Spin-Triplet Superconductivity due to Antiferromagnetic Spin-Fluctuation in Sr_2RuO_4

Takeshi Kuwabara* and Masao Ogata†
Department of Basic Science, Graduate School of Arts and Sciences, University of Tokyo, Komaba, Tokyo 153-8902, Japan
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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 $\boldsymbol{d}$ vector are examined in the one-band Hubbard model with random-phase approximation. The gap equations for the anisotropic case are derived and applied to Sr_2RuO_4. It is found that a nesting property of the Fermi surface together with the anisotropy leads to the triplet superconductivity with the $\boldsymbol{d} = \hat{z}(\sin k_x \pm i \sin k_y)$, which is consistent with experiments.

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Since the discovery of the superconducting phase in Sr_2RuO_4 [1], much effort has been paid for understanding its exotic properties. Among its several interesting features, the most fascinating one is that it is a spin-triplet superconductor confirmed by NMR experiment [2]. While most superconductors found during the last several decades are singlet, the only exceptions were ^{3}He and UPt_3. Therefore, the fact that the triplet pairing is realized in Sr_2RuO_4 has attracted much attention. While UPt_3 has a complicated electronic structure, Sr_2RuO_4 has a rather simple electronic state [1]. Thus clarifying the microscopic mechanism of superconductivity in Sr_2RuO_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 $\boldsymbol{q} = \boldsymbol{0}$ [3,4]. Therefore it is natural to expect that the origin of the triplet pairing in Sr_2RuO_4 is also ferromagnetic spin-fluctuation [5,6]. This assumption has been believed to be justified by NMR experiments [7–9]. However, the recent neutron scattering experiment has shown that there exists a significant peak near $\boldsymbol{q}_0 = (\pm 2\pi/3, \pm 2\pi/3)$ and no sizable ferromagnetic spin-fluctuation [10]. Thus it is difficult to assume that the spin-fluctuation near $\boldsymbol{q}_0$ plays no role in the Cooper pairing in Sr_2RuO_4. [In the following discussion we call this fluctuation antiferromagnetic (AF) spin-fluctuation, for simplicity.] However, this AF fluctuation leads to the singlet superconductivity rather than triplet, as expected in analogy to high-T_c cuprates [5].

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_2RuO_4 are twofold: One is the anisotropy of the spin-fluctuation found in NMR experiments [8,9] and the other is a nesting property with momentum $\boldsymbol{q}_0$ of the two-dimensional Fermi surface. We show that these two features explain the pairing in Sr_2RuO_4. In addition to this, it is found that the anisotropy of the spin-fluctuation explains the experimental fact that the $\boldsymbol{d}$ vector is parallel to the z direction [2]. First we extend the random-phase approximation (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_2RuO_4, becomes the most stable.

For one of the three bands in Sr_2RuO_4 [11], we assume a two-dimensional effective Hamiltonian

$$H = H_0 + \frac{I}{2N} \sum_{kk'q\sigma} c^\dagger_{k\sigma} c^\dagger_{k'-\sigma} c_{k'-q-\sigma} c_{k+q\sigma} , \quad (1)$$

where $c_{k\sigma}$ is the annihilation operator of an electron and only the on-site Coulomb repulsion, I, is considered as in the previous studies of spin-fluctuation mechanism. In the following we consider a band with Fermi surface similar to the β or γ band in Sr_2RuO_4. Although the spin-fluctuation near $\boldsymbol{q}_0$ is understood from the nesting effect of α and β bands [5], the wave-number dependence of spin-fluctuation can be common in the three bands due to some interactions.

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 of anisotropy in detail [12,13] but to examine the role of anisotropy on Cooper pairing. Therefore we introduce a phenomenological parameter α by

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

where $\chi_{(\uparrow\uparrow,0)}(\boldsymbol{q})$ [$\chi_{(+-,0)}(\boldsymbol{q})$] is the unperturbed static susceptibility of the z axis (xy plane), which originates from H_0. The parameter α represents the anisotropy of spin-fluctuation and we take $\alpha \le 1$ [12] since NMR experiments show that $\chi_{(xx)} < \chi_{(zz)}$ [8,9].

Using this one-band model, we discuss the effective interactions between Cooper pairs due to spin-fluctuations.

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Summation of bubble and ladder diagrams (i.e., RPA) gives

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

with

$$V_{\rm b.o}(\boldsymbol{k}-\boldsymbol{k}') = \frac{I}{N} \frac{(I/N)\chi_{(\uparrow\uparrow,0)}(\boldsymbol{k}-\boldsymbol{k}')}{1-(I/N)^2\chi^2_{(\uparrow\uparrow,0)}(\boldsymbol{k}-\boldsymbol{k}')},$$
$$V_{\rm b.e}(\boldsymbol{k}-\boldsymbol{k}') = \frac{I}{N} \frac{(I/N)^2\chi^2_{(\uparrow\uparrow,0)}(\boldsymbol{k}-\boldsymbol{k}')}{1-(I/N)^2\chi^2_{(\uparrow\uparrow,0)}(\boldsymbol{k}-\boldsymbol{k}')}, \quad (4)$$
$$V_{\rm lad}(\boldsymbol{k}-\boldsymbol{k}') = \frac{I}{N} \frac{(I/N)\chi_{(+-,0)}(\boldsymbol{k}-\boldsymbol{k}')}{1-(I/N)\chi_{(+-,0)}(\boldsymbol{k}-\boldsymbol{k}')}.$$

Here $V_{\rm b.o}$ ($V_{\rm b.e}$) comes from the summation of diagrams with odd (even) number of bubbles, and $V_{\rm lad}$ from the ladder diagrams.

In order to derive the gap equations, we introduce the operators

$$t_k^{(0)} = \sum_{ss'} (\sigma_2)_{ss'} c_{-ks} c_{ks'}, \quad (5)$$

$$t_k^{(a)} = \sum_{ss'} (\sigma_2\sigma_a)_{ss'} c_{-ks} c_{ks'}, \quad \text{for } a = 1,2,3, \quad (6)$$

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

$$H_{\rm int} = \frac{1}{4}\sum_{kk'} V_{\rm sin}(\boldsymbol{k}-\boldsymbol{k}') t_k^{(0)\dagger} t_{k'}^{(0)} + \frac{1}{4}\sum_{kk'}\sum_{a=1}^{3} V_{\rm tri}^{(a)}(\boldsymbol{k}-\boldsymbol{k}') t_k^{(a)\dagger} t_{k'}^{(a)}, \quad (7)$$

with

$$V_{\rm sin}(\boldsymbol{k}-\boldsymbol{k}') \equiv 2[V_{\rm b.e}(\boldsymbol{k}-\boldsymbol{k}') + V_{\rm lad}(\boldsymbol{k}-\boldsymbol{k}')],$$
$$V_{\rm tri}^{(1)}(\boldsymbol{k}-\boldsymbol{k}') = V_{\rm tri}^{(2)}(\boldsymbol{k}-\boldsymbol{k}') \equiv -2V_{\rm b.o}(\boldsymbol{k}-\boldsymbol{k}'), \quad (8)$$
$$V_{\rm tri}^{(3)}(\boldsymbol{k}-\boldsymbol{k}') \equiv 2[V_{\rm b.e}(\boldsymbol{k}-\boldsymbol{k}') - V_{\rm lad}(\boldsymbol{k}-\boldsymbol{k}')].$$

Since Sr_2RuO_4 has a long coherence length in the *ab* plane, $\xi_{ab} \approx 660$ Å [14], we use mean-field approximation to $H_{\rm int}$. We restrict the discussion to unitary states because it is unrealistic to assume nonunitary states in Sr_2RuO_4 [15]. Requiring that there is no coexistence of singlet and triplet pairs, we obtain the gap equations

$$\Delta(\boldsymbol{k}) = -\sum_{k'} V_{\rm sin}(\boldsymbol{k}-\boldsymbol{k}')\Delta(\boldsymbol{k}')\Theta[E_{\rm sin}(\boldsymbol{k}')],$$
$$d^{(a)}(\boldsymbol{k}) = -\sum_{k'} V_{\rm tri}^{(a)}(\boldsymbol{k}-\boldsymbol{k}') d^{(a)}(\boldsymbol{k}')\Theta[E_{\rm tri}(\boldsymbol{k}')], \quad (9)$$

where $\Theta(E) \equiv \frac{1}{2E}\tanh\frac{\beta E}{2}$, $E^2_{\rm sin}(\boldsymbol{k}) = \xi_k^2 + \Delta(\boldsymbol{k})\Delta^*(\boldsymbol{k})$, and $E^2_{\rm tri}(\boldsymbol{k}) = \xi_k^2 + \boldsymbol{d}(\boldsymbol{k})\cdot\boldsymbol{d}^*(\boldsymbol{k})$ with $\xi_k = \varepsilon_k - \mu$. The singlet and triplet order parameters are defined as $\Delta(\boldsymbol{k}) = -\frac{1}{2}\sum_{k'} V_{\rm sin}(\boldsymbol{k}-\boldsymbol{k}')\langle t_{k'}^{(0)}\rangle$ and $d^{(a)}(\boldsymbol{k}) = -\frac{1}{2}\sum_{k'} V^{(a)}_{\rm tri}(\boldsymbol{k}-\boldsymbol{k}')\langle t_{k'}^{(a)}\rangle$, respectively. Here $\boldsymbol{d}(\boldsymbol{k})$ is the so-called $\boldsymbol{d}$ vector for the triplet superconductivity.

In the system with the rotational symmetry in spin space, $\chi_{(\uparrow\uparrow,0)}(\boldsymbol{q}) = \chi_{(+-,0)}(\boldsymbol{q})$ is satisfied and thus the relation $V_{\rm b.o} + V_{\rm b.e} = V_{\rm lad}$ holds. In this case, it is easy to see $V_{\rm tri}^{(1)}(\boldsymbol{k}-\boldsymbol{k}') = V_{\rm tri}^{(2)}(\boldsymbol{k}-\boldsymbol{k}') = V_{\rm tri}^{(3)}(\boldsymbol{k}-\boldsymbol{k}')$.

On the other hand, the gap equation in Eq. (9) for the triplet pairing becomes dependent on the direction of the $\boldsymbol{d}$ vector in the anisotropic case. It means that *$\boldsymbol{d}$ vector has some preferred direction if the triplet pairs are formed by anisotropic spin-fluctuations.* This is naturally understood because the $\boldsymbol{d}$ vector is orthogonal to the spin direction of triplet Cooper pairs. For the present case with $\chi_{(+-,0)}(\boldsymbol{q}) < \chi_{(\uparrow\uparrow,0)}(\boldsymbol{q})$ (i.e., $\alpha < 1$) which is applied to the Sr_2RuO_4, we can see from Eq. (4) that $V_{\rm lad}(\boldsymbol{k}-\boldsymbol{k}')$ is suppressed and the effective interaction $V_{\rm tri}^{(3)}(\boldsymbol{k}-\boldsymbol{k}')$ approaches $V_{\rm sin}(\boldsymbol{k}-\boldsymbol{k}')$. Consequently, the triplet superconductivity with $d^{(3)}(\boldsymbol{k})$ (i.e., $\boldsymbol{d} \parallel \hat{z}$) 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 (π,π) stabilizes the singlet $d_{x^2-y^2}$-wave superconductivity. In that case, the singlet order parameters $\Delta(\boldsymbol{k}')$ with $\boldsymbol{k}' = (\pi,0)$ and $\Delta(\boldsymbol{k})$ with $\boldsymbol{k} = (0,\pi)$ have the opposite sign, so that the gap equation in (9) is satisfied with $V_{\rm sin}(\pi,\pi) > 0$.

For Sr_2RuO_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 β or γ band. Since the AF fluctuation in Sr_2RuO_4 has momentum $\boldsymbol{q}_0$, 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 2π. 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 $V_{\rm tri}^{(a)}(2\pi/3, 2\pi/3) > 0$. 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 order parameter symmetries in (9). Near the transition temperature T_c, we rewrite the gap equations as

$$\phi(\boldsymbol{k}) = -\sum_{k'} V_\phi(\boldsymbol{k}-\boldsymbol{k}')\phi(\boldsymbol{k}')\frac{1}{2\xi_{k'}}\tanh\frac{\beta_c\xi_{k'}}{2}, \quad (10)$$

where $\phi(\boldsymbol{k})$ represents $\Delta(\boldsymbol{k})$ or $d^{(a)}(\boldsymbol{k})$, and V_ϕ is determined from Eqs. (8) depending on ϕ. In the weak

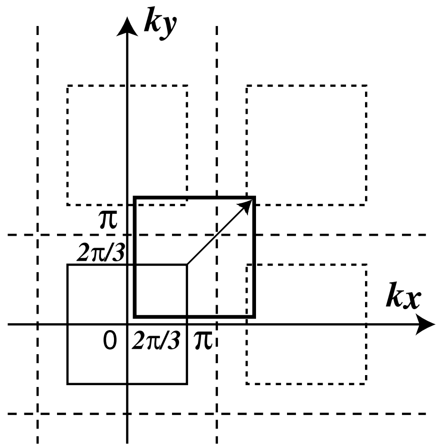

FIG. 1. A schematic Fermi surface for the β or γ band of Sr_2RuO_4. In order to show the nesting property, the Fermi surface shifted by the incommensurate AF wave number, $\boldsymbol{q}_0$, is also shown by a bold line. The thin dashed lines indicates the Fermi surfaces in the extended Brillouin zone.

coupling approximation, T_c is given by

$$k_B T_c = 1.13 \hbar v_F k_c \exp\left[-\frac{1}{N(0)\langle\langle V_\phi \rangle\rangle_{FS}}\right], \tag{11}$$

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

$$\langle\langle V_\phi \rangle\rangle_{FS} \equiv -\frac{\int_{FS} d\boldsymbol{k} \int_{FS} d\boldsymbol{k}' V_\phi(\boldsymbol{k}-\boldsymbol{k}')\phi(\boldsymbol{k})\phi(\boldsymbol{k}')}{[\int_{FS} d\boldsymbol{k}'] \int_{FS} d\boldsymbol{k}\, \phi^2(\boldsymbol{k})}. \tag{12}$$

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

For Sr_2RuO_4 we choose order parameters $\phi(\boldsymbol{k})$ as follows:

$$\begin{aligned} \phi_1(\boldsymbol{k}) &= \cos k_x + \cos k_y, \\ \phi_2(\boldsymbol{k}) &= \cos k_x - \cos k_y, \\ \phi_3(\boldsymbol{k}) &= \sin k_x \sin k_y, \\ \phi_4(\boldsymbol{k}) &= \sin k_x, (\hat{\boldsymbol{d}} \perp \hat{z}), \\ \phi_5(\boldsymbol{k}) &= \sin k_x, (\hat{\boldsymbol{d}} \parallel \hat{z}), \end{aligned} \tag{13}$$

where $\phi_1 \sim \phi_3$ correspond to singlet pairings, and ϕ_4, ϕ_5 to triplet pairings, respectively. The most probable candidate for Sr_2RuO_4 is $\hat{z}(\sin k_x \pm i \sin k_y)$ which is equivalent to ϕ_5 just below T_c, because the gap equation (10) for $\sin k_x \pm i \sin k_y$ is exactly the same as that for ϕ_5. If $N(0)\langle\langle V_{\phi_5} \rangle\rangle_{FS}$ is the largest, we expect that the order parameter $\boldsymbol{d}(\boldsymbol{k}) = \hat{z}(\sin k_x \pm i \sin k_y)$ is realized, because it acquires a larger energy gap than ϕ_5 near zero temperature.

To emphasize the characteristic feature of the nesting, we first use a simplified Fermi surface as shown in Fig. 1. For the $\boldsymbol{q}$ dependence of $\chi_{(\uparrow\uparrow,0)}(\boldsymbol{q})$ with a maximum at $\boldsymbol{q}_0$, we use the susceptibility obtained in the LDA calculation [5], and fix $S(\boldsymbol{0}) = 0.8$ with $S(\boldsymbol{q}) \equiv \frac{I}{N}\chi_{(\uparrow\uparrow,0)}(\boldsymbol{q})$. We regard $S(\boldsymbol{q}_0)$ as a phenomenological parameter.

Figure 2 shows the α dependence of $N(0)\langle\langle V_{\phi_n} \rangle\rangle_{FS}$ ($n = 1$–5) for $S(\boldsymbol{q}_0) = 0.95$. Other choices of $S(\boldsymbol{q}_0)$ from 0.90 to 0.99 do not change the results qualitatively. When the anisotropy is weak ($\alpha \sim 1$), the singlet $d_{x^2-y^2}$-wave superconductivity, ϕ_2, is stabilized. On the other hand, when α is small, the order parameter ϕ_5 is stabilized which is consistent with experiments.

The phase diagram as a function of α and $S(\boldsymbol{q}_0)$ is determined by examining various values of $S(\boldsymbol{q}_0)$ (Fig. 3). When the spin-fluctuation is isotropic (i.e., $\alpha = 1$), the singlet $d_{x^2-y^2}$-wave superconductivity, $\cos k_x - \cos k_y$, is the most stable. This is consistent with the previous study [5]. However, we find a fairly large parameter region where the state corresponding to $\hat{z}(\sin k_x \pm i \sin k_y)$ is realized.

We carry out the same calculation for the Fermi surfaces which resemble those in band-structure calculations. We find that the parameter region for the triplet pairing slightly shrinks, but still it is within the reasonable range. For example, $S(\boldsymbol{q}_0) = 0.95$ and $\alpha = 0.7$ still favors the triplet pairing. Therefore our mechanism is not so sensitive to the perfect nesting property of the Fermi surface.

The anisotropy of the total spin susceptibility $[\chi_{(\uparrow\uparrow)}(\boldsymbol{q}_0)/\chi_{(+-)}(\boldsymbol{q}_0)]$ is $\frac{1}{1-S(\boldsymbol{q}_0)}/\frac{\alpha}{1-\alpha S(\boldsymbol{q}_0)}$. This is in the range between 4 and 7 when we use the values at the phase boundary in Fig. 3. Even if we use values such as $S(\boldsymbol{q}_0) = 0.95$ and $\alpha = 0.7$, the anisotropy is less than 10. In order to compare these values with NMR experiments, however, it should be noted that the above anisotropy is only at $\boldsymbol{q} = \boldsymbol{q}_0$, and away from $\boldsymbol{q}_0$ the anisotropy becomes smaller since $S(\boldsymbol{q}) < S(\boldsymbol{q}_0)$. Because NMR $1/T_1T$ is proportional to the $\boldsymbol{q}$ summation of $\chi''(\boldsymbol{q}, \omega_N)$, we expect the anisotropy of $1/T_1T$ is smaller than the above values.

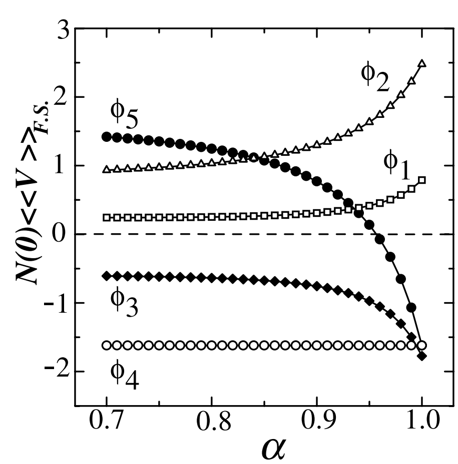

FIG. 2. The dependence of the anisotropy parameter, α, of $N(0)\langle\langle V_{\phi_n} \rangle\rangle_{FS}$ ($n = 1$–5) for $S(\boldsymbol{q}_0) = 0.95$.

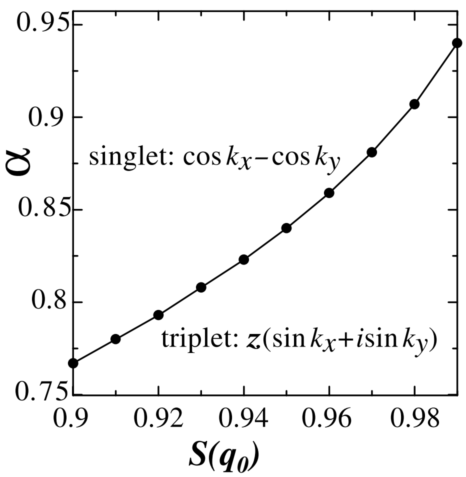

FIG. 3. Phase diagram as a function of the anisotropy parameter, α, and $S(\boldsymbol{q}_0)$ which is the maximum of $S(\boldsymbol{q}) = (I/N)\chi_{(\uparrow\uparrow,0)}(\boldsymbol{q})$, with $\boldsymbol{q}_0 = (\pm 2\pi/3, \pm 2\pi/3)$.

Actually NMR data [8,9] shows anisotropies which are consistent with our mechanism.

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_{ϕ_n}, 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 as shown in Fig. 1. This can be checked easily if we assume V_{ϕ_n} is enhanced very strongly and approximated as δ functions. Such an estimation shows that the triplet pairing utilizes the peak of $\chi_{(\uparrow\uparrow,0)}(\boldsymbol{q})$ more effectively than the singlet pairing does.

In determining the phase diagram in Fig. 3, we have assumed simple functional forms of the order parameters, $\phi_n(\boldsymbol{k})$. For the detailed calculations, it will be necessary to optimize the $\boldsymbol{k}$ dependence of $\phi_n(\boldsymbol{k})$. 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. It is shown that our mechanism is robust even if the nesting is weaker. In this paper we have not specified the band in Sr_2RuO_4. The γ band has the largest density of states at Fermi energy, while the nesting property will be stronger in α and β bands than for the γ band. Thus even if $\chi_0(\boldsymbol{q})$ for the γ band does not have a peak near $\boldsymbol{q}_0$, the β band has a mechanism for triplet superconductivity.

It is reported that Sr_2RuO_4 has an exotic property called "3K phase" [16] 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 α) near the interface region between Sr_2RuO_4 and Ru metal. We consider investigating the origin of the anisotropy to be very important both for understanding the superconductivity and for finding the new exotic phenomena.

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*Email address: t-kuwabara@bea.hi-ho.ne.jp
†Present address: Department of Physics, University of Tokyo, Hongo, Bunkyo-ku 113-0033 Tokyo, Japan.
Email address: ogata@phys.s.u-tokyo.ac.jp

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