Spin gap and $L$ modulated intensity at the low-energy incommensurate magnetic fluctuations in the superconducting state of Sr$_2$RuO$_4$

Kazuki Iida,¹,² Maiko Kofu,¹,³ Katsuhiko Suzuki,⁴ Naoki Murai,³ Seiko Ohira-Kawamura,³ Ryoichi Kajimoto,³ Yasuhiro Inamura,³ Motoyuki Ishikado,² Shunsuke Hasegawa,⁵ Takatsugu Masuda,⁵ Yoshiyuki Yoshida,⁶ Kazuhisa Kakurai,² Kazushige Machida,⁷ and Seunghun Lee¹

¹Department of Physics, University of Virginia, Charlottesville, Virginia 22904-4714, USA
²Neutron Science and Technology Center, Comprehensive Research Organization for Science and Society (CROSS), Tokai, Ibaraki 319-1106, Japan
³J-PARC Center, Japan Atomic Energy Agency (JAEA), Tokai, Ibaraki 319-1195, Japan
⁴Research Organization of Science and Technology, Ritsumeikan University, Kusatsu, Shiga 525-8577, Japan
⁵Neutron Science Laboratory, Institute for Solid State Physics, University of Tokyo, Kashiwa, Chiba 277-8581, Japan
⁶National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki 305-8565, Japan
⁷Department of Physics, Ritsumeikan University, Kusatsu, Shiga 525-8577, Japan

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Low-energy incommensurate (IC) magnetic fluctuations in the multiband superconductor Sr$_2$RuO$_4$ is investigated by high-resolution inelastic neutron scattering measurements and random phase approximation (RPA) calculations. Below $T_c$, the substantial spin gap is observed at $Q_{IC} = (0.3, 0.3, L)$ where the quasi-one-dimensional $\alpha$ and $\beta$ sheets consisting of the Fermi surfaces are in good nesting conditions. $L$ modulated intensity of the low-energy IC magnetic fluctuations and our RPA calculations indicate that the superconducting gaps regarding the $\alpha$ and $\beta$ sheets have the horizontal line nodes.

Strontium ruthenate Sr$_2$RuO$_4$ with $T_c = 1.5$ K has attracted a great deal interest as the prime candidate for a chiral $p$-wave superconductor. Although many theoretical and experimental studies have been performed, superconducting order parameter and driving force underlying unconventional superconductivity are still matters of intense debate. Nuclear magnetic resonance and polarized neutron scattering measurements reported spin-triplet superconductivity whereas muon spin rotation and Kerr effect measurements showed spontaneously time reversal symmetry breaking. They are the key ingredients of the chiral $p$-wave superconductor. On the other hand, there are some experimental results such as absence of the chiral edge currents, first-order superconducting transition, and strong $H_{c2}$ suppression, all of which are against for the chiral $p$-wave superconductivity.

Electrical structure of the normal state in Sr$_2$RuO$_4$ has been well established. The $t_{2g}$ electrons of the Ru$^{4+}$ ions form three cylindrical sheets at the Fermi surfaces. The $d_{xz}$ and $d_{yz}$ orbitals form quasi-one-dimensional $\alpha$ and $\beta$ sheets, while $d_{xy}$ forms a two-dimensional $\gamma$ sheet. Inelastic neutron scattering (INS) technique can directly measure imaginary part of generalized spin susceptibility ($\chi''$) as a function of momentum ($Q$) and energy ($\hbar \omega$) transfers, yielding abundant information of Fermi surface topology. The most pronounced magnetic signal is incommensurate (IC) magnetic fluctuations at $Q_{IC} = (0.3, 0.3, L)$ owing to the Fermi surface nesting between (or within) the $\alpha$ and $\beta$ sheets. The IC magnetic fluctuations persist up to at least 80 meV, while the IC magnetic fluctuations exhibit the anisotropic behavior as energy approaches to zero. In contrast to the pronounced signal from the IC magnetic fluctuations, only blurred signals are observed around the $\Gamma$ point. The broad excitation is considered to be ferromagnetic fluctuations originating from the $\gamma$ sheet.

Upon decreasing temperature below $T_c$, a spin gap is expected to evolve at each magnetic fluctuation owing to the opening of the superconducting gaps at the Fermi surfaces. No clear spin gap larger than 0.3 meV was, however, observed regarding the IC magnetic fluctuations at $(0.3, 0.3, 0)$. Moreover, spin resonance as a consequence of the Bardeen-Cooper-Schrieffer (BCS) coherence factor is not observed. So far, various experimental techniques reported that the superconducting gaps of Sr$_2$RuO$_4$ have line nodes. Based on the horizontal line nodes model, the spin gap and the neutron spin resonance are expected to emerge at $Q_{IC} = (0.3, 0.3, L)$ with finite $L$. In this letter, we investigate in detail the low-energy IC magnetic fluctuations in Sr$_2$RuO$_4$ along both in-plane and out-of-plane directions below and above $T_c$ using the combination of high-resolution INS measurements and random phase approximation (RPA) calculations.

Three single crystals of Sr$_2$RuO$_4$ with a total mass of ~10 g were prepared by the floating-zone method.
and each crystal shows $T_c \sim 1.4$ K (onset). They were co-aligned in a way that the $(HHL)$ plane is perpendicular to the rotating axis. Time-of-flight neutron scattering measurements at 0.3 and 1.8 K were performed using the disk chopper spectrometer AMATERAS installed at Japan Proton Accelerator Research Complex [37, 38]. The disk chopper was rotated in a frequency of 300 Hz, yielding the combinations of multiple incident neutron energies ($E_i$) 2.64, 5.93, and 23.7 meV with the energy resolutions 0.046, 0.146, and 1.07 meV, respectively, at the elastic channel.

Overall features of the IC magnetic fluctuations in Sr$_2$RuO$_4$ obtained by our INS measurements are summarized in Fig. 1. Figures 1(b) and 1(d) depict INS intensity maps at 0.3 K by averaging neutron scattering intensities over the energy window of [1.5, 3.5] meV. IC magnetic fluctuations are observed at $Q_{IC} = (0.3, 0.3)$, (0.3, 0.7), and (0.7, 0.7) [Fig. 1(b)] [22, 25, 28, 30]. In addition to the IC magnetic peaks, the Fermi surface nesting also induces the ridge scattering connecting $Q_{IC}$ around (0.5, 0.5) [23]. The INS intensity of the IC magnetic fluctuations along (0.3, 0.3, $L$) monotonically decreases with increasing $L$ [Fig. 1(d)], indicating the quasi-two-dimensional feature of the IC magnetic fluctuations [25, 30].

To explore the energy evolution of the IC magnetic fluctuations, the INS intensity map as a function of $HH$ and $\hbar \omega$ is shown in Fig. 1(a). Steep magnetic excitation evolves at $Q_{IC}$ [23]. The INS intensity is converted to the imaginary part of the spin susceptibility $\chi''(\hbar \omega)$ via the fluctuation dissipation theorem $\chi''(\hbar \omega) = (1 - e^{-\hbar \omega/\hbar \omega}) I(\hbar \omega)$ after subtracting the background. The $\chi''(\hbar \omega)$ spectra at $Q_{IC} = (0.3, 0.3)$ at 0.3 and 1.8 K are plotted in Fig. 1(e). The $\chi''(\hbar \omega)$ spectra above 0.6 meV are well fitted by the relaxation response model $\chi''(\hbar \omega) = \chi' \Gamma \hbar \omega/[(\hbar \omega)^2 + \Gamma^2]$ where $\chi'$ is the static susceptibility and $\Gamma$ is the relaxation rate [or the peak position of $\chi''(\hbar \omega)$], yielding $\Gamma = 5.7(2)$ meV [6.2(2) meV] at 0.3 K (1.8 K) [23, 30]. As such, observed IC magnetic fluctuations are quantitatively consistent with the previous INS works.

In the following, we concentrate on the low-energy IC magnetic fluctuations. As described below, in the superconducting state, a substantial spin gap appears at $Q_{IC} = (0.3, 0.3)$ [Fig. 1(a)] and $L$ modulated intensity of the IC magnetic fluctuations is also observed at the low energy channel [Fig. 1(c)]. For quantitative analysis on the spin gap and the $L$ modulated intensity of the low-energy IC magnetic fluctuations, $Q$ and $\hbar \omega$ dependences of the INS intensities [I(Q) and I(\hbar \omega)] are investigated.

Series of I(Q) cuts along $HH$ at 0.3 and 1.8 K are plotted in Figs. 2(a) and 2(b). The I(Q) cut with [0.35, 0.75] meV at each temperature is fitted by a Gaussian function with linear background. The peak center and width (full width at half maximum) are found to be $Q_{IC} = (0.303(2), 0.303(2))$ and $\sigma = 0.045(4)$ at 0.3 K [$Q_{IC} = (0.304(2), 0.304(2))$ and $\sigma = 0.044(4)$ at 1.8 K]. Since the low-energy IC magnetic fluctuations are very weak in intensity, we fix the center and width of the Gaussian to these values for all subsequent fits at different energy windows. This is reasonable because the dispersion of the IC magnetic fluctuations is very steep [22]. While the INS intensities above 0.3 meV exhibit the peaks at $Q_{IC} = (0.3, 0.3)$, almost no peak is observed below 0.2 meV at 0.3 K [Fig. 2(a)]. This result
suggests that the spin gap of \( \sim 0.2 \) meV at the \( Q_{IC} \) position gets open in the superconducting state. Meanwhile, there is a sizable peak even at the low energy in the normal state [Fig. 2(b)]. Evolution of the spin gap below \( T_c \) is more directly demonstrated by the energy cuts. Energy cuts at \( Q_{IC} \) and \( Q_{BG} \) (\( I_{IC} \) and \( I_{BG} \)) at 0.3 K are plotted in Fig. 2(c). Although bifurcation between \( I_{IC} \) and \( I_{BG} \) can be seen above 0.29 meV (see the arrow), no bifurcation is observed below 0.25 meV, indicating the evolution of the spin gap below \( T_c \). In contrast to the superconducting state, above \( T_c \), \( I_{IC} \) is always bigger than \( I_{BG} \) down to the lowest energy accessible in the current measurements [Fig. 2(d)], suggesting the gapless magnetic fluctuations in the normal state. By subtracting \( I_{BG} \) from \( I_{IC} \) and converting to the dynamical spin susceptibility, \( \chi''(\hbar \omega) \) of the low-energy IC magnetic fluctuations at 0.3 and 1.8 K are plotted in Figs. 2(e) and 2(f). Almost no spectral weight of \( \chi''(\hbar \omega) \) can be seen below \( \sim 0.25 \) meV at 0.3 K [see the arrow in Fig. 2(e)] while nonnegligible spectral weight persists down to at least 0.1 meV at 1.8 K [Fig. 2(f)]. By fitting the \( \chi''(\hbar \omega) \) spectrum at 0.3 K using the modified relaxation response model 

\[
\chi''(\hbar \omega) = \chi'(\hbar \omega - \langle \Delta_{SC} \rangle)/[(\hbar \omega - \langle \Delta_{SC} \rangle)^2 + \Gamma^2]
\]

where \( \langle \Delta_{SC} \rangle \) represents the \( L \) averaged spin gap and \( \Gamma \) is fixed to the value obtained from the high energy data in Fig. 1(e), the spin gap at 0.3 K is obtained to be \( \langle \Delta_{SC} \rangle = 0.11(4) \) meV. The same fit is also performed for \( \chi''(\hbar \omega) \) at 1.8 K, yielding \( \langle \Delta_{SC} \rangle = 0.01(2) \) meV. Therefore, within the accuracy of our INS measurements, we conclude that the IC magnetic fluctuations in \( Sr_2RuO_4 \) is gapless in the normal state while the substantial spin gap evolves in the superconducting state. As in the previous works \cite{28, 30}, no clear spin resonance but small enhancement at \( 0.5 \leq \hbar \omega \leq 0.8 \) meV is detected in our INS measurements. This is due to the small amount of the spectral weight of the low-energy IC magnetic fluctuations [Fig. 1(e)] and the small size of the spin gap, which only gives the tiny enhancement around twice the superconducting gap \( \hbar \omega \sim 2\Delta = 0.56 \) meV \cite{40}.

\( L \) dependence of the low-energy IC magnetic fluctuations provides us the crucial information to clarify the line nodes at the superconducting gaps \cite{33, 34}. Contour map of the INS intensities at 0.3 K with the energy window \([0.5, 0.8]\) meV is illustrated in Fig. 1(c). In contrast to the monotonically decreasing intensity at the higher energy window [Fig. 1(d)], \( L \) modulated IC mag-
netic fluctuations are observed in the lower energy. Figures 2(g) and 2(h) show the \( L \) dependences of the INS intensities of the IC magnetic fluctuations at 0.3 K with several different energies. The \( L \) dependences above \( h \omega \geq 4\Delta \) (\( \simeq 1.1 \text{ meV} \)) follow the squared magnetic form factor \[39\] [Figs. 2(g) and 2(h)], while the \( L \) dependence at the low energy does not simply follow the squared magnetic form factor but shows the \( L \) modulated intensity with the maximum around \( L = 0.5 \) [Fig. 2(i)]. Since the energy window \([0.5, 0.8] \text{ meV}\) is close to the amplitude of twice the superconducting gaps \[40\], the symmetry of the superconducting gaps is expected to be the origin of the \( L \) modulated intensities of the low-energy IC magnetic fluctuations in the superconducting state. To theoretically elucidate the origin of the \( L \) modulated intensity of the low-energy IC magnetic fluctuations, RPA calculations assuming the horizontal line nodes at the superconducting gaps are further performed.

To construct a realistic model, we perform density functional theory (DFT) calculations using the Wien2k package \[41\]. We obtain an effective 3-orbital model considering the \( \text{Ru} \) \( d_{xz}, d_{yz}, d_{xy} \)-orbitals using the maximum localized Wannier functions \[42\]. The generalized gradient approximation (GGA) exchange-correlation functional \[43\] is adopted with the cut-off energy \( RK_{\max} = 5 \) and 512 \( k \)-point mesh. We renormalize the bandwidth considering the effective mass \( m^* = 3.5 \), and the resulting renormalized bandwidth is \( W \sim 1.05 \text{ eV} \). We consider the following gap function with horizontal line nodes:

\[
\Delta(k) = \Delta_0 \cos c k_z
\]

within the standard BCS framework. We take the gap amplitude \( \Delta_0 = 4.8 \times 10^{-3} \text{W} \). In the body center tetragonal system, the period along to the \( k_z \) axis is \( 4\pi/c \), and thus we take \( k_z \) as \( 0 \leq k_z < 4\pi/c \). We obtain the dynamical spin susceptibility \( \chi^\text{total}_{\omega}(q, \omega) \) applying RPA as

\[
\chi^\text{total}_{\omega}(q, \omega) = \sum_{l,m} \chi^l_{m,m,0}(q, \omega)
\]

\[
\tilde{\chi}_0(q, \omega) = \tilde{\chi}_0(q, \omega)[I - \tilde{S}\tilde{\chi}_0(q, \omega)]^{-1}
\]

\[
\tilde{\chi}_0(q, \omega) = \tilde{\chi}_0(q, \omega) + \tilde{\chi}_0(q, \omega)
\]

\[
\chi^l_{m,m,0}(q, \omega) = \sum_{k} \sum_{n,m} \frac{f(E^m_{k+q}) - f(E^m_{k})}{\omega + i \delta - E^m_{k+q} + E^m_{k}} \times U_{l_1, \sigma_1, n}(k + q) U_{l_2, \sigma_2, m}(k)
\]

\[
\times U_{l_3, \sigma_3, n}(k) U^\dagger_{l_4, \sigma_4, m}(k + q)
\]

where \( l_1 \sim l_4 \) and \( \sigma_1 \sim \sigma_4 \) are the orbital \( d_{xz}, d_{yz}, d_{xy} \) and spin \((\uparrow \text{ and } \downarrow)\) indices. \( \tilde{\chi}_0(q, \omega) \) denotes the normal (anomalous) part of the irreducible bare susceptibility \( \chi_0 \) at \( \sigma_1 = \sigma_2 = \sigma_3 = \sigma_4 \) \( (\sigma_1 = \sigma_2 \neq \sigma_3 = \sigma_4) \).
coupling BCS value 1.76k_BTc ∼ 0.46 meV. This result indicates that the quasi-one-dimensional α and β sheets are active bands for the bulk superconductivity, resulting in the L modulated intensity of the low-energy IC magnetic fluctuations as the feedback effect from the superconducting gaps. Our RPA calculations reveal that the observed L modulated intensity originates from the horizontal line nodes at the superconducting gaps, in agreement with the field-angle-dependent specific heat capacity measurements [33]. The proposed chiral order parameters with the horizontal nodes (kx + iky) cosckz 45, 46 or (kx + iky)kz 47 are incompatible with the combined experimental facts: the absence of the spin gap and spin resonance at (1/3, 1/3, 0) probed by the triple-axis neutron scattering experiment 28 and the presence of the spin gap at (1/3, 1/3, 1/2) since the α and β band is fully responsible for superconductivity. As such, the present results give a strong constraint on the superconducting order parameter and stimulate further theoretical and experimental works to reconsider the pairing mechanism in Sr2RuO4.

In summary, we investigated in detail the low-energy IC magnetic fluctuations in Sr2RuO4. The substantial spin gap comparable to the superconducting gap appears at QIC below Tc. The L modulated intensity at the low-energy IC magnetic fluctuations and our RPA calculations indicate that the superconducting gaps regarding the α and β sheets have horizontal line nodes.

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