Microscopic Determination of the D-vector in Sr_2RuO_4

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Abstract

We perform a microscopic calculation to investigate how the chiral state $\hat{d}(k) = (k_{\rm x} \pm {\rm i} k_{\rm y})\hat{z}$ is stabilized in the triplet superconductor Sr_2RuO_4. Starting from the three band Hubbard model with spin-orbit interaction, we estimate the superconducting instability using the perturbation theory. The D-vector is microscopically determined by taking the spin-orbit interaction into account. It is shown that the chiral state is stabilized under the reasonable condition. The p-wave symmetry of order parameter and the properties of the γ-band are essential for the chiral state.

Key words: triplet superconductivity ; Sr_2RuO_4 ; D-vector ; spin-orbit coupling

1. Introduction

The spin triplet superconductivity (TSC) in Sr_2RuO_4 is one of the most interesting issues in the unconventional superconductivity [1]. The TSC has already been observed in heavy Fermion compounds [2], however, the microscopic investigation in these materials is generally difficult because of their complicated electronic structure. Then, Sr_2RuO_4 is the most favorable compound for the microscopic investigation on the TSC. Such studies will give various informations on the unconventional superconductivity.

The internal degree of freedom is an interesting character of the TSC and described by the D-vector [3]. However, the identification of the D-vector using the microscopic Hamiltonian is usually difficult, and actually not performed. In this paper, we focus on Sr_2RuO_4 and perform a microscopic calculation to identify the D-vector for the first time.

2. SU(2) symmetric case

We start from the three band model which is constructed from the $t_{2\rm g}$-orbitals in the Ru ions [4].

$$H = H_0 + H_I, \tag{1}$$

$$H_0 = \sum_{a=1}^{3} \sum_{\boldsymbol{k},s} \varepsilon_a(\boldsymbol{k}) c^{\dagger}_{\boldsymbol{k},a,s} c_{\boldsymbol{k},a,s} + 2\lambda \sum_i \boldsymbol{L}_i \boldsymbol{S}_i, \tag{2}$$

$$H_I = U \sum_{i,a} n_{i,a,\uparrow} n_{i,a,\downarrow} + U' \sum_{i,a>b} n_{i,a} n_{i,b} + 2J_{\rm H} \sum_{i,a>b} \boldsymbol{S}_{i,a} \boldsymbol{S}_{i,b} + J \sum_{a \neq b} \sum_{\boldsymbol{k},\boldsymbol{k'},\boldsymbol{q}} c^{\dagger}_{\boldsymbol{q}-\boldsymbol{k'},a,\downarrow} c^{\dagger}_{\boldsymbol{k'},a,\uparrow} c_{\boldsymbol{k},b,\uparrow} c_{\boldsymbol{q}-\boldsymbol{k},b,\downarrow}, \tag{3}$$

where $\varepsilon_1(\boldsymbol{k}) = -2t'_{\rm xy} \cos k_{\rm x} - 2t_{\rm xy} \cos k_{\rm y}$ (α'-band), $\varepsilon_2(\boldsymbol{k}) = -2t_{\rm xy} \cos k_{\rm x} - 2t'_{\rm xy} \cos k_{\rm y}$ (β'-band) and $\varepsilon_3(\boldsymbol{k}) = -2t_{\rm z}(\cos k_{\rm x} + \cos k_{\rm y}) - 4t'_{\rm z} \cos k_{\rm x} \cos k_{\rm y} - \mu_{\rm z}$ (γ-band). The α' and β'-bands construct the α and β-bands through a weak hybridization. The reasonable parameter set is chosen as $(t_{\rm xy}, t'_{\rm xy}, t_{\rm z}, t'_{\rm z}) = (1.5, 0.2, 1, 0.4)$ where the γ-band has about 57% of the density of states [5]. The particle number is fixed to $n_a = 1.33$. The interaction term H_I describes the on-site Coulomb interactions and 2λ is the coupling constant of the spin-orbit interaction.

First, we discuss the case $\lambda = 0$, where the SU(2) symmetry in the spin space is conserved and therefore the six fold degeneracy remains [6]. The unconventional superconductivity is generally caused by the momentum dependence of the effective interaction which arises from the many body effects. We calculate the or-

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der parameter and T_c using the Éliashberg theory [7] and the perturbation method. The effective interaction is estimated within the all second order terms and the third order terms with coefficient U^3. This procedure is justified in the perturbative region $U', |J_H|, |J| < U \leq W$. ($W$ is the band width.)

It has been shown that the TSC is obtained in the third order perturbation theory [8]. We have confirmed the validity of the perturbation by comparing the second order perturbation and the third order one [9]. The reasonable $T_c \sim 1.5$K is obtained in the moderately weak coupling region $U/W \sim 0.4$ where the third order term is smaller than the second order one. The momentum dependence of the third order term is suitable for the TSC, and considerably enhances T_c . Therefore, we also take into account the third order terms.

The pairing symmetry is the p-wave in the wide parameter region, although the higher order symmetry is obtained in the weak coupling limit [9].

One of the interesting results is the orbital dependent superconductivity (ODS) [10]. That is, the order parameter strongly depends on the orbital. We find that the ODS is robustly obtained in Sr_2RuO_4 [9]. This is mainly because the mixing between the γ and the other bands is negligible. The main band is γ under the reasonable parameter set. When t_{xy} is excessively decreased, the α' or β'-band becomes the main band.

3. Determination of the *D*-vector

Next, we take the spin-orbit interaction into account. Here, we can use the approximation based on the ODS; we have only to calculate the effective interaction between the γ-band. This is justified because the condensation energy is almost determined by the γ-band. We further perform the perturbation with respect to λ because λ/W is sufficiently small in Sr_2RuO_4. We find that the lowest order terms are in the second order. Therefore, we perform the calculation within the second order with respect to λ.

We find that the SU(2) symmetry is violated owing to the spin-orbit interaction combined with the Hund coupling term J_H. The six fold degeneracy is lifted to the three levels (1) $\hat{d}(k) = k_x\hat{x} \pm k_y\hat{y}$, (2) $\hat{d}(k) = k_x\hat{y} \pm k_y\hat{x}$ and (3) $\hat{d}(k) = (k_x \pm ik_y)\hat{z}$. Experimental results for Sr_2RuO_4 have supported the chiral state (3) [11,12].

The stabilized state is shown in Fig. 1. We can see that the chiral state (3) is stabilized under the reasonable parameter set. The state (1) is stabilized only when the γ-Fermi surface is hole-like, which is inconsistent with experiment [5]. Thus, we have microscopically determined the D-vector in Sr_2RuO_4 and shown that the perturbation theory gives the consistent pairing state including the D-vector.

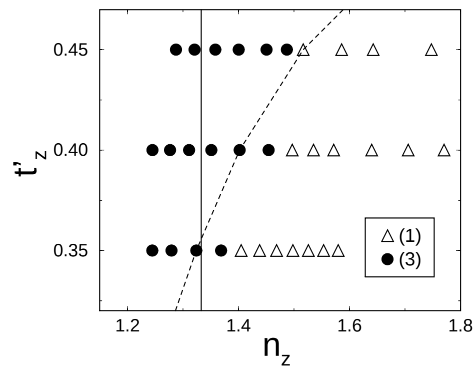

Fig. 1. Phase diagram for the parameters of the γ-band. $U = 5$ and $U' = J_H = J = 1$. The state (2) does not appear. The solid line corresponds to $n_z = 1.33$. The Fermi surface is electron-like (hole-like) in the left (right) side of the dashed line.

	γ-band	α-, β-band
p-wave	$(k_x \pm ik_y)\hat{z}$	$k_y\hat{x} \pm k_x\hat{y}$
p-wave (with node)	none	$k_y\hat{x} \pm k_x\hat{y}$
$f_{x^2-y^2}$-wave	$(k_x^2 - k_y^2)(k_y\hat{x} \pm k_x\hat{y})$	$(k_x^2 - k_y^2)(k_x\hat{x} \pm k_y\hat{y})$
f_{xy}-wave	$k_xk_y(k_x\hat{x} \pm k_y\hat{y})$	none

Table 1
Stabilized state for each pairing symmetry and main band.

We furthermore investigate the several pairing states by phenomenologically assuming the pairing interaction. The splitting of the degeneracy is microscopically estimated, similarly. The results are shown in Table I. We can see that the chiral state is stabilized only when the symmetry is the p-wave and the main band is γ. That is, this pairing state is essential for the chiral state. It is expected that this result is an important restriction on the pairing symmetry of Sr_2RuO_4.

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