Spin-triplet superconductivity due to antiferromagnetic spin-fluctuation in Sr$_2$RuO$_4$

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(March 21, 2022)

A mechanism leading to the spin-triplet superconductivity is proposed based on the antiferromagnetic spin fluctuation. The effects of anisotropy in spin fluctuation on the Cooper pairing and on the direction of $d$ vector are examined in the one-band Hubbard model with RPA approximation. The gap equations for the anisotropic case are derived and applied to Sr$_2$RuO$_4$. It is found that a nesting property of the Fermi surface together with the anisotropy leads to the triplet superconductivity with the $d = \hat{z}(\sin k_x \pm i \sin k_y)$, which is consistent with experiments.

Since the discovery of superconducting phase in Sr$_2$RuO$_4$ [1], much effort has been paid for understanding its exotic properties. Among several interesting natures, the most fascinating one is that it is a spin-triplet superconductor confirmed by NMR experiment [2]. While most superconductors found during several decades are singlet, the only exceptions were $^3$He and UPt$_3$. Therefore the fact that the triplet pairing is realized in Sr$_2$RuO$_4$ has attracted much attention. While UPt$_3$, the second example of spin-triplet superconductor, has a complicated electronic structure, Sr$_2$RuO$_4$ has a rather simple electronic state [3]. Thus clarifying the microscopic mechanism of superconductivity in Sr$_2$RuO$_4$ is very important for understanding the triplet superconductors in general.

In $^3$He, Cooper pairs are formed due to ferromagnetic spin fluctuations peaked at $q = 0$ [4]. Therefore it is natural to expect the origin of the triplet pairing in Sr$_2$RuO$_4$ is also ferromagnetic spin fluctuation [4]. This assumption has been believed to be justified by NMR experiments [5]. However the recent neutron scattering experiment has shown that there exists a significant peak near $q_0 = (\pm 2\pi/3, \pm 2\pi/3)$ and no sizable ferromagnetic spin fluctuation [6]. Thus it is difficult to assume that the spin fluctuation near $q_0$ plays no role in the Cooper pairing in Sr$_2$RuO$_4$. (In the following discussion we call this fluctuation as antiferromagnetic (AF) spin fluctuation, for simplicity.) However this AF fluctuation leads to the singlet superconductivity rather than the triplet superconductivity as expected in analogy to high-$T_c$ cuprates [7].

In this paper we propose a mechanism which gives the triplet pairing even if the spin fluctuation is AF. We find that the characteristic features of Sr$_2$RuO$_4$ are twofold: One is the anisotropy of the spin fluctuation found in NMR experiments [6], and the other is a nesting property with momentum $q_0$ of the two-dimensional Fermi surface. We show that these two features explain the pairing in Sr$_2$RuO$_4$. In addition to the competition between singlet and triplet pairing, the direction of the $d$ vector, which is the order parameter of triplet superconductivity, is another interesting problem. We show that the anisotropy of the spin fluctuation also explains the experimental fact that the $d$ vector is parallel to the $z$-direction [7]. First we extend the RPA formulation to the case of anisotropic spin fluctuation. Using the obtained effective interactions, we investigate the most stable pairing based on the weak-coupling gap equations. When the spin fluctuation is isotropic, the so-called $d_{x^2-y^2}$-wave pairing is the most stable. However when the anisotropy is increased, the state corresponding to $\hat{z}(\sin k_x \pm i \sin k_y)$, which is the prime candidate of Sr$_2$RuO$_4$, becomes the most stable.

For the $\gamma$ band which is one of the three bands in Sr$_2$RuO$_4$ [1], we assume a two-dimensional effective Hamiltonian

$$H = H_0 + \frac{I}{2N} \sum_{\mathbf{k} \mathbf{k}' \sigma} c_{\mathbf{k} \sigma}^\dagger c_{\mathbf{k}' - \mathbf{q} \sigma} c_{\mathbf{k}' - \mathbf{q} - \mathbf{q} + \sigma} c_{\mathbf{k} + \mathbf{q} \sigma},$$

where $c_{\mathbf{k} \sigma}$ is the annihilation operator of an electron with momentum $\mathbf{k}$ and spin $\sigma$. We consider only the on-site Coulomb repulsion, $I$, as in the previous studies of spin-fluctuation mechanism. Among the three bands, we consider the $\gamma$ band consisting of the antibonding band of Ru 4$d_{x^2-y^2}$ and O 2$p_x$ orbitals in this paper, because it has the largest density of states at Fermi energy and the superconductivity is considered to be realized predominantly in the $\gamma$ band [1]. Although the spin fluctuation near $q_0$ is understood from the nesting effect of $q_0$, it is the most fascinating problem of Sr$_2$RuO$_4$.

The anisotropy of spin fluctuation observed experimentally is implicitly included in the two-body Hamiltonian, $H_0$. Our purpose is not to investigate the origin

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74.20-z, 74.20Mn, 74.25Dw
of anisotropy in details but to examine the role of the anisotropy to Cooper pairing. Therefore we introduce a phenomenological parameter $\alpha$ by

$$\chi_{(+,0)}(q) = \alpha \chi_{(\uparrow\uparrow,0)}(q), \quad (2)$$

where $\chi_{(\uparrow\uparrow,0)}(q)$ (or $\chi_{(+,0)}(q)$) is the unperturbed static susceptibility of $z$ axis $(xy$ plane$)$, which originates from $H_0$. The parameter $\alpha$ represents the anisotropy of spin fluctuation and we take $\alpha \leq 1$ since NMR experiments show that $\chi_{(\uparrow\uparrow,0)} < \chi_{(+,0)}$ [13].

Using this one-band model, we discuss the effective interactions between Cooper pairs due to spin fluctuations. Summation of bubble and ladder diagrams (i.e., RPA approximation) gives

$$H_{\text{int}} = -\sum_{kk's} V_{b.o}(k-k')c_{ks}^{\dagger}e_{-ks}c_{k's} + \sum_{kk's} V_{b.e}(k-k')c_{ks}^{\dagger}c_{-ks}^{\dagger}e_{-ks}c_{k's} - \sum_{kk's} V_{\text{lad}}(k-k')c_{ks}^{\dagger}c_{-ks}^{\dagger}e_{ks}c_{k's}^{\dagger}, \quad (3)$$

with

$$V_{b.o}(k-k') = \frac{I}{N} \frac{(I/N)\chi_{(\uparrow\uparrow,0)}(k-k')}{1 - (I/N)^2\chi_{(\uparrow\uparrow,0)}(k-k')},$$

$$V_{b.e}(k-k') = \frac{I}{N} \frac{(I/N)^2\chi_{(\uparrow\uparrow,0)}(k-k')}{1 - (I/N)^2\chi_{(\uparrow\uparrow,0)}(k-k')},$$

$$V_{\text{lad}}(k-k') = \frac{I}{N} \frac{(I/N)\chi_{(+,0)}(k-k')}{1 - (I/N)\chi_{(+,0)}(k-k')}.$$ \quad (4)

Here $V_{b.o}$ ($V_{b.e}$) comes from the summation of diagrams with odd (even) number of bubbles, and $V_{\text{lad}}$ from the ladder diagrams. It is apparent that $V_{b.o}$ is between the electrons with equal spins while $V_{b.e}$ and $V_{\text{lad}}$ are between those with the opposite spins.

It is straightforward to derive the gap equations in the anisotropic case, using the method developed by Leggett [13]. First we introduce the operators

$$t_k^{(0)} = \sum_{ss'}(\sigma_2)_{ss'}c_{ks}^{\dagger}c_{ks'},$$

$$t_k^{(a)} = \sum_{ss'}(\sigma_a\sigma_2)_{ss'}c_{ks}^{\dagger}c_{ks'}, \quad \text{for} \quad a = 1, 2, 3,$$ \quad (5)

where $\sigma_a (a = 1, 2, 3)$ are Pauli matrices. The operator $t_k^{(0)}$ ($t_k^{(a)}$) corresponds to spin singlet (triplet) Cooper pairs. In terms of these operators, the effective interaction [8] can be rewritten as

$$H_{\text{int}} = \frac{1}{4} \sum_{kk'} V_{\text{sin}}(k-k')t_k^{(0)t_k^{(0)}},$$

$$+ \frac{1}{4} \sum_{kk'} \sum_{a=1}^{3} V_{\text{tri}}^{(a)}(k-k')t_k^{(a)t_{k'}^{(a)}},$$ \quad (7)

where

$$V_{\text{sin}}(k-k') = 2[V_{b.o}(k-k') + V_{\text{lad}}(k-k')],$$

$$V_{\text{tri}}^{(1)}(k-k') = V_{\text{tri}}^{(2)}(k-k') \equiv -2V_{b.o}(k-k'),$$

$$V_{\text{tri}}^{(3)}(k-k') \equiv 2[V_{b.e}(k-k') - V_{\text{lad}}(k-k')].$$ \quad (8)

Since Sr$_2$RuO$_4$ has a long coherence length in $ab$ plane, $\xi_{ab} \approx 660$ Å [13], we use field-mean approximation to $H_{\text{int}}$. We restrict the discussion to unitary states because it is unrealistic to assume non-unitary states in Sr$_2$RuO$_4$ [13]. Requiring that there is no coexistence of singlet and triplet pairs, we obtain the gap equations

$$\Delta(k) = -\sum_{k'} V_{\text{sin}}(k-k')\Delta(k')\Theta(E_{\text{sin}}(k')),$$

$$d^{(a)}(k) = -\sum_{k'} V_{\text{tri}}^{(a)}(k-k')d^{(a)}(k')\Theta(E_{\text{tri}}(k')),$$ \quad (9)

where $\Theta(E) = \frac{1}{2}\tanh\frac{E}{kT}$, $E_{\text{sin}}(k) = 2\sin k_x \alpha + \Delta(k)\Delta^*(k)$, and $E_{\text{tri}}(k) = 2\sin k_x + d(k) - d^*(k)$ with $\xi_k = \varepsilon_k - \mu$.

The singlet and triplet order parameters are defined as

$$\Delta(k) = -\frac{i}{2} \sum_{k'} V_{\text{sin}}(k-k')\langle t_k^{(0)} \rangle$$

$$d^{(a)}(k) = -\frac{i}{2} \sum_{k'} V_{\text{tri}}^{(a)}(k-k')\langle t_k^{(a)} \rangle$$

and $\langle t_k^{(0)} \rangle$ and $\langle t_k^{(a)} \rangle$ are the expectation values of $t_k^{(0)}$ and $t_k^{(a)}$, respectively. Here $d(k)$ is the so-called $d$ vector for the triplet superconductivity.

In the system with the rotational symmetry in spin space, $\chi_{(+,0)}(q) = \chi_{(+,0)}(q)$ is satisfied and thus the relation $V_{b.o} + V_{b.e} = V_{\text{lad}}$ holds. In this case, it is easy to see $V_{\text{tri}}^{(1)}(k-k') = V_{\text{tri}}^{(2)}(k-k') = V_{\text{tri}}^{(3)}(k-k')$. On the other hand, the gap equation in Eq. (9) for the triplet pairing becomes dependent on the direction of the $d$ vector in the anisotropic case. It means that the vector has some preferred direction if the triplet pairs are formed by anisotropic spin fluctuations. This is naturally understood because the $d$ vector is orthogonal to the spin direction of triplet Cooper pairs [13]. For the present case with $\chi_{(+,0)}(q) < \chi_{(+,0)}(q)$ (i.e., $\alpha < 1$) which is applied to the Sr$_2$RuO$_4$, we can see from Eq. (9) that $V_{\text{lad}}(k-k')$ is suppressed and the effective interaction $V_{\text{tri}}^{(3)}(k-k')$ approaches $V_{\text{sin}}(k-k')$. Consequently the triplet superconductivity with $d^{(0)}(k)$ (i.e., $d || z$) can be stabilized even due to the AF spin fluctuations.

In order to determine the symmetry of the superconducting order parameter, we have to take account of their sign change along the Fermi surface. For the high-$T_c$ superconductors, the AF spin fluctuation with momentum $(\pi,\pi)$ stabilizes the singlet $d_{x^2-y^2}$-wave superconductivity. In that case, the singlet order parameters $\Delta(k')$ with $k' = (\pi, 0)$ and $\Delta(k)$ with $k = (0, \pi)$ have the opposite sign, so that the gap equation in Eq. (9) is satisfied with $V_{\text{sin}}(\pi, \pi) > 0$.

For Sr$_2$RuO$_4$ we consider that a kind of nesting property of the Fermi surface plays an important role. This is the second point of our mechanism. Figure 1 shows a schematic Fermi surface for the $\gamma$ band. Since the AF fluctuation in Sr$_2$RuO$_4$ has momentum $q_0$, the Fermi surface is also shifted by $(2\pi/3, 2\pi/3)$ in Fig. 1. It is apparent that some part of the shifted Fermi surface overlaps
with the original Fermi surface with modulo $2\pi$. In analogy to the case of high-$T_c$ superconductivity, if the superconducting order parameters have the opposite sign on these overlapping portions of the Fermi surface, the gap equation is satisfied with $V_{\text{tri}}(\phi) = 0$. From Fig. 1, it is natural to consider the p-wave pairing instead of the singlet $d_{x^2-y^2}$-wave pairing.

In order to clarify this point quantitatively, we compare various kinds of anisotropic superconductivity using the effective interaction and the simplified Fermi surface. Near the transition temperature $T_c$, we rewrite the gap equations as

$$\phi(\mathbf{k}) = -\sum_{k'} V_\phi(\mathbf{k} - \mathbf{k'}) \phi(\mathbf{k'}) \frac{1}{2k'} \tanh \frac{\beta k}{2},$$

where $\phi(\mathbf{k})$ represents one of the order parameters $\Delta(\mathbf{k})$ or $d^\phi(\mathbf{k})$, and $V_\phi$ is determined from Eqs. (3) depending on $\phi$. In the weak coupling approximation, $T_c$ is obtained as

$$k_B T_c = 1.13\hbar v_F k_c \exp \left[ -\frac{1}{N(0) \langle \langle \phi \rangle \rangle_{FS}} \right],$$

where $v_F$, $k_c$, and $N(0)$ are the Fermi velocity, cut-off of the wave number, and the density of states at the Fermi energy, respectively. $\langle \langle \phi \rangle \rangle_{FS}$ means the average over the Fermi surface,

$$\langle \langle \phi \rangle \rangle_{FS} = \frac{\int_{FS} d\mathbf{k} \int_{FS} d\mathbf{k}' V_\phi(\mathbf{k} - \mathbf{k'}) \phi(\mathbf{k}) \phi(\mathbf{k}')}{\int_{FS} d\mathbf{k}} \int_{FS} d\mathbf{k} \phi^2(\mathbf{k}).$$

We identify that the order parameter which gives the largest $N(0) \langle \langle \phi \rangle \rangle_{FS}$ is realized.

For Sr$_2$RuO$_4$ we choose order parameters $\phi(\mathbf{k})$ as follows

$$\phi_1(\mathbf{k}) = \cos k_x + \cos k_y,$$
$$\phi_2(\mathbf{k}) = \cos k_x - \cos k_y,$$
$$\phi_3(\mathbf{k}) = \sin k_x \sin k_y,$$
$$\phi_4(\mathbf{k}) = \sin k_x, (d \perp z),$$
$$\phi_5(\mathbf{k}) = \sin k_x, (d || z),$$

where $\phi_1 \sim \phi_3$ correspond to singlet pairings, and $\phi_4$, $\phi_5$ to triplet pairings, respectively. The most probable candidate for Sr$_2$RuO$_4$ is $\hat{z}(\sin k_x \pm i \sin k_y)$ which is equivalent to $\phi_5$ just below $T_c$, because the gap equation (10) for $\sin k_x \pm i \sin k_y$ is exactly same as that for $\phi_5$. If $N(0) \langle \langle \phi_5 \rangle \rangle_{FS}$ is the largest, we expect that the order parameter $d(\mathbf{k}) = \hat{z}(\sin k_x \pm i \sin k_y)$ is realized, because near zero temperature it acquires a larger energy gap than $\phi_5$.

To emphasize the characteristic feature of the nesting, we assume the simplified Fermi surface as shown in Fig. 1. For the $q$ dependence of $\chi(q,q')$ with a maximum at $q_0$, we use the susceptibility obtained in the LDA calculation [2], and fix $S(0) = 0.8$ with $S(q) = \frac{1}{N} \chi(q,q')(q')$. We regard $S(q_0)$ as a phenomenological parameter.

Figure 2 shows the $\alpha$ dependence of $N(0) \langle \langle \phi_5 \rangle \rangle_{FS}$ ($n = 1 \sim 5$) for $S(q_0) = 0.95$. We examined various choices of $S(q_0)$ from 0.90 to 0.99 to find that the results do not change qualitatively. When the anisotropy is weak ($\alpha \sim 1$), the singlet $d_{x^2-y^2}$-wave superconductivity, $\phi_2$, is stabilized. On the other hand, when $\alpha$ is small, the order parameter $\phi_5$ is stabilized which is consistent with experiments.

![FIG. 1. A schematic Fermi surface for the $\gamma$ band of Sr$_2$RuO$_4$. In order to show the nesting property, the Fermi surface shifted by the AF wave number, $q_0$, is also shown by the solid line. The thin dashed lines indicates the Fermi surfaces in the extended Brillouin zone.](image)

![FIG. 2. The dependence of the anisotropy parameter, $\alpha$, of $N(0) \langle \langle \phi_5 \rangle \rangle_{FS}$ ($n = 1 \sim 5$) for $S(q_0) = 0.95$.](image)
region where the state corresponding to \( \hat{z} (\sin k_x \pm i \sin k_y) \) is realized.

Finally we discuss the competition between the singlet \( \cos k_x - \cos k_y \) pairing and the triplet \( \hat{z} (\sin k_x \pm i \sin k_y) \) pairing in terms of the effective interaction and the nesting property. From the explicit form of \( V_{\phi_n} \) for \( n = 2 \) and 5, we can see that a relation \( V_{\phi_2} \geq V_{\phi_5} \) is satisfied. Therefore if we consider only the magnitude of the effective interaction, the singlet pairing is favorable. However the nesting property favors the triplet pairing. Let us assume that \( V_{\phi_n} \) is enhanced very strongly by the AF fluctuation and approximated as

\[
V_{\phi_n}(q) = \frac{I}{N} A_n \delta(q_x \pm 2\pi/3) \delta(q_y \pm 2\pi/3),
\]

with \( \delta \) being the \( \delta \) function with modulo 2\( \pi \). Using this approximated form of \( V_{\phi_n}(n = 2 \) and 5), we obtain

\[
\begin{align*}
N(0) \langle \langle V_{\phi_2} \rangle \rangle_{FS} &= [-2.79 \times 10^{-2}\delta(0) + 4.91 \times 10^{-2}] A_2, \\
N(0) \langle \langle V_{\phi_5} \rangle \rangle_{FS} &= [4.24 \times 10^{-2}\delta(0) + 5.06 \times 10^{-2}] A_5.
\end{align*}
\]

This estimation shows that the \( \hat{z} (\sin k_x \pm i \sin k_y) \) pairing utilizes the peak of \( \chi(\uparrow \uparrow, 0)(q) \) at \( q_0 \) more effectively than \( \cos k_x - \cos k_y \) pairing does. Therefore, even if \( A_2 > A_5 \), the triplet pair can be stabilized.

In determining the phase diagram in Fig. 3, we have assumed simple functional forms of the order parameters, \( \phi_n(k) \). For the detailed calculations, it will be necessary to optimize the \( k \)-dependence of \( \phi_n(k) \). However the global feature of the phase diagram will not change.

In summary, we have generalized the RPA formulation of the effective interaction due to the spin fluctuations and derived gap equations including the anisotropic case. We have shown that the state corresponding to \( \hat{z} (\sin k_x \pm i \sin k_y) \) becomes the most stable even if the AF spin fluctuation is dominant, when the anisotropy is strong enough and the nesting property of the Fermi surface is present. Although the nesting for the actual Fermi surface will be weaker than what we assumed here, it is reasonable to think that our mechanism is the most promising one as far as the AF fluctuation is dominant.

In this paper we have investigated the pairing in the \( \gamma \) band. However it is straightforward to consider the other bands (\( \alpha \) and \( \beta \) bands) in Sr\(_2\)RuO\(_4\). Since the nesting property will be comparable or even stronger for these bands than for the \( \gamma \) band, we expect the same mechanism for triplet superconductivity for \( \alpha \) and \( \beta \) bands even if the \( \gamma \) band does not have the peak near \( q_0 \).

It is reported that Sr\(_2\)RuO\(_4\) has exotic property called as 3K phase \[17\] when Ru metal is embedded in the single crystal. We speculate that the enhancement of \( T_c \) is due to the increase of the anisotropy (i.e., decrease of \( \alpha \)) near the interface region between Sr\(_2\)RuO\(_4\) and Ru metal. We consider that to investigate the origin of the anisotropy is very important both for understanding the superconductivity and for finding the new exotic phenomena.

We are grateful for useful discussions with M. Sigrist, Y. Maeno and Y. Matsuda. One of the authors (T.K.) thanks to H. Namaizawa for useful instructions.

\[1\] Y. Maeno, H. Hashimoto, K. Yoshida, S. NishiZaki, T. Fujita, J. G. Bednorz, and F. Lichtenberg, Nature 372, 532 (1994).
\[2\] K. Ishida, H. Mukuda, Y. Kitaoka, K. Asayama, Z.Q. Mao, Y. Mori and Y. Maeno, Nature 396, 658 (1998).
\[3\] For a review, see D. J. Scalapino, Proceedings of MOS99, [cond-mat/9908287].
\[4\] S. Nakajima, Prog. Theor. Phys. 50, 1101 (1973).
\[5\] I. I. Mazin and D. J. Singh, Phys. Rev. Lett. 82, 4324 (1999).
\[6\] M. Sigrist, et al., Physica C317-318, 134 (1999).
\[7\] T. Imai, A. W. Junt, K. R. Thurber, and F. C. Chou, Phys. Rev. Lett. 81, 3006 (1998).
\[8\] H. Mukuda, et al., J. Phys. Soc. Jpn. 67, 3945 (1998).
\[9\] H. Mukuda, et al., Phys. Rev. B60, 12279 (1999).
\[10\] Y. Sidis, et al., Phys. Rev. Lett. 83, 3320 (1999).
\[11\] T. Oguchi, Phys. Rev. B51, 1385 (1995); D. J. Singh, Phys. Rev. B52, R505 (1997).
\[12\] D. Agterberg, T. M. Rice, and M. Sigrist, Phys. Rev. Lett. 78, 3374 (1997).
\[13\] A. J. Leggett, Ann. Phys. 85, 11 (1974).
\[14\] T. Akima, S. NishiZaki, and Y. Maeno, J. Phys. Soc. Jpn. 68, 694 (1999).
\[15\] K. Ishida, et al., Phys. Rev. B56, R505 (1997).
\[16\] D. Vollhardt and P. Wölfle, The Superfluid Phases of Helium 3, Taylor&Francis (1990).
\[17\] Y. Maeno, T. Ando, Y. Mori, E. Ohmichi, S. Ikeda, S. NishiZaki, and S. Nakatsuji, Phys. Rev. Lett. 81, 3765 (1998).