Spin and Orbital Contributions to Magnetically Ordered Moments
in 5d Layered Perovskite Sr2IrO4

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The ratio of orbital (L) and spin (S) contributions to the magnetically ordered moments of a 5d transition metal oxide, Sr2IrO4 was evaluated by non-resonant magnetic x-ray diffraction. We applied a new experimental setting to minimize the error in which we varied only the linear-polarization of incident x-ray at a fixed scattering angle. Strong polarization dependence of the intensity of magnetic diffraction was observed, from which we conclude that the ordered moments contain substantial contribution from the orbital degree of freedom with the ratio of ⟨L⟩/⟨S⟩ ≈ 5.0, evidencing the pronounce effect of spin-orbit coupling. The obtained ratio is close to but slightly larger than the expected value for the ideal J_{eff} = 1/2 moment of a spin-orbital Mott insulator, |⟨J_{1/2}|L_{1/2}|⟩|^2 / |⟨J_{1/2}|S_{1/2}|⟩|^2 = 4, which cannot be accounted by the redistribution of orbital components within the t_{2g} bands associated with the elongation of the IrO6 octahedra.

Magnetic moments of 3d transition metal complexes predominantly originate from the spins of the d electrons rather than the orbital momenta because of the quenching of the orbital momenta by the crystal fields. The orbital contribution is treated as a perturbation to the spin, the effect of which is renormalized to the g factor of electrons resulting in a magnetic anisotropy. In heavier elements like 5d transition metals, however, the spin-orbit coupling (SOC) is pronounced and drastic change of the electronic states is anticipated. An unconventional Mott state was recently found in a layered perovskite with Ir^{4+} (5d^5), Sr2IrO4, where a half-filled band of J_{eff} = 1/2 (J_{eff} = S + L_{eff} = S - L ) is formed by a strong SOC and a moderate Coulomb repulsion opens a charge gap within the J_{eff} = 1/2 band. Experimental supports for the J_{eff} = 1/2 character of the ordered moments were given by the measurements of XAS and resonant magnetic x-ray scattering (RXS). The strong suppression of the magnetic x-ray scattering at the L_{II} edge (2p_{3/2} → 5d) indicated that the wave function of electrons in charge of magnetism should be reasonably close to that of J_{eff} = 1/2 state. The J_{eff} = 1/2 character of the ordered moments was also identified in other complex iridium oxides.

In reality, even in the prototypical spin-orbital Mott insulator Sr2IrO4, there should be certain deviation from the ideal J_{eff} = 1/2 state. Factors to destabilize the ionic J_{eff} = 1/2 band could be the followings.

1. The refinement of the crystal structure of Sr2IrO4 showed an elongation (~ 4 % along the c-axis) and the rotation within a plane of IrO6 octahedra (Fig. 1(a)) [1]. Those should lift the degeneracy of t_{2g}.
2. The octahedral ligand field splitting, 10 Dq, is finite, which could give rise to admixture of the e_g states [2,3].
3. The system is close to metallic states and not a strong insulator. Band effect should influence the nature of the ordered moment [4,11,12].

To fully understand the nature of the magnetic moment of a spin-orbital Mott insulator, Sr2IrO4 estimates of orbital ⟨L⟩ ≡ ⟨ψ|L|ψ⟩) and spin ⟨S⟩ ≡ ⟨ψ|S|ψ⟩ moments of the ordered moment should be the first step to determine the precise wave function, |ψ⟩. The deduced ⟨L⟩/⟨S⟩ ratio would specify the competing source to destabilize the ionic J_{eff} = 1/2 band. Determination of ⟨L⟩ and ⟨S⟩ was performed by X-ray magnetic circular dichroism (XMCD) technique, which probed only the canted component as the field-induced weak ferromagnetic moments [13]. Our approach to tackle this problem is to probe the orbital and spin magnetizations separately by a polarization analysis of non-resonant magnetic X-ray scattering (NRMXS).

The principle of individual observation of ⟨L⟩ and ⟨S⟩ by NRMXS was formulated by Blume and Gibbs [14]. While spins in the target material can be treated as stationary objects like electron charges, the interaction between orbital motion of electrons around nuclei and incident x-ray is expected to include a relativistic process. The scattering amplitude at a wave vector K of magnetic scattering is a summation of spin and orbital contributions as

\[ \langle M_m \rangle = -i\tau [S(K) \cdot B + L(K) \cdot B_0], \]  

where

\[ B = (\epsilon' \times \epsilon) - (\hat{k}_i \times \epsilon') \times (\hat{k}_i \times \epsilon) + (\hat{k} \times \epsilon') \times (\hat{k}_i \times \epsilon'), \]

and

\[ B_0 = (\epsilon' \times \epsilon). \]
The \( \hat{k}_i (\hat{k}_f) \) and \( \epsilon (\epsilon') \) denote the unit vectors pointing the propagation and the polarization of the incident (scattered) x-ray, as shown in Fig. 1(b). It should be stressed that spin and orbital densities \( \langle S(K) \rangle \) and \( \langle L(K) \rangle \) are coupled with different matrices. This is a crucial advantage of magnetic x-ray diffraction over neutron diffraction in identifying the orbital and spin contributions. The magnetic scattering matrix of neutrons is simply written as \( \langle M \rangle = \left[ \frac{1}{2} L(K) + S(K) \right] \cdot C \). Here, \( \left[ \frac{1}{2} L + S \right] \) couples to a matrix \( C = K \times (\sigma \times \vec{K}) \), using \( \vec{K} \), the unit vector along \( K \), and neutron spin operator \( \sigma \). For this reason, one cannot separate the orbital and spin contributions to the ordered moments by neutron scattering.

In this Letter, we report the ratio of orbital and spin contributions to the magnetically ordered moments of \( \text{Sr}_2\text{IrO}_4 \), by utilizing the merit of the magnetic scattering of x-ray. We applied a new experimental setting of NR-MXS with fixed \( K \) and azimuthal angle, \( \Psi \), which minimizes the experimental error in estimating the \( \langle L \rangle / \langle S \rangle \) ratio \( 13 \). The ratio \( \langle L \rangle / \langle S \rangle = |\langle \psi | L_z | \psi \rangle | / |\langle \psi | S_z | \psi \rangle | \) is estimated to be \( 5.0 \pm 0.7 \) at a magnetic Bragg reflection \( K = (1 0 22) \). The obtained ratio is close to the expected value for the \( J_{\text{eff}} = 1/2 (J_{1/2}) \) state at \( K = 0 \), \( |\langle J_{1/2} | L_z | J_{1/2} \rangle | / |\langle J_{1/2} | S_z | J_{1/2} \rangle | = 4 \), but certainly shows an enhancement of the orbital component. The deviation from the ideal \( J_{\text{eff}} = 1/2 \) cannot be explained by the admixture of the \( J_{\text{eff}} = 3/2 \) state associated with the elongation of an \( \text{IrO}_6 \) octahedron. We also demonstrate the orientation of the magnetic moments by rotating the azimuthal angle (\( \Psi \)) with \( 1^\circ \) accuracy.

A single crystal of \( \text{Sr}_2\text{IrO}_4 \) with a dimension of 1 mm \( \times \) 0.3 mm \( \times \) 0.1 mm was synthesized by a flux method. Antiferromagnetic long-range order below \( T_N = 230 \) K was confirmed by magnetization and RXS \( 3, 5 \). NR-MXS measurements were performed at 10 K, where the magnitudes of the ordered moments were almost saturated upon cooling. We used BL19LXU at SPring-8 with a purely polarized x-ray \( 16 \), which enabled us to control the linear polarization of the incident x-ray precisely.

The configuration of NRMXS measurement is shown in Fig. 1(b). Hereafter we use a Cartesian coordinate system, defined by unit vectors \( \hat{u}_1, \hat{u}_2, \) and \( \hat{u}_3 \), which point to the direction of \( \hat{k}_i + \hat{k}_f, \hat{k}_i \times \hat{k}_f, \) and \( \hat{k}_i - \hat{k}_f \), respectively. The origin of the azimuth angle, \( \Psi \), is set to the crystalline b-axis \( \parallel \hat{u}_1 \) direction. Each experimental data set was taken by rotating the linear polarization direction \( \theta_{\text{pol}} \) with fixed \( \theta \) and \( \Psi \), and fit by the theoretical curve with a parameter \( \langle L \rangle / \langle S \rangle \). The ratios \( \langle L \rangle / \langle S \rangle \) were determined for three sets of azimuth angles, \( \Psi \), to confirm the accuracy of our estimate. The matrix form of NRMXS is given in Ref. 14 as

\[
\langle M \rangle = \left( \begin{array}{c}
\sin^2 \theta (L_1 + S_1 \cos \theta + S_3 \sin \theta) \\
\sin 2\theta (2L_2 \sin^2 \theta - S_2)
\end{array} \right). 
\]

\[ \theta = \frac{1}{2} \theta \] 19. The scattering-angle (\( \theta \)) dependent ratio of \( \pi' \) and \( \sigma' \) detections,

\[
I_{\pi'}/I_{\sigma'} = \sin^2 \left( \frac{\theta}{2} \right) \frac{2L_1(K) + S_1(K) - S_3(K) \tan (\theta/2)^2}{S_2(K)^2}
\]

yielded a ratio of orbital and spin contributions of the magnetic moments. However, this approach using an analyzer crystal for the polarization analysis was subject to a large experimental error due to the insufficient intensities of diffraction. Besides, the magnetic moments of holmium and of uranium compounds are well-localized \( f \) electrons where \( \langle L(K) \rangle \) and \( \langle S(K) \rangle \) have small \( \theta \) dependences. In case of \( 5d \) electrons, the \( \theta \) dependence could
be much more significant and the measurement of the $K$ dependent $I_c/I_{\sigma}$ would cause a large error. An experimental approach without an analyzer crystal that is precise enough to estimate $(L)/\langle S \rangle$ ratio even at a fixed $K$ has been anticipated, which is particularly crucial for $5d$ transition metal oxides. We examined the $\vartheta_{\text{pol}}$ dependence of the diffraction with fixed $K$, by controlling two $\pi/2$ phase plates of diamond to realize $\Delta \vartheta_{\text{pol}} \sim 1^\circ$.

We measured the $\vartheta_{\text{pol}}$-dependent intensity of $(1\,0\,22)$ magnetic reflection. The photon energy of incident x-ray was set to 10.45 keV. The scattering angle was $\theta = 31.1^\circ$ corresponding to the $(1\,0\,22)$ magnetic Bragg reflection. The experimental configuration with fixed diffraction angle ($\vartheta$) and azimuth angle ($\Psi$) maintained the irradiated area on the surface unchanged.

![Figure 2](image.png)

**FIG. 2.** $\vartheta_{\text{pol}}$ dependence of magnetic and charge scatterings in the antiferromagnetic state for $\Psi = 90^\circ$. The diffractions for $\vartheta_{\text{pol}} = 0^\circ$ and $90^\circ$ are shown in the inset.

The obtained $\vartheta_{\text{pol}}$ dependence of charge and magnetic scatterings for $\Psi = 90^\circ$ ($a \perp \hat{u}_2$) is shown in Fig. 2. Charge scattering is expressed as $I_c \propto \gamma_{c,\sigma'}^2 + \gamma_{c,\pi'}^2$ with

$$
\begin{pmatrix}
\gamma_{c,\sigma'}^2 \\
\gamma_{c,\pi'}^2
\end{pmatrix} = \rho(K) \begin{pmatrix}
1 & 0 \\
0 & \cos 2\theta
\end{pmatrix} \begin{pmatrix}
\cos \vartheta_{\text{pol}} \\
\sin \vartheta_{\text{pol}}
\end{pmatrix}.
$$

Both the charge and magnetic diffraction intensities show sinusoidal $\vartheta_{\text{pol}}$ dependence. Large amplitude of the sinusoidal curve for the magnetic scattering evidences considerable contribution of the orbital component to the ordered moments. The antiphase $\vartheta_{\text{pol}}$ dependence to that of the charge scattering indicates $b$-collinear antiferromagnetic moments ($\hat{u}_2 \parallel M$). We rotated the sample around the $Q$ vector, and measured the magnetic diffraction for other azimuthal angles, $\Psi = 0^\circ, \pm 45^\circ$ corresponding to $\hat{u}_2 \perp b$, $\hat{u}_2 \parallel a \pm b$, respectively, as shown in Fig. 3 (a). One prominent finding is that $I_m$ becomes nearly independent of $\vartheta_{\text{pol}}$ for $\Psi = 0^\circ$, which we could obtain only in the case that the magnetic moments lie along the $\hat{u}_1$ direction. This firmly establishes that the magnetic moments lie along the $b$-axis, and combined with the antiparallel alignment of moments by the RXS measurements [3], we determined the magnetic structure as shown in Fig. 3 (b). By fitting the data with Eq. 4 by taking $M \parallel b$ into account, we estimate the ratio of orbital and spin contributions to the ordered moment $(L)/\langle S \rangle$ as $5.0 \pm 0.7$. The ratios obtained by other azimuthal angles are consistent with the value $(L)/\langle S \rangle \sim 5.0$ as shown in Fig. 3 (a). These results confirm the vital role of the large spin-orbit coupling.

![Figure 3](image.png)

**FIG. 3.** (a) The $\vartheta_{\text{pol}}$ dependence of magnetic and charge scattering for three azimuth angles. The charge scattering did not depend on $\Psi$. The solid and dashed lines represent fitted curves for three azimuthal angles with a fixed $(L)/\langle S \rangle = 5.0$. It should be noted that no fitting parameter other than the scaling factor is used. The phases of the sinusoidal $\vartheta_{\text{pol}}$ dependence are well reproduced by Eq. 4. (b) Magnetic structure of the ordered state in SrIrO$_3$ determined by the measurements of the azimuth angle ($\Psi$) dependent magnetic diffraction.

Considering the ionic wave function with the magnetic moment along the $b$-axis, the $J_{\text{eff}} = 1/2$ state is written by choosing the quantized axis $Z \equiv 1/\sqrt{2}(x + y)$ as

$$
|J_{\text{eff}} = 1/2, \pm \rangle = \left(\frac{1}{\sqrt{6}}\right) \left(|yx, + \rangle \pm |yz, - \rangle\right)
\pm \left(|zx, + \rangle \mp |zx, - \rangle\right) \mp \sqrt{2}|xy, \mp \rangle
\mp \left(i/2\sqrt{3}\right) |R_{5z2}\rangle \left[(1 \pm i) \left(|Y_2^1, + \rangle \pm |Y_2^{-1}, - \rangle\right)\right.
\pm \left(1 \mp i\right) \left(|Y_2^1, - \rangle \pm |Y_2^{-1}, + \rangle\right) \pm \sqrt{2}|Y_2^2, \mp \rangle.
$$

Here, $|R_{5z2}\rangle$ and $|Y_2^1\rangle$ are the radial and spherical wave functions of 5d electrons respectively, and the $\pm$ signs denote up and down spins quantized to the $b$ direction. Using this $J_{\text{eff}} = 1/2$ wave function, the ratio of the expectation values of $L_z = 1/\sqrt{2}(L_x + L_y)$ and $S_z = 1/\sqrt{2}(S_x + S_y)$ is $|\langle J_{1/2}/L_z|J_{1/2}/S_z\rangle|/(|\langle J_{1/2}/S_z|J_{1/2}/S_z\rangle|) = 0$ at $K = 0$. The present measurements were performed with $K = (0\, 0\, 22)$ ($\theta = 31.1^\circ$) and the expected ratio is shifted by spin and orbital form factors of $d$-electrons, which are composed of Fourier transforms of three $t_{2g}$ wave functions. The calculated form factors defined by $f_{1(2)}(K) \equiv \int |R_{5z2}\rangle |Y_2^{1(2)}\rangle \exp(-2\pi i(K \cdot r)) dr$ are 0.636
for \( l_z = 1(|yz\rangle, |zx\rangle) \) and 0.873 for \( l_z = 2(|xy\rangle) \) spherical wave functions. Using the form factors at \( K = (1\ 0\ 22) \), the expected ratio of orbital and spin contributions is shifted to \( [1/3 \cdot (f_1 + f_2)] / [1/6 \cdot f_2] = 3.5 \) [20], that is slightly smaller than 4, the value at \( K = 0 \). The observed ratio of orbital and spin contributions to the moment, \( \langle L \rangle / \langle S \rangle \sim 5.0 \) is not far away from 3.5, showing that the wave function of Sr\(_2\)IrO\(_4\) is approximated as the \( J_{\text{eff}} = 1/2 \) function. This is in support of the dominant effect of the spin-orbit coupling.

Since the expected ratio for the ideal \( J_{\text{eff}} = 1/2 \) is \( |(J_{1/2}|LZ|J_{1/2})| / |(J_{1/2}|SZ|J_{1/2})| < 4 \) because of \( f_1 < f_2 \) for any \( K \), the observed \( \sim 40\% \) overshoot of \( \langle L \rangle / \langle S \rangle \) is not an experimental error but shows a physically significant hybridization of the \( J_{\text{eff}} = 1/2 \) with other states. We discuss possible sources for this enhancement of the orbital contribution.

The crystal structure analysis shows a \( \sim 4\% \) elongation of IrO\(_6\) octahedra along the \( c \)-axis, which causes a ligand field splitting of the triply degenerated \( t_{2g} \) manifold into \( |xy\rangle \) with upper energy level and doubly degenerated \( |yz\rangle \) and \( |zx\rangle \) orbitals. Considering only \( |xy\rangle \), \( |yz\rangle \), and \( |zx\rangle \), the wave function in the tetragonal field can be described as

\[
|\psi\rangle = 1/\sqrt{6}\left((1-\delta)(|yz+,+\rangle \pm |yz,-\rangle) \pm (1-\delta)(|zx,+=\rangle \mp |zx,=\rangle) \mp \sqrt{2}(1+2\delta)|xy,=\rangle\right).
\]

To justify the observed \( \langle L \rangle / \langle S \rangle \) ratio at \( K \), \( |\langle \psi|LZ|\psi\rangle| / |\langle \psi|SZ|\psi\rangle| = 5.0 \), we obtain \( \delta = -0.11 \), which implies the reduction of the \( |xy\rangle \) orbital with a down spin. The elongated IrO\(_6\) octahedra along the \( c \)-axis should enhance \( |xy\rangle \) character resulting in a positive value of \( \delta \), which is opposite to the observed coefficient. The \( t_{2g} \) redistribution of orbital states caused by the elongation of an IrO\(_6\) octahedron is clearly insufficient to understand the enhancement of the orbital contribution. Other hybridization effect should be invoked. For example, the staggered in-plane rotation of IrO\(_6\) octahedra could induce the hybridization of \( e_g \) and \( t_{2g} \) states due to the finite 10 Dq by the cubic crystal field. The weak Mott character of electrons proximity to a bad metal can also destabilize the ionic picture.

To conclude, we present a quantitative estimate of the ratio of orbital and spin contributions to the magnetically ordered moment of 5\( d \) based antiferromagnet, Sr\(_3\)IrO\(_4\), utilizing NRMXS. The experimental setting applied to this material offers a unique opportunity to unveil the real electronic state produced by the novel interplay of the strong spin-orbit coupling, lattice distortion, and hybridizations with other orbital states. The magnetic moment is dominated by orbital angular momentum with the value \( \langle L \rangle / \langle S \rangle \sim 5.0 \pm 0.7 \), which is not far from the \( J_{\text{eff}} = 1/2 \) spin-orbital Mott picture for this material. A nearly 40\% enhancement of the orbital contribution from the ideal \( J_{\text{eff}} = 1/2 \) state was observed. This cannot be ascribed to an intra-\( t_{2g} \) redistribution of the orbital component associated with the elongated IrO\(_6\) octahedron but clearly points the importance of the hybridization with other orbital states. We have also succeeded in determining the magnetic structure including both the wave vector and the direction of ordered moments by analyzing the polarization dependence of NRMXS.

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[20] The expectation values of $L_Z$ and $S_Z$ are expressed using the spherical wave functions as

$$\langle J_{1/2, +} | L_Z | J_{1/2, +} \rangle = 1/6 \langle R_{52} | R_{52} \rangle \left[ \langle Y^2, - | Y^2, - \rangle + \langle Y^{-2}, - | Y^{-2}, - \rangle + \langle Y^{-1}, - | Y^{-1}, - \rangle + \langle Y^{-1}, - | Y^{-1}, - \rangle \right]$$

and

$$\langle J_{1/2, +} | S_Z | J_{1/2, +} \rangle = 1/6 \langle R_{52} | R_{52} \rangle \langle Y^2, - | Y^2, - \rangle.$$