Spin triplet superconductivity with line nodes in Sr$_2$RuO$_4$

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Several possible odd-parity states are listed up group-theoretically and examined in light of recent experiments on Sr$_2$RuO$_4$. Those include some of the f-wave pairing states, $d(k) \propto \hat{z}(k_x + ik_y)$ and $\hat{z}(k_x^2 - k_y^2)(k_x + ik_y)$ and other $\hat{z}(k_x + ik_y) \cos ck_z$ ($c$ is the c-axis lattice constant) as most plausible candidates. These are time-reversal symmetry broken states and have line nodes running either vertically (the former two) or horizontally (the latter), consistent with experiments. Characterizations of these states and other possibilities are given.

KEYWORDS: spin triplet superconductivity, line node of the energy gap, time-reversal symmetry breaking

The possibility of the spin triplet pairing in Sr$_2$RuO$_4$ is pointed out soon after the discovery of the superconductivity. Experimental evidence for the spin triplet pairing is accumulated. The temperature-independent Knight shift for the external magnetic field parallel to the conducting plane (the basal plane) is thought to be the evidence for the spin triplet pairing with the $d$-vector aligned to the $z$-axis. The $\mu$SR experiments indicates that the magnetic field is spontaneously induced and the time reversal symmetry seems to be broken in the superconducting state. These experiments were explained by the $p$-wave spin triplet state with the order parameter

$$d(k) = \Delta_0 \hat{z}(k_x + ik_y),$$

where $\Delta_0$ is a constant. This state is analogous to the Anderson-Brinkman-Morel (ABM) state, which is identified as the A phase in superfluid $^3$He. The AMB state in superfluid $^3$He has point nodes of the energy gap at $k_x = k_y = 0$ on the spherical Fermi surface. However, since the Fermi surface of Sr$_2$RuO$_4$ consists of three cylindrical surfaces, the above $p$-wave state has a finite energy gap on the Fermi surface. The previous experiments of specific heat $C(T)$ and NMR relaxation rate $T_1^{-1}$ showed that about a half of the density of states remains at $T = 0$ in the superconducting state. In order to explain this residual density of states, the non-unitary states and the orbital dependent superconductivity are proposed.

However, it is reported in very recent experiments that the residual density of states are very small in the better samples, i.e. $C(T) \propto T^2$ and $T_1^{-1} \propto T^3$ at low temperatures. These temperature dependences are interpreted as a consequence of the line nodes of the energy gap. The residual density of states observed in the previous experiments may be due to the impurity effects on the anisotropic superconductivity with line nodes.

An anisotropic energy gap model caused by the finite range interaction in the two-dimensional plane is proposed to explain the line-node-like temperature dependences of the specific heat and relaxation rate in Sr$_2$RuO$_4$. The order parameter in this case is given by

$$d(k) = \Delta_0 \hat{z}(\sin ak_x + \sin ak_y),$$

where $a$ is the lattice constant in the basal plane of the tetragonal crystal $D_{4h}$. This anisotropic energy gap should give the exponential temperature dependence as $\exp(-\alpha \Delta/T)$ at temperatures below the smallest energy gap $\Delta$ in clean samples, where $\alpha$ is a constant of the order 1. As far as we know, however, there are no experimental evidence for the existence of the small gap in Sr$_2$RuO$_4$.

The previously classified pairing states with a line node either (A) break the four-fold symmetry in the basal plane such as $\hat{x}k_x$, belonging to the two-dimensional representation $E_u$, which is incompatible with the four-fold symmetric $H_2$ behavior or (B) have the two component $d$ vector such as a non-unitary bipolar state: $\hat{x}k_x + i\hat{y}k_y$, which is incompatible with the Knight shift experiments. Thus, if we accept these experiments, all the previous states becomes unlikely to explain. This is also true for those states listed by Rice and Sigrist and Sigrist and Zhitomirsky.

Here we are going to first list several possible odd-parity states with lower angular momentum allowed under the tetragonal symmetry $D_{4h}$ of Sr$_2$RuO$_4$, then we argue plausibility of these states in light of the existing data where a pairing mechanism is also examined for stabilizing some of the classified states.

In Table I the orbital functions allowed in $D_{4h}$ are derived from the product of the two irreducible representations, which are listed up in Table II.

Among these allowed states the following $f$-pairing states are particularly attractive:
where the order parameter in this class is not the partial kder parameters characterized by the two wave vectors \( m \) and \( \mathbf{n} \).

The experimental facts seem to decomposing. At the moment we do not know how well this out the desired line node except for some special case. 

\[ \gamma \] with \( d \)

So far we only consider the purely two-dimensional order parameters characterized by the two wave vectors \( k_x \) and \( k_y \) in the basal plane. However, there is another class of the states compatible with the experimental data, namely,

\[ d(\mathbf{k}) = \Delta_0 \hat{z}(k_x^2 - k_y^2)R(k_x + ik_y) \]

and

\[ d(\mathbf{k}) = \Delta_0 \hat{z}k_xk_y(k_x + ik_y) \]

because (1) they are both odd-parity states and have single d-vector component, and (2) the four vertical line nodes run along the c-axis and the four-fold symmetry in the basal plane is preserved.

Here we should point out a possibility that these f-pairing states can mix \( p \)-wave pairing in general for D_{\text{hn}}, namely,

\[ d(\mathbf{k}) = \Delta_0 \hat{z}\{k_xk_y(k_x + ik_y) + \gamma(k_y + ik_z)\} \]

with \( \gamma \) being a complex number. This mixing washes out the desired line node except for some special case. Within the present framework we assume that the angular decomposition is nearly complete, neglecting their mixing. At the moment we do not know how well this decomposition is, but the experimental facts seem to demand it.

So far we only consider the purely two-dimensional order parameters characterized by the two wave vectors \( k_x \) and \( k_y \) in the basal plane. However, there is another class of the states compatible with the experimental data, namely,

\[ d(\mathbf{k}) = \hat{z}[f_o(k_x, k_y)(a_0 + a_1 \cos(ck_z) + a_2 \cos(2ck_z) + \ldots) + f_e(k_x, k_y)(b_1 \sin(ck_z) + b_2 \sin(2ck_z) + \ldots)], \]

where the order parameter in this class is not the partial wave in \( k_z \) but the Fourier series with \( c \) being the lattice constant along the c-axis. \( f_o(k_x, k_y) \) and \( f_e(k_x, k_y) \) are the odd and even functions with respect to the inversion in the \( k_x - k_y \) plane, respectively. The previously considered states (eq.(3) and eq.(4)) are two-dimensional states with \( a_0 = 1 \) and \( a_n = b_n = 0 \) \((n > 0)\). We propose the state with \( a_1 \neq 0 \) and other \( a_n \) and \( b_n \) are zero. The order parameter is written as

\[ d(\mathbf{k}) = \Delta_0 \hat{z}(k_x + ik_y)\cos(ck_z). \]

This particular state can be regarded as derived from a product representation \( A_{1g} \times E_u \) and is periodical along the c-axis. This lattice periodicity might be important because all the three Fermi surfaces are open along the c-axis, but close within the basal plane. In fact, this state has horizontal line nodes at \( k_z = \pm \frac{\pi}{\xi_c} \), which run parallel to the basal plane, and breaks the time reversal symmetry. Even if the \( a_0 \) term is mixed, i.e.

\[ d(\mathbf{k}) = \Delta_0 \hat{z}(k_x + ik_y)(\cos(ck_z) + a_0), \]

the horizontal line nodes exist as long as \( a_0 \) is real and \( |a_0| < 1 \).

If we take account of the tetragonal \( \text{K}_2\text{NiF}_4 \) type crystal structure or the body centered tetragonal lattice of Ru, the order parameter,

\[ d(\mathbf{k}) = \Delta_0 \hat{z}(\sin \frac{ak_x}{2} + i \sin \frac{ak_y}{2})\cos \frac{ck_z}{2}, \]

is preferable. This state has the horizontal line nodes at \( k_z = \pm \frac{\pi}{\xi_c} \). This state is possible if the effective intralayer interaction is repulsive and interlayer coupling is attractive, as we discuss below.

Due to the Coulomb interaction the effective interaction will be repulsive between electrons in the same plane. We assume the effective interaction is attractive for electrons at \( r_i \) and \( r_i + r \), if \( r' = r \pm \frac{a}{2} \pm \frac{b}{2} \pm \frac{c}{2} \).

\[ V(r, r') = -V_0, \]

where \( V_0 > 0 \), \( r_i \) and \( r_i + r \) are the lattice sites of \( \text{Ru} \), and \( a \) and \( c \) are the lattice constant in the body centered tetragonal lattice. The Fourier transform of the effective interaction is

\[ V(\mathbf{k}, \mathbf{k}') = -8V_0 \cos \frac{a(k_x - k_x')}{2} \cos \frac{a(k_y - k_y')}{2} \]

where \( k'_x \) is the wave vector of the desired line node.

\[ V(\mathbf{k}, \mathbf{k}') = -8V_0 \cos \frac{a(k_x - k_x')}{2} \cos \frac{a(k_y - k_y')}{2} \]

\[ \times \cos \frac{c(k_z - k_{z}')}{2} \]

\[ = -8V_0 \cos \frac{a(k_x - k_x')}{2} \sin \frac{a(k_y - k_y')}{2} \]

\[ \times \cos \frac{c(k_z - k_{z}')}{2} \]

\[ \times \sin \frac{a(k_x - k_x')}{2} \sin \frac{a(k_y - k_y')}{2} \]

\[ \times \sin \frac{c(k_z - k_{z}')}{2} \sin \frac{c(k_z - k_{z}')}{2} \]

The orbital part of the order parameter caused by this interaction should have the form

\[ \sin \frac{a(k_x - k_x')}{2} \sin \frac{a(k_y - k_y')}{2} \]

\[ \cos \frac{c(k_z - k_{z}')}{2} \]

\[ \sin \frac{c(k_z - k_{z}')}{2} \sin \frac{c(k_z - k_{z}')}{2} \]

\[ \sin \frac{a(k_x - k_x')}{2} \sin \frac{a(k_y - k_y')}{2} \]
in the triplet pairing. These four states have different transition temperature in the weak coupling limit, but the first two states are degenerate. Although we have to calculate in more detail to find which state is most stable, we think the order parameter
d(k) = \tilde{\Delta}_0 \left( \sin \frac{ak_x}{2} \cos \frac{ak_y}{2} + i \cos \frac{ak_x}{2} \sin \frac{ak_y}{2} \right) \times \cos \frac{ck_z}{2} \tag{13}

will possibly be the stable state. If we neglect the \( k_x \) and \( k_y \) dependences in \( \cos \frac{ak_x}{2} \) and \( \cos \frac{ak_y}{2} \), we get the order parameter given in eq. (9).

We propose some experiments to test the horizontal and vertical line nodes. The thermal conductivity will have weak dependence on the direction in the \( x-y \) plane and have a power low dependence on temperature, if the line nodes are horizontal. On the other hand it will show strong four-fold symmetry and exponential dependences in some direction if the superconducting state has the vertical nodes of the energy gap. The penetration depth will also show the orientation of the line node. This kind of the orientation dependent transport measurements, including the ultrasound attenuation was decisive in identifying the intricate gap structure of another triplet superconductor \( \text{UPt}_3 \).\footnote{[3] K. Ishida, H. Mukuda, Y. Kitaoka, K. Asayama, Z.Q. Mao, Y. Mori and Y. Maeno: Nature (London) 396 (1998) 658.}

The Josephson effect between conventional superconductors and \( \text{Sr}_2\text{RuO}_4 \) is observed and shows the interesting temperature dependences.\footnote{[4] A. Sumiyama, M. Ichioka and A.G. Lebed for helpful discussions.} Some explanations are given. Although the experimental study of the direction-dependence of the Josephson effect will be difficult because of the roughness of the interface, the existing of the Ru lamellas and 3K phases can consider the ideal Josephson junction. Since all the states considered in this paper have \( d \parallel \hat{z} \), the Josephson current \( I \parallel \hat{z} \) between the triplet and the singlet superconductors is forbidden in the first order in the spin-orbit coupling.\footnote{[5] Y. Maeno, H. Hashimoto, K. Yoshida, S. Nishizaki, T. Fujita, J.G. Bednorz and F. Lichtenberg: Nature (London) 372 (1994) 532.} The Josephson current between spin triplet and spin singlet is possible, if the \( d \) vector is not parallel to the current and the total (spin plus angular) momentum is conserved. In the states given in eq. (3), eq. (9) or eq. (13), the Josephson current in the \( x-y \) plane is canceled, since the order parameter changes the sign in the \( k_z \)-direction. However, the Fermi surface is corrugated as observed by angle-dependent magnetoresistance oscillation and the angle dependence of the de Haas van Alphen effect and as a result the cancellation will not be perfect. In the presence of the mixing of the \( k_z \) independent term (as in eq. (5)) the Josephson current is also finite.

The horizontal line nodes will be most clearly seen by the neutron scattering. Since the quasi-particles are excited around \( k_z = \pm \frac{\pi}{c} \) in the superconducting state eq. (1) or eq. (13), the excitations between these quasi-particles, i.e. excitations with \( q_z = \pm \frac{2\pi}{c} \) will become large. The neutron scattering experiment below \( T_c \) will have peaks at \( q_z = \pm \frac{2\pi}{c} \), while it is almost independent of \( q_z \) above \( T_c \).

As a final remark, we point out the following additional possibilities:

1. Suppose that we disregard the \( \mu \text{SR} \) experiment.\footnote{[1] T.M. Rice and M. Sigrist: J. Phys. Condens. Matter 7 (1995) L643.}

Among the previous states, the non-unitary bipolar state, described by

\[ d(k) = \Delta_0 (\hat{z}k_x + i\hat{y}k_y) \tag{14} \]

has line nodes for both up-spin and down-spin pair branches, thus there is no residual \( T \)-linear specific heat. This state does not exhibit the macroscopic spontaneous moment averaged over the Fermi surfaces below \( T_c \). Since the effective spin-orbit coupling felt by the Cooper pairs may be small in \( \text{Sr}_2\text{RuO}_4 \), the \( d \) vector can rotate in the spin space. When the external field \( H \) is in the basal plane, the non-unitary bipolar state becomes

\[ d(k) = \Delta_0 (\hat{z}k_x + \hat{j}k_y) \tag{15} \]

with \( \hat{j} \) being a vector lying in the basal plane which is rotatable so as to keep \( H \parallel \hat{j} \), being consistent with the Knight shift experiment.\footnote{[2] Y. Maeno, H. Hashimoto, K. Yoshida, S. Nishizaki, T. Fujita, J.G. Bednorz and F. Lichtenberg: Nature (London) 372 (1994) 532.} As another possibility, the time reversal symmetry conserved state becomes a candidate such as \( \hat{z}k_x \) or \( \hat{z}k_y \) which are degenerate in \( D_{4h} \). They form a domain structure in real system which may preserve the overall four-fold symmetry. Note that there is no four-fold symmetric states without the variable \( k_z \) in our classified states.\footnote{[3] K. Ishida, H. Mukuda, Y. Kitaoka, K. Asayama, Z.Q. Mao, Y. Mori and Y. Maeno: Nature (London) 396 (1998) 658.}

(2) Suppose further that we disregard the Knight shift experiment in addition to the \( \mu \text{SR} \) experiment.\footnote{[4] A. Sumiyama, M. Ichioka and A.G. Lebed for helpful discussions.} Then the following singlet pairings with line nodes are another candidates, including

\[ \Delta(k) = \Delta_0 k_x k_y (k_x^2 - k_y^2) \quad \text{for } A_{2g} \tag{16} \]

\[ \Delta(k) = \Delta_0 k_x^2 - k_y^2 \quad \text{for } B_{1g} \tag{17} \]

\[ \Delta(k) = \Delta_0 k_x k_y \quad \text{for } B_{2g}. \tag{18} \]

These singlet states might be stabilized by the observed antiferromagnetic fluctuations,\footnote{[3] K. Ishida, H. Mukuda, Y. Kitaoka, K. Asayama, Z.Q. Mao, Y. Mori and Y. Maeno: Nature (London) 396 (1998) 658.} whose wave vector is \( \mathbf{Q} \sim (\frac{2\pi}{3c}, 0, 0) \).

In conclusion, we list up and examine the several possible superconducting states in \( \text{Sr}_2\text{RuO}_4 \), including some of the \( f \)-pairing states, \( \hat{z}k_x k_y (k_x + ik_y) \) and \( \hat{z}(k_x^2 - k_y^2)(k_x + ik_y) \) and other \( \hat{z}(k_x + ik_y) \cos ck_z \). These states explain the experiments of \( \mu \text{SR} \), NMR and the specific heat. Experiments to distinguish these states are proposed.

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\[ \Delta(k) = \Delta_0 k_x k_y \quad \text{for } B_{2g}. \tag{18} \]
[4] G.M. Luke, Y. Fudamoto, K.M. Kojima, M.I. Larkin, J. Mer- rin, B. Nachumi, Y.J. Uemura, Y. Maeno, Z.Q. Mao, H. Nakamura and M. Sigrist: Nature (London) 394 (1998) 558.
[5] K. Machida, M. Ozaki and T. Ohmi: J. Phys. Soc. Jpn. 65 (1996) 3720.
[6] M. Sigrist and M. Zhitomirsky: J. Phys. Soc. Jpn. 65 (1996) 3452.
[7] A.J. Leggett: Rev. Mod. Phys. 47 (1975) 331.
[8] S. Nishizaki, Y. Maeno, S. Farner, S. Ikeda and T. Fujita: J. Phys. Soc. Jpn. 67 (1998) 560.
[9] K. Ishida, Y. Kitaoka, S. Ikeda, K. Asayama, Y. Maeno, K. Yoshida and T. Fujita: Phys. Rev. B 56 (1997) R505.
[10] Y. Maeno, S. Nishizaki, K. Yoshida, S. Ikeda and T. Fujita: J. Low Temp. Phys. 105 (1996) 1577.
[11] D.P. Agterberg, T.M. Rice and M. Sigrist: Phys. Rev. Lett. 78 (1997) 3374.
[12] K. Ishida: private communications.
[13] Y. Maeno: private communications.
[14] K. Miyake and O. Narikiyo: Phys. Rev. Lett. 83 (1999) 1423.
[15] Z.Q. Mao, Y. Maeno, T. Akima and T. Ishiguro, preprint.
[16] Note that we cannot improve this situation by extending the $p$-wave basis function to the periodic form: $k_x \rightarrow \sin ak_x$

$\ k_y \rightarrow \sin ak_y$ such as shown in eq. 17.

[17] See, for example, K. Machida, T. Nishira and T. Ohmi: J. Phys. Soc. Jpn. 68 (1999) No.10.
[18] R. Jin, Y. Zadorozhny, Y. Liu, D.G. Schlom, Y. Mori and Y. Maeno: Phys. Rev. B 59 (1999) 4433.
[19] C. Honerkamp and M. Sigrist: Prog. Theor. Phys. 100 (1998) 53.
[20] M. Yamashiro, Y. Tanaka and S. Kashiwaya: J. Phys. Soc. Jpn. 67 (1998) 3364.
[21] A. Sumiyama et al.: unpublished.
[22] V.B. Geshkenbein and A.I. Larkin: JETP Lett. 43 (1986) 395.
[23] Y. Hasegawa: J. Phys. Soc. Jpn. 67 (1998) 3699.
[24] Y. Yoshida, A. Mukai, R. Settai, Y. Onuki and H. Takei: J. Phys. Soc. Jpn. 67 (1998) 2551.
[25] E. Ohmichi, H. Adachi, Y. Mori, Y. Maeno, T. Ishiguro and T. Oguchi: Phys. Rev. B 59 (1999) 7263.
[26] Y. Yoshida, R. Settai, Y. Onuki, H. Takei, K. Betsuyaku and H. Harima: J. Phys. Soc. Jpn. 67 (1998) 1677.
[27] I.I. Mazin and D.J. Singh: Phys. Rev. Lett. 82 (1999) 4324.
[28] Y. Sidis, M. Braden, P. Bourges, B. Hennion, S. Nishizaki, Y. Maeno and Y. Mori: e-print, cond-mat/9904343.