\kappa_n \simeq \frac{2}{\pi} \frac{vv'eH}{\Delta^2} (0.955 + 0.0286 \cos(4\tilde{\theta}))^2$$  \hspace{1cm} (16)

and

$$\kappa_\perp/\kappa_n \simeq -\frac{2}{\pi} \frac{vv'eH}{\Delta^2} (0.955 + 0.0286 \cos(4\tilde{\theta}))(0.29 \sin(2\tilde{\theta}))$$  \hspace{1cm} (17)

For $\frac{T}{\Delta} \gg C_0$, $\kappa_\parallel$ is given by

$$\kappa_\parallel(H=0) = \frac{3\sqrt{3} \zeta(3) T^2}{2\Delta \sqrt{3}\Gamma \Delta} \left[ \ln(2\sqrt{\frac{\Delta}{\sqrt{3}\Gamma}}) \right] \frac{n}{m}$$  \hspace{1cm} (18)
and $\zeta(3) = 1.202\ldots$. In this limit the thermal conductivity increase like $T^2$ as in $d$-wave superconductors.

b) clean limit ($\langle x \rangle \ll C_0 \ll 1$, i.e. $\Gamma \ll H_{c2} \ll 1$)

$$
\kappa_{\parallel}/\kappa_0 \simeq 1 + \frac{1}{3} \frac{\langle(1 + \cos(2\phi))x^2\rangle}{C_0^2}
$$

$$
= 1 + \frac{1}{12\sqrt{3}}(1 - \frac{1}{2} \cos(2\tilde{\theta})) \frac{v v' eH}{\Gamma \Delta} \ln(2\sqrt{\frac{\Delta}{\sqrt{3} \Gamma}}) \ln(\frac{2\Delta}{\sqrt{v v' eH}})
$$

(19)

$$
\kappa_{\perp}/\kappa_0 \simeq -\frac{1}{24\sqrt{3}} \sin(2\tilde{\theta}) \frac{v v' eH}{\Gamma \Delta} \ln(2\sqrt{\frac{\Delta}{\sqrt{3} \Gamma}}) \ln(\frac{2\Delta}{\sqrt{v v' eH}})
$$

(20)

where $\kappa_0 = \frac{\pi^2 T n}{6\sqrt{3} \Delta m}$ is Lee’s universal thermal conductivity. Therefore $\kappa_{\perp} \sim -\sin(2\tilde{\theta})$ appears to be the universal behavior for $p$-wave, $d$-wave, and $f$-wave superconductors.

For $\mathbf{H} \parallel \mathbf{c}$, we can derive the corresponding expressions readily, though we don’t expect any angular dependence. The quasi-particle density of states is given by for the superclean limit,

$$
N(H)/N_0 \simeq \frac{\pi}{2\sqrt{3}} \frac{v \sqrt{eH}}{\Delta^2} + \frac{2}{\pi} \frac{\Gamma}{v \sqrt{eH}} \ln(\frac{4\Delta}{v \sqrt{eH}})
$$

(21)

for the superclean limit, and

$$
N(H)/N_0 \simeq \frac{N_{\text{imp}}}{N_0} (1 + \frac{v^2 eH}{4\sqrt{3} \Gamma \Delta} \ln(\frac{2\Delta}{v \sqrt{eH}}))
$$

(22)

for the clean limit. Also the thermal conductivity tensor is given by

$$
\kappa_{\parallel}/\kappa_n \simeq \frac{\pi^2}{24} \frac{v^2 eH}{\Delta^2}
$$

(23)

for the superclean limit, and

$$
\kappa_{\parallel}/\kappa_0 \simeq 1 + \frac{1}{6\sqrt{3}} \frac{v^2 eH}{\Gamma \Delta} \ln(2\sqrt{\frac{\Delta}{\sqrt{3} \Gamma}}) \ln(\frac{2\Delta}{v \sqrt{eH}})
$$

(24)

for the clean limit. Finally, off-diagonal thermal conductivity has the simple relation like $\kappa_{\perp} = \kappa_{\parallel}(eB/m)\Gamma_H$ where $\Gamma_H$ is the scattering rate related to the Hall coefficient.

Conclusions. – We have studied theoretically the specific heat and the thermal conductivity tensor in the vortex state of $f$-wave superconductivity in a planar magnetic field when $H \ll H_{c2}$ and $T \ll T_c$. The quasi-particle relaxation is assumed to be due to the impurity scattering in the unitarity limit.

We find for $H \ll H_{c2}$ and $T \ll T_c$ appreciable $\tilde{\theta}$-dependence for both the diagonal and the off-diagonal component of the planar thermal conductivity tensor in a planar magnetic field. Although the present $\tilde{\theta}$-dependences are much smaller than those expected for $p$-wave superconductors, it is not certain if they are consistent with the thermal conductivity data of $\text{Sr}_2\text{RuO}_4$ crystals. Therefore, further works on the thermal conductivity tensor in $f$-wave superconductors and other unconventional superconductors are highly desirable. On the other hand, the present result should apply for $\text{UPt}_3$ in phase B in a low magnetic field.
Acknowledgments. – We thank I. Bonalde and Y. Maeno for providing us the digitized version of their figure, which we used in construction of Fig.1 and Fig.2. We are also benefited from discussions with K. Izawa, T. Ishiguro, Y. Maeno, Y. Matsuda and M.A. Tanatar on their experimental data of thermal conductivity in Sr$_2$RuO$_4$. HW acknowledges the support from the Korea Research Foundation under the Professor Dispatching Scheme. Also HW thanks Dept. of Physics and Astronomy, USC for their hospitality during her stay.

REFERENCES

[1] Maeno Y. et al, Nature bf 372 (1994) 532; Maeno Y., Physica C 282-287 (1997) 206.
[2] Rice T.M., and Sigrist M., J. Phys. Cond. Matters 7 (1995) L643; Sigrist M. et al, Physica C 317-318 (1999) 134.
[3] Luke G. et al, Nature 394 (1998) 558.
[4] Ishida K. et al, Nature 396 (1998) 658.
[5] Nishizaki S., Maeno Y. and Mao Z.Q., J. Phys. Soc. Jpn. 69 (2000) 572.
[6] Bonalde I., Yanoff B.D., Salamon M.B., Van Harlingen D.J., Chia E.M.E., Mao Z.Q. and Maeno Y., preprint.
[7] Maki K. and Puchkaryov E., Europhys Lett. 50 (2000) 533.
[8] Maki K. and Yang G., Fizika 8 (1999) 345.
[9] Heffner R.H. and Norman M.R., comments on Cond. Matter Phys. 17 (1996) 361.
[10] Kosztin I. and Leggett A., Phys.Rev. Lett. 79 (1997) 135.
[11] Maki K., and Won H., Physica C (in press).
[12] Maki K., Yang G., and Won H., in Proceedings of M2S-HTSC VI (Houston, Feb. 2000).
[13] Salamon M.B., Yu F., and Kopylov V.N., J. Superconductivity 8 (1995) 44 ; Yu F., Salamon M.B., Leggett A.J., Lee W.C. and Ginsberg D.M., Phys. Rev. Lett. 74 (1995) 5136.
[14] Aubin H., Behnia K., Ribault M., Gagnon R. and Taillefer L., Phys Rev. Lett.78 (1997) 2624.
[15] Volovik G.E., JETP Lett. 58 (1993) 469; Kopnin N.B. and Volovik G.E. JETP Lett. 64 (1996) 690.
[16] Barash Yu S., Svidzinski A.A., and Mineev V.P., JETP Lett.65 (1997) 638.
[17] Kübert C. and Hirschfeld P.J., Solid State Commun. 105 (1998) 459; Phys. Rev. Lett. 80 (1998) 4963.
[18] Vekhter L., Carbotte J.P., and Nicol E.J., Phys. Rev. B 59 (1999) 1417; Vekhter I., Hirschfeld P.J., Carbotte J.P., and Nicol E.J., Phys Rev. B 59 (1999) R9023.
[19] Won H. and Maki K., cond-mat/0004105
[20] Maki K., and Tsuento T., Prog. Theor. Phys. 27 (1962) 228.
[21] Tanatar M.A. et al, in Proceedings of M2S-HTSC IV (Houston, Feb. 2000); Tanatar M.A. and Maeno Y. (private communication)
[22] Izawa K. et al (private communication).
[23] Won H. and Maki K., in preparation.
[24] Suderow H., Aubin H., Behnia K., and Huxley A., Phys. Lett. A 234 (1997) 64.
[25] Won H. and Maki K., Europhys. Lett. 30, (1995) 427; Phys. Rev. B 53 (1996) 5927.
[26] Griffin A. and Ambegaokar V., Phys. Rev. 137 (1964) A1151.
[27] Lee P.A., Phys. Rev. Lett. 71 (1993) 1887.
H. Won and K. Maki, Fig. 1
H. Won and K. Maki, Fig. 2