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Probing pairing symmetry in Sr_2RuO_4

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Abstract. We study the spin dynamics in a p-wave superconductor at the nesting vector associated with the α- and β-bands in Sr_2RuO_4. We find a collective mode at the nesting vector in the superconducting phase identified as the odd-parity pairing state which breaks time-reversal symmetry. This mode in the spin channel exists only in a p-wave superconductor, not in s- or d-wave superconductors. We propose that probing this mode would clarify the pairing symmetry in Sr_2RuO_4.

The nature of superconductivity in Sr_2RuO_4 [1] has been the subject of intense theoretical and experimental activity. Although Sr_2RuO_4 has the same layered perovskite structure as La_2CuO_4, the prototype of the cuprates, the behaviour is remarkably different. At present, not much is known about any possible relation to the cuprates.

While it is clear that electron correlation effects are important in Sr_2RuO_4, the normal state is characterized as essentially a Fermi liquid below 50 K. The resistivities in all directions show T^2-behaviour for $T \leqslant 50$ K. The effective mass is about 3–4 m_{electron} and the susceptibility is also about 3–4 χ_0 where χ_0 is the Pauli spin susceptibility. There is considerable evidence that, in contrast to the conventional normal state (below 50 K), the superconducting state (below about 1 K) is unconventional. The nuclear quadrupole resonance (NQR) does not show a Hebel–Slichter peak [2]. The transition temperature is very sensitive to non-magnetic impurities [3]. ^{17}O NMR Knight shift experiments show that the spin susceptibility undergoes no change across T_c but stays the same as in the normal state for magnetic field parallel to the RuO_2 plane [4].

Shortly after the discovery of superconductivity in Sr_2RuO_4, it was proposed that odd-parity (spin-triplet) Cooper pairs are formed in the superconducting state in analogy with the case for ^{3}He [5]. Further evidence favouring spin-triplet pairing is provided by the observation of the ferromagnetic metallic state in $SrRuO_3$ which is the three-dimensional analogue of layered Sr_2RuO_4 [6]. Since a weak-coupling analysis of the spin-triplet state implies a nodeless gap [5], it is puzzling that the specific heat and NQR measurements show a large residual density of states (DOS)—50–60% of the DOS of the normal state—in the superconducting phase [2, 7]. As a consequence, a non-unitary superconducting state like the ^{3}He A_1 phase has been proposed [8]. However, a recent specific heat measurement [9] shows that the residual DOS is about 25% of the normal DOS, which indicates that the non-unitary state may not be stabilized.

An alternative explanation, the so-called *orbital-dependent superconductivity*, has been proposed [10]. Since four 4d electrons in Ru^{4+} partially fill the t_{2g} band, the relevant orbitals are d_{xy}, d_{xz}, and d_{yz} which determine the electronic properties. Using the quasi-two-dimensional

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nature of the electronic dispersion, the authors of [10] show that there are two superconducting order parameters for two different classes of the orbitals. The gap of one class of bands is substantially smaller than that of the other class of bands. The presence of gapless excitations for temperatures greater than that of the smaller gap would account for a residual DOS. The recent analysis of the London penetration depth and coherence length led to evidence being found for orbital-dependent superconductivity, with d_{xy} identified as the orbital relevant for superconductivity [11]. The possibility of a second superconducting phase transition when the pairing symmetries are different for different classes of the bands was also discussed .

Sigrist *et al* proposed [12] the following order parameter which is claimed to be compatible with all currently available experimental data:

$$\boldsymbol{d} = \hat{\boldsymbol{d}}(k_1 \pm \mathrm{i}k_2) \tag{1}$$

where $\hat{\boldsymbol{d}}$ is parallel to the $\hat{\boldsymbol{c}}$-axis and the gap is described as a tensor represented in terms of $\boldsymbol{d}$ in the following way.

$$\hat{\boldsymbol{\Delta}}(\boldsymbol{k}) = \boldsymbol{\sigma} \cdot \boldsymbol{d}\, \mathrm{i}\sigma_2 \tag{2}$$

where $\boldsymbol{\sigma}$ is the vector of Pauli matrices. Here $\hat{\boldsymbol{d}}$ is the spin vector whose direction is perpendicular to the direction of the spin associated with the condensed pair [13]. Notice that the direction of the order parameter vector is frozen along the $\hat{\boldsymbol{c}}$-direction due to the crystal field and there is a full gap over the whole Fermi surface.

The details of the Fermi surface have been observed from quantum oscillations [14]. The Fermi surface consists of three nearly cylindrical sheets, which is consistent with the electronic band calculations [15]. The three Fermi sheets are labelled α, β, and γ. While the γ-sheet of the Fermi surface can be attributed solely to the d_{xy} Wannier function, the α- and β-sheets are due to the hybridization of the d_{xz} and d_{yz} Wannier functions. Combining the orbital-dependent superconductivity and experimental observation [11], we find that the gap associated with the γ-band is larger than that associated with the α- and β-bands. Therefore the γ-band, which is essentially a quasi-isotropic two-dimensional one, is responsible for the existing superconductivity. On the other hand, the α- and β-sheets are quasi-one-dimensional, and can be visualized as a set of parallel planes separated by $Q = 2\pi/3$ running in both the k_x- and k_y-directions. Therefore, it is natural to expect sizable nesting effects at the wave vector $\boldsymbol{Q} = (2\pi/3, 2\pi/3)$ originating from the α- and β-bands. In the normal state, one can see that there should be a collective mode in the spin channel due to nesting, as has been shown by numerical calculation of the static susceptibility [16]. Neutron scattering experiments also show a peak at the wave vector $(0.6\pi, 0.6\pi, 0)$, close to the nesting vector [16], with energy transfer 6.2 meV [17]. Mazin and Singh discussed the possibility of a competition between p-wave and d-wave superconductivity in Sr_2RuO_4. The experimental result [17] also casts some doubt on a predominant role for ferromagnetic spin fluctuations in the mechanism of spin-triplet superconductivity. Although it is generally accepted that the pairing symmetry in Sr_2RuO_4 has odd parity, further theoretical and experimental studies are still necessary to determine the pairing symmetry of the possible order parameters [5] which have odd parity.

In this paper, we propose a way to probe the pairing symmetry in Sr_2RuO_4. We calculate the spin–spin correlation function at the nesting vector, $\boldsymbol{Q} = (2\pi/3, 2\pi/3)$, using the Green function method. It is important to include the coupling between the spin density and the vectorial order parameter fluctuation which is a property unique to p-wave superconductors. We find a collective mode in the spin channel in the superconducting state only for a p-wave superconductor with pairing symmetry which breaks time-reversal symmetry. Since the position of the resonant peak is just below 2Δ, this will also determine the size of the smaller gap related to the α- and β-bands which have nesting. On the other hand, no observation of the mode will indicate that the pairing symmetry associated with the α- and β-bands is different from that associated with the γ-band, assuming that the pairing symmetry in the γ-band, which does not have any nesting effect on the Fermi surface, is the one proposed as equation (1). Therefore there must be a second superconducting phase transition at a rather low temperature.

Using the Nambu representation, the Green function can be written as [18, 19]

$$G^{-1}(\omega_n, \boldsymbol{k}) = \mathrm{i}\omega_n - \xi_{\boldsymbol{k}}\rho_3 - \Delta\rho_1\boldsymbol{\sigma}\cdot\hat{\boldsymbol{d}}\,\mathrm{i}\sigma_2 \tag{3}$$

where $\boldsymbol{\rho}$ and $\boldsymbol{\sigma}$ are Pauli matrices which operate in the particle–hole and spin spaces, respectively. Here $\xi_{\boldsymbol{k}} = k^2/(2m) - \mu$, where μ is the chemical potential. In the superconducting state, the bare transverse susceptibility which represents the spin-flip procedure can be written by using Green functions [19, 20]:

$$\chi^{00}(\omega_\nu, \boldsymbol{q}) = T\sum_n\sum_{\boldsymbol{k}}\mathrm{Tr}[G(\omega_n, \boldsymbol{k})\alpha_+G(\omega_n+\omega_\nu, \boldsymbol{k}+\boldsymbol{q})\alpha_-] \tag{4}$$

where ω_n is the Matsubara frequency and the spin vertex $\boldsymbol{\alpha}$ is given by [21]

$$\boldsymbol{\alpha} = \frac{1+\rho_3}{2}\boldsymbol{\sigma} + \frac{1-\rho_3}{2}\sigma_2\boldsymbol{\sigma}\sigma_2 \tag{5}$$

and $\alpha_\pm = \alpha_1 \pm \mathrm{i}\alpha_2$.

Since the gap order parameter fluctuation couples to the spin density, the susceptibility renormalized by order parameter fluctuations consists of two parts:

$$\chi^0(\omega, \boldsymbol{q}) = \chi^{00}(\omega, \boldsymbol{q}) - \frac{V(\omega, \boldsymbol{q})g'\bar{V}(\omega, \boldsymbol{q})}{1 - g'\Pi(\omega, \boldsymbol{q})} \tag{6}$$

where g' is the coupling constant of the spin density and the order parameter fluctuation. Here $V(\omega, \boldsymbol{q})$ and $\Pi(\omega, \boldsymbol{q})$ can be computed as follows:

$$\begin{aligned} V(\omega_\nu, \boldsymbol{q}) &= T\sum_n\sum_{\boldsymbol{k}}\mathrm{Tr}[G(\omega_n, \boldsymbol{k})\alpha_+G(\omega_n+\omega_\nu, \boldsymbol{k}+\boldsymbol{q})(\alpha_-\rho_1\sigma_1)] \\ \Pi(\omega_\nu, \boldsymbol{q}) &= T\sum_n\sum_{\boldsymbol{k}}\mathrm{Tr}[G(\omega_n, \boldsymbol{k})(\alpha_+\rho_1\sigma_1)G(\omega_n+\omega_\nu, \boldsymbol{k}+\boldsymbol{q})(\alpha_-\rho_1\sigma_1)]. \end{aligned} \tag{7}$$

Using $\xi_{\boldsymbol{k}} = -\xi_{\boldsymbol{k}+\boldsymbol{Q}}$ for the nesting vector $\boldsymbol{Q}$, we found the following results at $T = 0$:

$$\begin{aligned} \mathrm{Re}\,\chi^{00}(\omega, \boldsymbol{Q}) &= \begin{cases} -g^{-1} - N_0\dfrac{|\omega|\arcsin(|\omega|/2\Delta)}{2\sqrt{|\omega^2-4\Delta^2|}} & |\omega| < 2\Delta \\ -g^{-1} - N_0|\omega|\ln\left(\dfrac{4\Delta^2}{\omega^2-4\Delta^2}\right)\Big/(2\sqrt{\omega^2-4\Delta^2}) & |\omega| > 2\Delta \end{cases} \\ \mathrm{Im}\,\chi^{00}(\omega, \boldsymbol{Q}) &= \begin{cases} 0 & |\omega| < 2\Delta \\ -N_0\dfrac{\pi\omega}{2\sqrt{\omega^2-4\Delta^2}} & |\omega| > 2\Delta \end{cases} \end{aligned} \tag{8}$$

$$\begin{aligned} \mathrm{Re}\,V(\omega, \boldsymbol{Q}) &= \begin{cases} -N_0\dfrac{\Delta\,\mathrm{sgn}(\omega)\arcsin(|\omega|/2\Delta)}{\sqrt{|\omega^2-4\Delta^2|}} & |\omega| < 2\Delta \\ -N_0\Delta\,\mathrm{sgn}(\omega)\ln\left(\dfrac{4\Delta^2}{\omega^2-4\Delta^2}\right)\Big/\sqrt{\omega^2-4\Delta^2} & |\omega| > 2\Delta \end{cases} \\ \mathrm{Im}\,V(\omega, \boldsymbol{Q}) &= \begin{cases} 0 & |\omega| < 2\Delta \\ -N_0\dfrac{\pi\Delta}{\sqrt{\omega^2-4\Delta^2}} & |\omega| > 2\Delta \end{cases} \end{aligned} \tag{9}$$

$$\mathrm{Re}\,\Pi(\omega, \boldsymbol{Q}) = \begin{cases} N_0 \dfrac{2\Delta^2 \arcsin(|\omega|/2\Delta)}{|\omega|\sqrt{|\omega^2 - 4\Delta^2|}} & |\omega| < 2\Delta \\ N_0 2\Delta^2 \ln\left(\dfrac{4\Delta^2}{\omega^2 - 4\Delta^2}\right) \Big/ (|\omega|\sqrt{\omega^2 - 4\Delta^2}) & |\omega| > 2\Delta \end{cases}$$

$$\mathrm{Im}\,\Pi(\omega, \boldsymbol{Q}) = \begin{cases} 0 & |\omega| < 2\Delta \\ N_0 \dfrac{2\pi\Delta^2}{\omega\sqrt{\omega^2 - 4\Delta^2}} & |\omega| > 2\Delta \end{cases} \tag{10}$$

where N_0 is the DOS at the Fermi level. Using the above result, the renormalized susceptibility is obtained as follows for $|\omega| < 2\Delta$:

$$\begin{aligned} \mathrm{Re}\,\chi^0(\omega, \boldsymbol{Q}) &= -g^{-1} - \frac{N_0}{2} \frac{|\omega| \arcsin(|\omega|/2\Delta)}{\sqrt{4\Delta^2 - \omega^2}} \\ &\quad + \frac{N_0^2 \Delta^2 |\omega| (\arcsin(|\omega|/2\Delta))^2}{g'^{-1}|\omega|(4\Delta^2 - \omega^2) - 2N_0\Delta^2 \arcsin(|\omega|/2\Delta)\sqrt{4\Delta^2 - \omega^2}} \\ \mathrm{Im}\,\chi^0(\omega, \boldsymbol{Q}) &= 0 \end{aligned} \tag{11}$$

where g is the strength of the interaction which is responsible for the superconductivity.

Including the effect of the exchange interaction within the random phase approximation (RPA), the full dynamical spin susceptibility is expressed as

$$\chi(\omega, \boldsymbol{q}) = \frac{\chi^0(\omega, \boldsymbol{q})}{1 - I_q \chi^0(\omega, \boldsymbol{q})} \tag{12}$$

where the exchange interaction $I_{\boldsymbol{Q}} \equiv -I$ for $\boldsymbol{Q}$. Since $\mathrm{Im}\,\chi^0 = 0$ and $\mathrm{Re}\,\chi^0$ diverges as ω approaches 2Δ, there exists a collective mode which is a bound state of excited pairs. The mode is positioned at

$$\omega = 2\Delta - \frac{\pi^2}{4} I^2 \Delta N_0^2. \tag{13}$$

Here we have used the fact† that $g \gg I, g'$. We also assumed that $\arcsin(|\omega|/2\Delta) \approx \pi/2$, consistent with the result. Notice that the position of the mode is very close to 2Δ. The intensity of the peak is

$$\frac{\pi^2}{2} I \Delta N_0^2. \tag{14}$$

Now, let us investigate the case of the spin-singlet superconductors, such as s- or d-wave superconductors. In the case of the spin-singlet superconductors, the bare spin–spin correlation function can be obtained through the following expression:

$$\chi^0(\omega, \boldsymbol{Q}) = \sum_{\boldsymbol{k}} \left(1 - \frac{\xi_k \xi_{k+Q} + \Delta_k \Delta_{k+Q}}{E_k E_{k+Q}}\right) \left(\frac{1}{\omega - E_k - E_{k+Q}} - \frac{1}{\omega + E_k + E_{k+Q}}\right). \tag{15}$$

For an s-wave superconductor, i.e., $\Delta_{\boldsymbol{k}} = \Delta_{\boldsymbol{k+Q}} = \Delta$, one can obtain the following results for $|\omega| < 2\Delta$:

$$\begin{aligned} \mathrm{Re}\,\chi^0(\omega, \boldsymbol{Q}) &= -N_0 \ln\left(\frac{\sqrt{|\omega^2 - 4\Delta^2|}}{\Delta} + \frac{\sqrt{|\omega^2 - 3\Delta^2|}}{\Delta}\right) + \ln(C) \\ \mathrm{Im}\,\chi^0(\omega, \boldsymbol{Q}) &= 0 \end{aligned} \tag{16}$$

† Because I represents the exchange interaction between the spin waves formed in the superconducting state, I is smaller than g for the stability of the ground state. $1/g' - 1/g = \Omega_d/(4\Delta^2)$ where the Ω_d is the pinning frequency [19]. Here we neglect it since it is much smaller than the gap.

where C is a constant. This implies that one needs an enormously large interaction I to get a collective mode, i.e., $I \gg 1/N_0$, which is practically impossible.

Let us study the possibility of having a resonance peak in a d-wave superconductor at the nesting vector $\boldsymbol{Q} = (2\pi/3, 2\pi/3)$. Assuming that the superconducting phase is described by the conventional BCS superconductor with the d-wave pairing symmetry:

$$\Delta(\boldsymbol{k}) = (\Delta/2)[\cos(k_x) - \cos(k_y)]$$

we use the same expression as equation (15) for the bare spin–spin correlation function. Due to the coherence factor, there is a collective mode at $\boldsymbol{Q} = (\pi, \pi)$ even without nesting in the electronic dispersion [22]. However, in the case of $\boldsymbol{Q} = (2\pi/3, 2\pi/3)$, we do not have a simple relation like that for $\boldsymbol{Q} = (\pi, \pi)$. In fact, $\Delta_{\boldsymbol{k}}$ is equal to $-\Delta_{\boldsymbol{k}+\boldsymbol{Q}}$ for the line from $\boldsymbol{k} = (-2\pi/3, 0)$ to $(0, -2\pi/3)$, which makes the coherence factor O(1), but $\Delta_{\boldsymbol{k}}$ and $\Delta_{\boldsymbol{k}+\boldsymbol{Q}}$ have linear dispersion in (k_x, k_y) so it does not produce any singularity in the spin susceptibility. If the momenta lie near nodes, then we have the same dispersion relation for $\boldsymbol{Q} = (\pi, \pi)$, and it was found [23] that there is no singularity in the spin channel if $\boldsymbol{k}$ and $\boldsymbol{k} + \boldsymbol{Q}$ are near nodes. Therefore we do not expect any collective mode in either s- or d-wave superconductors at the wave vector $\boldsymbol{Q} = (2\pi/3, 2\pi/3)$.

The possible Cooper pairing states were classified according to the irreducible representations of the tetragonal point group D_{4h} which include one two-dimensional and four one-dimensional representations for both even and odd parity [5, 24]. Assuming that the order parameter associated with the α- or β-bands has different pairing symmetry to that of equation (1), we also study the existence of a resonance peak with the following order parameters classified as odd-parity pairing:

$$\boldsymbol{d} = \begin{cases} \hat{\boldsymbol{x}}k_1 + \hat{\boldsymbol{y}}k_2 \\ \hat{\boldsymbol{x}}k_1 - \hat{\boldsymbol{y}}k_2 \\ \hat{\boldsymbol{x}}k_2 + \hat{\boldsymbol{y}}k_1 \\ \hat{\boldsymbol{x}}k_2 - \hat{\boldsymbol{y}}k_1. \end{cases} \tag{17}$$

We found that the spin–spin correlation function behaves as in equation (16). However, since the direction of the d-vector is now in the x–y plane, the spin–spin correlation function along the z-direction has the same singularity as equation (8).

Therefore, we conclude that the collective mode at the nesting vector exists only with the proposed order parameter, equation (1), unless there is unusually strong coupling between the spin density and the order parameter fluctuation. It is important to emphasize that the collective mode at the nesting vector cannot be obtained from the general expression for the spin wave given in reference [19], because this mode is a bound state which occurs only at the nesting vector.

In conclusion, we studied the spin dynamics in a p-wave superconductor at the nesting vector associated with the α- and β-bands in Sr_2RuO_4. We found that there is a collective mode at a frequency just below 2Δ where Δ is the smaller gap according to orbital-dependent superconductivity. We show that this mode exists only in a p-wave superconductor, not in s- or d-wave superconductors. We also demonstrated that the other odd pairing states do not produce the collective mode in the transverse susceptibility unless there is unusually strong coupling between the spin density and the order parameter fluctuation. Therefore we suggest that probing this mode will determine the pairing symmetry associated with the α- and β-bands, and possibly the γ-band provided that it has nesting. This will help to clarify the controversy regarding the pairing symmetry in Sr_2RuO_4.

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