Models of Superconductivity in Sr$_2$RuO$_4$

Thomas Dahm$^a$, Hyekyung Won$^{b,c}$, Kazumi Maki$^c$

$^a$Institut für Theoretische Physik, Universität Tübingen, Auf der Morgenstelle 14, D-72076 Tübingen, Germany
$^b$Department of Physics, Hallym University, Chuncheon 200-702, South Korea
$^c$Department of Physics and Astronomy, University of Southern California, Los Angeles, CA 90089-0484, U.S.A.

Recent experimental data on purest Sr$_2$RuO$_4$ single crystals clearly indicate the presence of nodes in the superconducting order parameter. Here, we consider one special p-wave order parameter symmetry and two two-dimensional f-wave order parameter symmetries having nodes within the RuO$_2$ plane. These states reasonably describe both specific heat and penetration depth data. We calculate the thermal conductivity tensor for these three states and compare the results with recent thermal conductivity data. This allows us to single out one of these states being consistent with both thermodynamic and thermal conductivity data: the planar f-wave state having B$_{1g}$×E$_u$ symmetry.

PACS: 74.70.Dd, 74.20.-z, 74.25.Bt, 74.25.Fy

I. INTRODUCTION

The recently discovered superconductivity in Sr$_2$RuO$_4$ has been interpreted in terms of a p-wave triplet superconducting state having a full energy gap. For example the spontaneous spin polarization seen by muon spin rotation experiments and the flat Knight-shift seen by nuclear magnetic resonance (NMR) are consistent with spin triplet pairing. However, recent specific heat data and the superfluid density of purest single crystals of Sr$_2$RuO$_4$ with $T_c \lesssim 1.5$K clearly show low temperature behavior consistent with nodes in the order parameter very similar to observations of d-wave superconductivity in the high-$T_c$ cuprate superconductors.

Here we shall study three examples of two-dimensional (2D) superconducting order parameters with spin triplet pairing having nodes within the RuO$_2$ a-b plane. The first one is the anisotropic p-wave state proposed by Miyake and Narikiyo with $\Delta(\vec{k}) \propto \sin(k_ya) \pm i \sin(k_xa)$. Here, $a$ denotes the lattice constant of the RuO$_2$ square lattice. In order to have a node with this state, however, we have to stretch the Fermi wavevector $k_F$ towards the particular value of $k_F a = \pi$, while a more realistic value would be $k_F a = 2.7$ as judged from bandstructure calculations.$^7$ In the following we will denote this particular p-wave state as the nodal p-wave state. As the second and third example we consider the planar f-wave states recently proposed by Hasegawa et al.$^3$ Here, the angular φ dependence of the order parameter is given by $\Delta(\vec{k}) \propto \cos(2\phi)e^{\pm i\phi}$ and $\Delta(\vec{k}) \propto \sin(2\phi)e^{\pm i\phi}$, respectively.

Within circular symmetric weak-coupling BCS theory one immediately realizes that the thermodynamics of the latter two states is identical to the one of d-wave superconductors.$^6$ We have worked out the thermodynamics of the anisotropic, nodal p-wave state here as well. In Figs. we show our results for the temperature dependence of the specific heat $C_s/\gamma T$ and the superfluid density $\rho_s(T)$ for the nodal p-wave and the 2D f-wave states together with the experimental data. For comparison, we also show the results of a 3D f-wave state, considered by two of us recently.$^2$ As is readily seen, the 2D f-wave states give a better description of the experimental data than the 3D f-wave or the nodal p-wave states, though the differences between the 2D f-wave and the 3D f-wave states are rather small.

![FIG. 1. The specific heat $C_s/\gamma T$ as a function of $T/T_c$ for the 2D f-wave states (solid line) and the nodal p-wave state (dashed line) considered in this work. Also shown are the experimental data by Nishizaki et al. (circles) and the 3D f-wave state considered in Ref. 12 (dotted line).](image)

Very recently the thermal conductivity of Sr$_2$RuO$_4$ in a planar magnetic field has been studied.$^4$ Both groups studied the thermal conductivity parallel to the a-axis in a magnetic field within the a-b plane in a direction tilted by an angle $\theta$ from the heat current. Both groups found no appreciable angular dependence. This experimental result is already inconsistent with the isotropic p-wave state having a full energy gap and the 3D f-wave state.$^1$ Indeed, we shall show that the thermal conductivity data is consistent with only one of the three nodal states considered here: the 2D f-wave state with angular dependence $\cos(2\phi)e^{\pm i\phi}$. The two other states exhibit
rather large angular dependence and therefore are inconsistent with the experiments.

In the next section we briefly summarize the thermodynamic properties of the nodal $p$-wave superconductor with $\Delta(\vec{k}) \propto \sin(k_x a) \pm i \sin(k_y a)$. In many respects the results are very similar to the ones for $d$-wave superconductors\textsuperscript{4} and 3D $f$-wave superconductors\textsuperscript{3}. Then we proceed to consider the thermal conductivity in a planar magnetic field. The result for the 2D $f$-wave state with angular dependence $\cos(2\phi)e^{\pm i\phi}$ is very similar to the one in $d$-wave superconductors discussed recently in Ref. 13.

II. THERMODYNAMICS OF THE NODAL $P$-WAVE SUPERCONDUCTOR

We consider the superconducting order parameter given by $\Delta(\vec{k}) = \frac{\Delta}{s_M} \sin(k_x a) \pm i \sin(k_y a)$ with $k_x a = \pi \cos(\phi)$ and $k_y a = \pi \sin(\phi)$ and the normalization $s_M = \sqrt{\pi} \sin(\pi a_F) = 1.125$. This is the model proposed in Ref. 9 except that we have chosen the Fermi wavevector $k_F a = \pi$ in order to have a node in $\Delta(\vec{k})$. The quasi-particle Green function in Nambu representation is given by

$$G(k, \omega) = (i \omega - \xi_k \rho_3 - \Delta(k) \rho_1 \sigma_1)^{-1}$$

where $\Delta(k) = \frac{\Delta}{s_M} [\sin(k_x a) \pm i \sin(k_y a)]$.

FIG. 2. The superfluid density $\rho_s(T)$ as a function of $T/T_c$ for the 2D $f$-wave states (solid line) and the nodal $p$-wave state (dashed line) together with the experimental data by Bonalde et al.\textsuperscript{12} (circles) and the 3D $f$-wave state considered in Ref. 13 (dotted line).

Then the quasi-particle density of states is given by

$$N(E)/N_0 = \text{Re}\left\langle \frac{E}{\sqrt{E^2 - \Delta^2(k)}} \right\rangle$$

where $\Delta(0) = \frac{\Delta}{s_M}$ and $\rho_3 = \frac{\Delta}{s_M}$. In particular we find $\Delta(0)/T_c = 2.00$, which has to be compared with 2.14 in the 2D $f$-wave case.

FIG. 3. The density of states for the 2D $f$-wave state (solid line) and the nodal $p$-wave state (dashed line).

The entropy $S$ is obtained from

$$S = -4 \int_0^\infty dE N(E) \left[ f \ln f + (1 - f) \ln(1 - f) \right]$$

$$= 4 \int_0^\infty dE N(E) \left[ \beta E (1 + e^{\beta E})^{-1} + \ln(1 + e^{-\beta E}) \right]$$

with $f$ being the Fermi function and $\beta = 1/T$. Then the specific heat $C_s(T)$ is given by

$$C_s(T) = T \frac{dS(T)}{dT}$$

$C_s(T)/\gamma T$ has been shown in Fig. 4. Finally, the superfluid density $\rho_s(T)$ is given by

$$\rho_s(T) = 1 - \frac{\beta \Delta}{2} \int_0^\infty dE N(E)/N_0 \text{sech}^2 \left( \frac{\beta E}{2} \right)$$

which behaves almost linearly in $T$ and is shown in Fig. 5. We note that at low temperatures an expansion of $\rho_s(T)$ leads to $\rho_s(T) = 1 - 2 \ln 2 \times 0.7162 \frac{T}{T_c} + \cdots$. 

$$= \frac{4}{\pi} y \int_0^{\pi/4} d\phi \text{Re} \left( \frac{1}{\sqrt{y^2 - f^2(\phi)}} \right)$$

where $f^2(\phi) = \frac{\Delta}{s_M}^2 (1 - \cos(\sqrt{2}\pi \cos(\phi)) \cos(\sqrt{2}\pi \sin(\phi)))$, $y = E/\Delta$, and $<>$ denotes an angular average. The density of states is calculated and shown in Fig. 3 together with the one for the 2D $f$-wave case. In particular for $E/\Delta \ll 1$, the density of states increases linearly as $N(E)/N_0 \approx 0.7162 E/\Delta$, while in the 2D $f$-wave case it varies like $N(E)/N_0 \approx E/\Delta$. Otherwise the two curves look very similar. Here, the gap equation

$$\lambda^{-1} = \langle f^2 \rangle^{-1} \int_0^E dE \langle f^2 \rangle \text{tanh}(\frac{E}{2T})$$

has been solved numerically. In particular we find $\Delta(0)/T_c = 2.00$, which has to be compared with 2.14 in the 2D $f$-wave case.
III. THERMAL CONDUCTIVITY TENSOR IN
THE A-B PLANE

As shown in earlier experiments on YBCO, the thermal conductivity tensor in a planar magnetic field is very sensitive to the nodal directions and thus may be used to further discriminate between the states studied above. We shall consider the thermal conductivity tensor in the vortex state of the nodal $p$-wave and the 2D $f$-wave separately. We will show that only one of these states appears to be consistent with the angular independence observed recently.

A. Nodal $p$-wave state

The necessary theoretical scheme, neglecting vortex core scattering, has been worked out during the past few years. We just apply this method for the present case. In particular for $\pi / 2 \ll 1$ in the superclean limit we obtain

$$\frac{\kappa_{xx}}{\kappa_n} = \frac{2}{\pi} \frac{2S}{\pi} \frac{2M}{\pi} \langle (1 + \cos(2\phi)) x \rangle$$

$$= \frac{2}{\pi} \frac{2S}{\pi} \frac{2M}{\pi} \frac{v}{\Delta^2} F(\theta)$$

(7)

where $v$ and $v'$ are the Fermi velocities within the $a$-$b$ plane and perpendicular to it, respectively, and $x = |v \cdot q| / \Delta$ denotes the Doppler shift due to the superflow around the vortex (see Ref. [3]). $\kappa_n = \pi^2 T_n / 61 m$ is the normal state thermal conductivity. The function $F(\theta)$ is given by

$$F(\theta) = \frac{2}{\pi^2} \sqrt{1 + \sin^2 \theta E} \left( \frac{1}{\sqrt{1 + \sin^2 \theta}} \right) \times$$

$$\left( \sqrt{1 + \sin^2 \theta E} \left( \frac{1}{\sqrt{1 + \sin^2 \theta}} \right) + \sqrt{1 + \cos^2 \theta E} \left( \frac{1}{\sqrt{1 + \cos^2 \theta}} \right) \right)$$

(8)

with $E$ being the complete elliptic integral of the second kind and

$$\kappa_{xy} / \kappa_n = 0$$

(9)

In the present situation there will be no off-diagonal component, because the heat current is parallel to the nodal direction. The angular dependence of $\kappa_{xx}$ is given by the function $F(\theta)$, which is shown in Fig. 1. Surprisingly, $\kappa_{xx}$ has a broad maximum for $\theta = \pi / 2$. Also, the anisotropy $\kappa_{xx}(\pi / 2) / \kappa_{xx}(0) = 1.910$ is quite strong. Therefore, in view of the thermal conductivity experimental data, we have to reject this possibility.

B. 2D $f$-wave state

As already mentioned we consider the two states $\sin(2\phi) e^{\pm i\phi}$ and $\cos(2\phi) e^{\pm i\phi}$. The order parameter $\propto \sin(2\phi) e^{\pm i\phi}$ has the same nodal structure as the nodal $p$-wave state studied in the last subsection and has been studied recently by Graf and Balatsky. Following the same procedure as above we find for the state $\sin(2\phi) e^{\pm i\phi}$

$$\kappa_{xx} / \kappa_n = \frac{2}{\pi} \langle (1 + \cos(2\phi)) x \rangle = \frac{2}{\pi} \frac{v}{\Delta^2} F(\theta)$$

(10)

and

$$\kappa_{xy} = 0$$

(11)

where $F(\theta)$ has been shown in Fig. 4.

FIG. 4. Angular variation of the functions $F(\theta)$, $I^2(\theta)$, and $I(\theta)L(\theta)$ as defined in Eqs. (6), (14), and (15). The angular variation of the thermal conductivity $\kappa_{xx}$ for the nodal $p$-wave state, as given by the function $F(\theta)$, is much stronger than for the $\cos(2\phi) e^{\pm i\phi}$ $f$-wave state ($I^2(\theta)$) due to the different position of the nodes in the gap function.

Therefore, also the state $\sin(2\phi) e^{\pm i\phi}$ gives a rather large $\theta$ dependence, which is inconsistent with the existing experiments.

Finally, let us consider the state $\cos(2\phi) e^{\pm i\phi}$, which has its nodes along the zone diagonal. As already noted, this state has the same thermodynamics as a $d$-wave superconductor. Further, the thermal conductivity tensor is now given by

$$\kappa_{xx} / \kappa_n = \frac{2}{\pi} \frac{v}{\Delta^2} I^2(\theta)$$

(12)

and

$$\kappa_{xy} / \kappa_n = -\frac{2}{\pi} \frac{v}{\Delta^2} I(\theta)L(\theta)$$

(13)
where

\[ I(\theta) = \frac{1}{\pi} \left( \sqrt{\frac{3+s}{2}} E \left( \sqrt{\frac{2}{3+s}} \right) + \sqrt{\frac{3-s}{2}} E \left( \sqrt{\frac{2}{3-s}} \right) \right) \]

and

\[ L(\theta) = \frac{1}{\pi} \left( \sqrt{\frac{3+s}{2}} E \left( \sqrt{\frac{2}{3+s}} \right) - \sqrt{\frac{3-s}{2}} E \left( \sqrt{\frac{2}{3-s}} \right) \right) \]

with \( s = \sin(2\theta) \).

In Fig. 4 the angular dependences of the functions \((I(\theta))^2\) and \(I(\theta)L(\theta)\) are shown together with \(F(\theta)\). Thus, as in \(d\)-wave superconductors, this state exhibits a fourfold symmetry in \(\kappa_{xx}\). But the angular dependence is about 10\% and may be compatible with the experiments.\[3,4\]. Thus, we conclude that the \(\cos(2\phi)e^{\pm i\phi}\) 2D \(f\)-wave state is the best candidate to describe all of these experimental observations.

As mentioned above, our analysis of the thermal conductivity tensor neglects vortex core scattering. At least in the high-\(T_c\) compounds in a small magnetic field and at low temperatures this contribution can be neglected.\[5,6\]. In Sr_2RuO_4 the vortex core size is larger and at present it is unclear to what extend this contribution plays a role. We expect that the angular dependences shown in Fig. 4 will be weakened both by vortex core scattering and finite temperatures, which will improve agreement with the experiments.

As an additional check on the position of the nodes of the order parameter we propose a measurement of the transverse thermal conductivity \(\kappa_{xy}\). As Eqs. (3) and (4) show, \(\kappa_{xy}\) vanishes, if the nodes lie along the a or b directions. However, we expect a finite transverse thermal conductivity \(\kappa_{xy}\) showing a \(\sin(2\theta)\) variation for the \(\cos(2\phi)e^{\pm i\phi}\) \(f\)-wave state having its nodes along the zone diagonal, as Eq. (3) shows.

\section*{IV. CONCLUSIONS}

We compared one \(p\)-wave and two \(2D\) \(f\)-wave superconducting states with recent experimental data from pure crystals of Sr_2RuO_4. We find that within weak-coupling theory the two \(2D\) \(f\)-wave states give the closest description of the thermodynamic data. Among these, the angular dependence of magnetotransport favors the \(\cos(2\phi)e^{\pm i\phi}\) \(f\)-wave state, since the other two states exhibit much stronger anisotropy than observed experimentally. Therefore, among the simplest states the \(\cos(2\phi)e^{\pm i\phi}\) \(f\)-wave state, having \(B_{1g} \times E_u\) symmetry appears to be the best candidate for superconductivity in Sr_2RuO_4.

\section*{ACKNOWLEDGMENTS}

We thank Y. Maeno and I. Bonalde for providing us with the digital form of their experimental data, which were used in Fig. 3 and Fig. 4.

We also thank K. Izawa, Y. Maeno, Y. Matsuda, and M. A. Tanatar for fruitful discussions on their ongoing experiments. One of us (KM) thanks for the hospitality of N. Schopohl and the University of T¨ubingen where part of this work has been done. HW acknowledges support from the Korean Science and Engineering Foundation (KOSEF) through grant No. 1999-2-114-005-5.

\begin{thebibliography}{99}

\bibitem{1} Y. Maeno \textit{et al}, Nature \textbf{372}, 532 (1994); Y. Maeno Physica C \textbf{282-287}, 206 (1997).
\bibitem{2} T. M. Rice and M. Sigrist, J. Phys. Cond. Mat. \textbf{7}, L643 (1995); M. Sigrist \textit{et al}, Physica C \textbf{317-318}, 134 (1999).
\bibitem{3} G. Luke \textit{et al}, Nature \textbf{394}, 558 (1998).
\bibitem{4} K. Ishida \textit{et al}, Nature \textbf{396}, 653 (1998).
\bibitem{5} S. Nishizaki, Y. Maeno, and Z. Mao, J. Phys. Soc. Jpn. \textbf{69}, 572 (2000); J. Low Temp. Phys. \textbf{117}, 1581 (1999).
\bibitem{6} I. Bonalde, B. D. Yanoff, M. B. Salamon, D. J. Van Harlingen, E. M. E. Chia, Z. Q. Mao and Y. Maeno, preprint.
\bibitem{7} H. Won and K. Maki, Phys. Rev. B \textbf{49}, 1397 (1994).
\bibitem{8} W. N. Hardy, D. A. Bonn, D. C. Morgan, R. Liang, and K. Zhang, Phys. Rev. Lett. \textbf{70}, 3999 (1993).
\bibitem{9} K. Miyake and O. Narikiyo, Phys. Rev. Lett. \textbf{83}, 1423 (1999).
\bibitem{10} I. I. Mazin and D. J. Singh, Phys. Rev. Lett. \textbf{79}, 733 (1997).
\bibitem{11} Y. Hasegawa, K. Machida, and M. Ozaki, J. Phys. Soc. Jpn. \textbf{69}, 336 (2000) (cond-mat/9909310).
\bibitem{12} G. Yang and K. Maki, Fizika \textbf{8}, 345 (1999); H. Won and K. Maki, preprint cond-mat/0006151.
\bibitem{13} M. A. Tanatar, S. Nishizaki, Z. Q. Mao, Y. Maeno, and T. Ishiguro, M2S-HTSC VI proceedings (Houston, February 2000); M. A. Tanatar and Y. Maeno (private communication).
\bibitem{14} K. Izawa and Y. Matsuda (private communication).
\bibitem{15} H. Won and K. Maki, preprint cond-mat/0004102.
\bibitem{16} M. B. Salamon, F. Yu, and V. N. Kopylov, J. Supercond. \textbf{8}, 449 (1995); F. Yu \textit{et al}, Phys. Rev. Lett. \textbf{74}, 5136 (1995).
\bibitem{17} H. Aubin, K. Behnia, M. Ribault, R. Gagnon, and L. Taillefer, Phys. Rev. Lett. \textbf{78}, 2624 (1997).
\bibitem{18} C. Kibert and P. J. Hirschfeld, Solid State Comm. \textbf{105}, 459 (1998); Phys. Rev. Lett \textbf{80}, 4963 (1999). I. Vekhter and P. J. Hirschfeld, preprint cond-mat/9912253.
\bibitem{19} Yu. S. Barash and A. A. Svidzinskii, Phys. Rev. B \textbf{58}, 6476 (1998).
\bibitem{20} M. J. Graf and A. V. Balatsky, preprint cond-mat/0005540.
\bibitem{21} M. Chiao, R. W. Hill, C. Lupien, B. Popic, R. Gagnon, and L. Taillefer, Phys. Rev. Lett. \textbf{82}, 2943 (1999).
\end{thebibliography}