Magnetism of Multi-Orbital Edge States in Sr$_2$RuO$_4$

Yoshiki Imai$^{a,b}$, Katsunori Wakabayashi$^c$, and Manfred Sigrist$^a$

$^a$Institute for Theoretical Physics, ETH Zürich, Zürich, Switzerland
$^b$Department of Physics, Saitama University, Saitama, Japan
$^c$International Center for Materials Nanoarchitectonics (MANA), NIMS, Tsukuba, Japan

E-mail: imai@phy.saitama-u.ac.jp

Abstract. Magnetic properties of edge states in the chiral $p$-wave superconductor Sr$_2$RuO$_4$ are investigated based on a multi-band model restricting to the two bands derived from the 4$d$-$t^{2}_g$ orbitals. While generally low-energy gapless Andreev bound states appear at the edges which carry spontaneous charge current, they are not topologically protected. Including spin-orbit coupling of the two orbitals we find additionally edge spin currents which are present in the normal as well as the superconducting phase. They contribute to the anomalous and the spin Hall effect and generate in the superconducting phase a finite spin polarization at the surface. Repulsive onsite interaction strengthens the spin polarization through the coupling to a nesting driven incipient magnetic phase of the system. We speculate that the magnetizations of the spin polarization and the chiral edge currents could partially compensate each other, in view of recent experimental results.

1. Introduction
The unconventional superconductor Sr$_2$RuO$_4$ as one of the best studied transition metal oxides has been considered as a good candidate for chiral $p$-wave pairing, $d^{\pm}_\pm = \hat{z}(k_x \pm i k_y)$ [1]. This time reversal symmetry violating state induces gapless quasiparticle states at surfaces normal to the $x$-y-directions, due to Andreev reflection. Such states are expected to carry charge current which would give rise to magnetic fields at the edges [2, 3]. However, very detailed studies with scanning SQUID probes have found only negative results for such currents so far [4]. In the present study we use a two-band model including spin-orbit coupling, as introduced in the next section in order to investigate the specific magnetic properties of edge states of the electron- and a hole-like Fermi surface sheets known for the $\alpha$ and $\beta$ sheets in Sr$_2$RuO$_4$ (Fig.1).

2. Model and Method
A convenient model to analyze edge state properties for our system is a multi-leg ribbon two-band model including the inter- and intra-orbital hybridization as well as local spin-orbit coupling (Fig.2). We introduce the labels $p_x$ and $p_y$ orbitals corresponding in symmetry to the Ru 4$d$-$t^{2}_g$ orbitals, $d_{xz}$ and $d_{yz}$, in Sr$_2$RuO$_4$. The Hamiltonian is given by $H = H_{\text{intra}} + H_{\text{inter}} + H_{\text{SO}} + H_{\text{int}}$, 
\begin{align}
H_{\text{intra}} &= t \sum_{i,\sigma} \left( \sum_{l=1}^{L} c_{i0p_x \sigma}^\dagger c_{i1p_x \sigma} + \sum_{l=1}^{L-1} c_{i0p_y \sigma}^\dagger c_{i1p_y \sigma} + h.c. \right) - \mu \sum_{ilm\sigma} n_{ilm\sigma}, \\
H_{\text{inter}} &= t' \sum_{i,m,\sigma} \left( \sum_{l=1}^{L} c_{ilm\sigma}^\dagger c_{i1l+1\bar{m}\sigma} - \sum_{l=2}^{L} c_{ilm\sigma}^\dagger c_{i1l-1\bar{m}\sigma} + h.c. \right),
\end{align}

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spin (charge) current is defined as No quantizations are expected in the quasiparticle conductivities \[5, 6\].

vanishes for the chiral channel. Figure 4(a) shows the both spin currents and the net spin current. While the absolute values of both spin-up and -down currents are same, the flowing directions become opposite. Thus the net charge current vanishes and the net spin current only appears.

3. Results

The self-consistent mean field calculations are performed numerically at zero temperature. For illustration we choose a rather large pairing interaction \(V = -2t\) and \(t' = 0.2t\) (\(t\) serves as unit of energy) with an overall particle density \(n = 4/3\). The resulting quasiparticle spectrum in Fig.3 includes low-energy Andreev bound states besides the fully gapped "bulk" states, which are located at the two boundaries. Because the Chern number within our two-band model vanishes for the chiral p-wave state, these edge states are not topologically protected and also no quantizations are expected in the quasiparticle conductivities \[5, 6\].

Nevertheless we find finite spontaneous charge and spin currents at the edge (Fig.4). The spin (charge) current is defined as \(J_l^{(sc)} = J_l^s \mp J_l^c\) where \(- (+)\) stands for the spin (charge) channel. Figure 4(a) shows the both spin currents and the net spin current. While the absolute values of both spin-up and -down currents are same, the flowing directions become opposite. Thus the net charge current vanishes and the net spin current only appears.

\[
H_{SO} = -\sum_{i\sigma} \sum_{l} (i\lambda\sigma c_{il\sigma}^{\dagger} \bar{c}_{il\sigma} + h.c.),
\]

\[
H_{\text{int}} = \frac{1}{2} \sum_{ilm,\sigma,\sigma'} [V(n_{ilm\sigma}n_{il+1m\sigma'} + n_{ilm\sigma'}n_{il+1m\sigma}) + U\delta_{\sigma,\sigma'}n_{ilm\sigma}n_{il\bar{m}\bar{\sigma}}]
\]
Figure 3. Energy spectrum in the low-energy region for \( U = 0 \) as a function of momentum \( k \) parallel to \( y \)-axis.

Figure 4. Spin-dependent currents and spin and charge currents for \( U = 0 \). (a) and (b) depict the normal and superconducting phases. The solid (dashed) line stands for the spin \( \uparrow (\downarrow) \) currents. The dotted (dash-dotted) line for the spin (charge) current. Insets: magnifications near the edge.

Figure 4(b) shows that both spin-up and -down currents flow in the same direction resulting in a finite chiral charge current (sum of the two components). Being different in size, however, they also give rise to a (helical) spin current (difference of the two components). The main contribution originates from hopping along the \( x \)-direction, so that they are essentially dominated by the \( p_x \)-orbital. The spin-orbit coupling introduces a spin-dependent phase factor yielding a spin-dependent effective field for the electrons [7]. This is the cause for the finite spin current and also induces contributions to the anomalous and the spin Hall effect near the surface. These effects disappear naturally with \( \lambda \to 0 \). There are two important aspects of

Figure 5. Spin polarization for various choices of the repulsive interaction \( U \). Panels (a) and (b) show the spin polarizations on \( p_x \)- and \( p_y \)-orbital, respectively.

Figure 6. Sum of spontaneous magnetic field for various choices of the repulsive interaction. Open (solid) symbols represent \( B^c (B^r) \).

the magnetism due to spin polarization in this system. On the one hand, the superconducting phase supports coexisting spin and charge currents flowing along at the edges. Based on the spin Hall effect this must yield a finite spin polarization. Since the dominant contributions are from the \( p_x \)-orbital the corresponding the magnetization is \( m_{lp_x} \), depicted in Fig. 5(a). Through spin-orbit coupling the polarization direction is tied to the chirality of the pairing state.

On the other hand, we have nesting features in the band structure, well visible in Fig.1. The repulsive interaction \( U \) has the trend to induce a spin density wave with the corresponding
nesting vector $Q \approx 2\pi/3$. Our calculation shows that the $p_y$-orbital is most susceptible to this ordering channel which is competition with the (gapful) chiral $p$-wave pairing state. Thus, the spin density wave state only occurs at the surface due to the presence of gapless Andreev bound states and decays on a certain length scale towards bulk such that the interior of the system does not show any magnetism. This order is related to the $p_y$ and can be seen as $m_{lp_y}$ in Fig.5(b). This magnetic moment $m_{lp_y}$ grows quickly with the value of $U$ and exceeds the magnetic moments $m_{lp_x}$. Again spin-orbit coupling is responsible for the fact that the orientation of the $m_{lp_y}$ is not independent of the orientation of the chirality of the pairing state. Note that the orientation of the magnetization along the $z$-axis is also enforced by spin-orbit coupling [8].

Both spontaneous edge currents as well as spin magnetization contribute to the surface magnetization (parallel to the $z$-axis) of the system. Here we would like to compare the magnitude to both components, defining the orbital current contribution as

$$B_c(l) = -a \sum_{l'} \langle J_c l' \rangle$$

and the spin contribution as

$$B_r(l) = -\mu_B a^3 \left( n_{l \uparrow} - n_{l \downarrow} \right).$$

Here $a$ is the lattice constant. In Fig.6 we display both magnetic fields as a function of $l$ for different values of the repulsive interaction $U$, ignoring the minor differences in the prefactors of the two expressions. Note that within our model the two magnetic fields are opposite to each other and depending on $U$ reach the same order of magnitude. Thus, the net spontaneous magnetic field detected near the edge can be strongly reduced. In this discussion the Meissner screening of the superconducting state is not taken into account.

This result is interesting in view of recent experiments searching for surface magnetism by scanning SQUID probes [4]. The negative result might be explainable by a compensation effect, also taking the current contributions of the third band ($\gamma$-band) into account, which has been neglected for simplicity in the present discussion.

4. Summary

Motivated by the magnetic and superconducting properties of Sr$_2$RuO$_4$ we have analyzed surface properties, restricting to the $\alpha$-$\beta$-bands which show the most pronounced spin magnetic properties. These two bands give rise to both spontaneous charge and spin currents at the surface. The former is induced by time reversal symmetry broken chiral $p$-wave superconducting phase, while the latter originates from the topology of spin-orbit coupling and inter-/intra-orbital hybridization and is also present in the normal state. The combination of the two currents produces a finite spin polarization at the surface as well as the exchange interaction $U$ does due to band nesting features. We note that this effect may have some relevance for the interpretation of the negative result by local magnetic probes trying to find the magnetism expected for chiral $p$-wave superconductivity in Sr$_2$RuO$_4$ [4]. A detailed discussion will be given elsewhere [6].

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