Topological aspect and transport property in multi-band spin-triplet chiral $p$-wave superconductor $\text{Sr}_2\text{RuO}_4$

Yoshiki Imai$^1$, Katsunori Wakabayashi$^2$, Manfred Sigrist$^3$

$^1$Department of Physics, Saitama University, Saitama, Japan
$^2$International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Tsukuba, Japan
$^3$Theoretische Physik, ETH-Honggerberg, Zürich, Switzerland

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

Abstract. Considering the superconductor $\text{Sr}_2\text{RuO}_4$, we analyze a three-band tight-binding model with one hole-like and two electron-like Fermi surfaces corresponding to the $\alpha$, $\beta$ and $\gamma$ bands of $\text{Sr}_2\text{RuO}_4$ by means of a self-consistent Bogoliubov-de Gennes approach for ribbon-shaped system to investigate topological properties and edge states. In the superconducting phase two types of gapless edge states can be identified, one of which displays an almost flat dispersion at zero energy, while the other, originating from the $\gamma$ band, has a linear dispersion and constitutes a genuine chiral edge states. Not only a charge current appears at the edges but also a spin current due to the multi-band effect in the superconducting phase. In particular, the chiral edge state from the $\gamma$ band is closely tied to topological properties, and the chiral $p$-wave superconducting states are characterized by an integer topological number, the so-called Chern number. We show that the $\gamma$ band is close to a Lifshitz transition. Since the sign of the Chern number may be very sensitive to the surface condition, we consider the effect of the surface reconstruction observed in $\text{Sr}_2\text{RuO}_4$ on the topological property and show the possibility of the hole-like Fermi surface at the surface.

1. Introduction

The transition metal oxide $\text{Sr}_2\text{RuO}_4$ has attracted much interest due to the unconventional nature of its superconducting phase [1, 2]. Various theoretical and experimental studies support the chiral $p$-wave state, $d=\Delta_0(\hat{z}(k_x\pm ik_y))$, as the leading candidate of the superconducting order parameter, which is a two-dimensional analog of the Anderson-Brinkman-Morel (ABM) state of $^3\text{He}$ superfluid [3]. This phase is doubly degenerate with the Cooper pair orbital angular momentum $L_z=\pm 1$, which provides the possibility of the formation of domains. While on theoretical grounds we expect the presence of a spontaneous charge current near the edge in the superconducting state, the experimental search so far gives negative results only [4].

In previous papers, we investigated the magnetic and topological properties of this system [5, 6]. While the $\alpha/\beta$ bands generate mainly the spin-polarization near the edges due to the presence of the small on-site repulsive interaction, which tends to compensate the spontaneous magnetic field originating from the charge current. The Chern number of these two bands vanishes because of the cancellation between the electron- and hole-like properties of Fermi surfaces. On
the other hand, there exist edge states with linear dispersion resulting from the $\gamma$ band which are topologically protected.

In this proceedings, we report on topological and edge state properties of the chiral $p$-wave superconducting phase in a three-band tight-binding model. We also consider the effect of surface reconstruction due to the RuO$_6$ octahedron rotation observed at the surface of Sr$_2$RuO$_4$ on the topological properties of the superconducting state.

2. Model and Method

The low-energy electronic states belong to the Ru 4$d_{2z}$ orbital and the effective band structure can be constructed by means of the two-dimensional three-band tight binding model. Hereafter $d_{xz}$, $d_{yz}$ and $d_{xy}$ orbitals are called as $x$, $y$ and $z$ orbitals, respectively. In order to study edge states giving insight into topological nature of the superconductor, a ribbon-shaped system with the number of legs $L$ is used, as depicted in Fig. 1. Open and periodic boundary conditions are imposed along the $y$- and $x$-directions, respectively.

The Hamiltonian consists of hopping, spin-orbit interaction and interaction terms, which are given by

$$H = H_{\alpha\beta} + H_\gamma + H_{SO} + H_a,$$

with

$$H_{\alpha\beta} = -t \sum_{i,\sigma} \left( \sum_{l=1}^{L} c_{ilx\sigma}^\dagger c_{i+l x\sigma} + \sum_{l=1}^{L-1} c_{ily\sigma}^\dagger c_{i+l y\sigma} + h.c. \right)$$

$$-t' \sum_{i,\sigma, m, m' \neq z} \sum_{l=1}^{L-1} \left( c_{ilm\sigma}^\dagger c_{i+l+1 m\sigma} - c_{il+1 m\sigma}^\dagger c_{i+l m\sigma} + h.c. \right) - \mu \sum_{ilm \neq z} n_{ilm\sigma},$$

$$H_\gamma = -t_z \sum_{i,\sigma} \left( \sum_{l=1}^{L} c_{ilz\sigma}^\dagger c_{i+l z\sigma} + \sum_{l=1}^{L-1} c_{ilz\sigma}^\dagger c_{i+l+1 z\sigma} + h.c. \right)$$

$$-t'_z \sum_{i,\sigma} \sum_{l=1}^{L-1} \left( c_{ilz\sigma}^\dagger c_{i+l+1 z\sigma} + c_{il+1 z\sigma}^\dagger c_{i+l z\sigma} + h.c. \right) - \mu \sum_{ilz\sigma} n_{ilz\sigma} - \Delta \sum_{ilz\sigma} n_{ilz\sigma},$$

$$H_{SO} = -\lambda \sum_{il} \sum_{mm'nn'} \sum_{\sigma\sigma'} \sum_{\sigma\sigma''} c_{ilm\sigma}^\dagger \sigma_{\sigma\sigma'} c_{il'm'\sigma''},$$

$$H_a = U_0 \sum_{il\sigma\sigma'} \left( \sum_{m=x, z} n_{ilm\sigma} n_{i+1lm\sigma'} + \sum_{m=y, z} n_{ilm\sigma} n_{il+1m\sigma'} \right).$$
where $c_{ilm\sigma}^\dagger$ ($c_{ilm\sigma}$) is the creation (annihilation) operator for electrons on the site $i$ of leg $l$, in the orbital $m$ (= $x$, $y$ or $z$ orbital) and with spin $\sigma$ (= $\uparrow$ or $\downarrow$). Moreover, $n_{ilm\sigma} = c_{ilm\sigma}^\dagger c_{ilm\sigma}$ is the corresponding number operator. $\mu$ and $\lambda$ stand for the chemical potential and the amplitude of the spin-orbit coupling, respectively. The energy difference between the $x$-$y$ orbitals and the $z$ orbital is denoted by $\Delta z$. $\epsilon_{m\mu'm''\sigma}$ and $\sigma$ in the spin-orbit interaction are the Levi-Civita symbol and the Pauli matrix, respectively. In order to introduce the superconducting state, attractive nearest neighbor interactions are introduced with $U_a (< 0)$.

We use here BCS-type mean field approximation to decouple the interaction terms. The gap functions for the spin-triplet sector are defined as

$$\Delta^x_{lm}=\frac{1}{2}\left(\langle c_{i+1lm\uparrow}c_{ilm\downarrow}\rangle + \langle c_{i+1lm\downarrow}c_{ilm\uparrow}\rangle\right), \Delta^y_{lm}=\frac{1}{2}\left(\langle c_{i+1lm\uparrow}c_{ilm\downarrow}\rangle + \langle c_{i+1lm\downarrow}c_{ilm\uparrow}\rangle\right),$$

which corresponds to in-plane equal-spin pairing.

3. Results

The model parameters are taken as $t'=0.1t$, $t_z=0.7t$, $t_0'=0.3t$, $\Delta_0=0.065t$ and $\lambda=0.1t$, whose amplitudes describe well the bulk energy dispersion and the two-dimensional Fermi surfaces obtained from the first principles calculation in the normal phase.

The superconducting order parameters are determined self-consistently in the ribbon system at zero temperature for $U_a = -1.5t$ which generates the larger gap function with a very short coherent length. Therefore the number of legs $L = 100$ gives the well-defined independent Andreev bound state at each edge where the gap function at the center of the ribbon corresponds to that of the bulk result.

The most stable pairing state has the chiral $p$-wave form with $d = \Delta_0\hat{z}(k_x + ik_y)$ avoiding nodes in the excitation gap, where the real and imaginary parts of the gap functions have the same amplitudes ($\text{Re}\Delta^x = \text{Im}\Delta^y$) at the center of the ribbon. Note that since $d = \Delta_0\hat{z}(k_x + ik_y)$ and $d = \Delta_0\hat{z}(k_x - ik_y)$ states are degenerate, we hereafter focus on $d = \Delta_0\hat{z}(k_x + ik_y)$ state.

Figure 2 shows the energy dispersion and the spectral function at $l = 1$ in the momentum space for the superconducting state. There exist two groups of subgap states within the fully opened superconducting gap. One is the almost flat dispersion except $k \sim \pm 2/3\pi$ resulting from the $\alpha$-$\beta$ band, which is isolated from the bulk dispersion. The other is the linear dispersion around $k = 0$ from the $\gamma$ band.

Since there are two edges in our ribbon model, the subgap spectrum consists of contributions from both edges. In order to focus on one edge, the local spectral function is depicted in Fig. 2(b) at $l = 1$, which is defined as

$$\rho_l(k, \omega) = \sum_{m\sigma} |u_k(lm\sigma, n)|^2 \delta(\omega - E_{kn}),$$

Figure 2. (a) Energy dispersion and (b) the energy spectrum at $l = 1$ of the ribbon model where bright area represents larger weight.
where \( u_k(\text{lm}\sigma, n) \) is the eigenstate wavefunction of the mean-field Hamiltonian with a quantum number \( n \). Due to the time-reversal symmetry breaking in the chiral \( p \)-wave superconducting state, the edge state is not symmetric with respect to \( k = 0 \), which leads to the spontaneous chiral edge current.

Thus we investigate the current densities, defining the spin-dependent current operators,

\[
\begin{align*}
 j_{\alpha\beta}^{(1)} &= \frac{1}{N} \sum_k (2t \sin k) c_{k\alpha\sigma}^\dagger c_{kl\beta\sigma}, \\
 j_{\alpha\sigma}^{(2)} &= \frac{1}{N} \sum_{m=x,y} \left\{ (-2it' \cos k) c_{klm\sigma}^\dagger c_{kl+1\bar{m}\sigma} + (2it' \cos k) c_{kl+1\sigma}^\dagger c_{klm\sigma} \right\}, \\
 j_{\gamma}^{(1)} &= \frac{1}{N} \sum_k (2t_z \sin k) c_{kl\sigma}^\dagger c_{kl\sigma}, \\
 j_{\gamma}^{(2)} &= \frac{1}{N} \sum_k (2t'_z \sin k) \left( c_{kl\sigma}^\dagger c_{kl+1\sigma} + c_{kl+1\sigma}^\dagger c_{kl\sigma} \right),
\end{align*}
\]

(8)

(9)

where \( \bar{m} \) means \( \bar{x} = y \) and \( \bar{y} = x \). Since the amplitude of the spin-dependent current decreases with distance from the edge and vanishes at the center of the ribbon, we can define the net spin and charge current densities near one edge as follows

\[
\begin{align*}
 j^n_{s} &= \frac{L}{2} \sum_{l=1,\sigma} \left( j_{l\sigma}^{n(1)} + j_{l\sigma}^{n(2)} \right), \\
 j^n_{c} &= -\frac{e}{\hbar} \sum_{l=1,\sigma} \left( j_{l\sigma}^{n(1)} + j_{l\sigma}^{n(2)} \right).
\end{align*}
\]

(10)

Figure 3 shows the net spin and charge currents resulting from the \( \alpha-\beta \) and the \( \gamma \) bands near one of the edges. The chiral edge current appears due to the time-reversal symmetry breaking so that both charge currents from the \( \alpha-\beta \) and the \( \gamma \) bands are rather little affected by the spin-orbit interaction. On the other hand, with increasing the amplitude of the spin-orbit interaction, the net spin current of the \( \alpha-\beta \) band increases. Since an electron on the \( x-y \) orbitals gets the spin-dependent phase factor moving on the smallest closed triangle sites, a spin-dependent effective magnetic field is induced. Therefore both the spin-orbit interaction and the next-nearest-neighbor hopping between the \( x \) and \( y \) orbitals lead to the spin-dependent currents and the net spin current near the edges [5]. On the other hand, the spin-orbit interaction affects the electron on the \( z \) orbital only via the \( x \) and \( y \) orbitals, so that the magnitude of the spin-current of the \( \gamma \) band is small regardless of the spin-orbit coupling. Therefore in our multi-band model of the chiral \( p \)-wave phase, there exist not only charge currents but also spin currents.

Next let us discuss the topological properties of the chiral \( p \)-wave superconducting state. For fully gapped systems the edge state is closely connected with topological properties due to the
bulk-edge correspondence. We define the topological invariant in the superconducting phase by using the two-dimensional bulk system with three orbitals, which is given by

$$N_T = \frac{-2\pi i}{N} \sum_{k} \sum_{ijkl} \langle J^\mu_k \rangle_{ij} \langle J^\nu_k \rangle_{kl} u_k^*(i,n) u_{k'}(j,n') u_k^*(k,n') u_{k'}(l,n') \left( \frac{E_{kn} - f(E_{kn'})}{(E_{kn} - E_{kn'})^2} \right)$$

where indices $i, j, k$ and $l$ include the site, orbital and spin. The operator $J^\mu_k$ is defined as $\langle J^\mu_k \rangle_{ij} = \langle i | \frac{\partial H_k}{\partial \mu_i} | j \rangle$ with the two-dimensional bulk mean-field Hamiltonian $H_{MF}^{2D} = \sum_k H_k$. $E_n$ stands for the energy eigenvalue of the quasiparticle state with index $n$ and $f(E_n)$ is the Fermi distribution function.

Figure 4 shows the topological number $N_T$ as a function of the chemical potential. In order to discuss the $\gamma$ band effect, the topological number for the two ($\alpha$-$\beta$) band model is also computed. At the chemical potential value which well fits the electron density and the Fermi surfaces of $\text{Sr}_2\text{RuO}_4$, the topological number vanishes for the $\alpha$-$\beta$-band part, but is $+1$ through the $\gamma$-band which is essential for topological property. Note that the topological number becomes a non-integer around $\mu = 2t$ where the superconducting gap vanishes partially due to having nodes at the van Hove points in $\gamma$-band. The topological number switches from 1 to $-1$ at $\mu = \mu_c \sim 1.15t$. This indicates that since $\text{Sr}_2\text{RuO}_4$ is near the Lifshitz transition and the amplitude of the fully opened superconducting gap is strongly suppressed, such that the chiral edge state may be sensitive to disorder.

Furthermore the scanning tunneling microscopy studies observed the doubling of the unit cell due to the rotation of the RuO$_6$ octahedron along the $c$ axis with a rotation angle $\theta = 9 \pm 3^\circ$ at the surface of $\text{Sr}_2\text{RuO}_4$ [7]. Since the surface reconstruction resulting from the rotation effect may give rise to the change of the electronic state, we also determine the band structure by means of the first principles calculation package WIEN2k [8] based on the density functional method (DFT). We assume that the lattice constants are identical with the values in the tetragonal structure (space group No.139 I4/mmm), where the muffin-tin (MT) sphere radii $R_{MT}$ are given by 1.95 for Ru, 2.3 for Sr and 1.68 for O a.u., respectively. $R_{MT}K_{MAX} = 7$ where $K_{MAX}$ is amplitude of the largest $K$ vector in plane wave expansion. We assume the lattice structure with rotated RuO$_6$ octahedron as uniform not only at the surface but also in the bulk material, for simplicity. Since $\text{Sr}_2\text{RuO}_4$ displays strong two-dimensional anisotropy, the electronic state has two-dimensional character and is almost independent of the effect from the other layers. Thus, the surface electronic state can be captured within this treatment.

Figure 5 shows the band structure obtained from the first principles calculation in the normal phase for two choices of the rotation angle around the $c$-axis. Note that the number of bands is doubled due to the doubling of unit cell, and the result for $\theta = 0$ is identical with that of the tetragonal structure (space group $I4/mmm$). For $\theta = 0$, the $\gamma$ band near X point is slightly above the Fermi level, which reveals the electron-like Fermi surface. With increasing $\theta$, the $\gamma$ band near X point is lowered and touches the Fermi level at $\theta \sim 5^\circ$ which leads to the Lifshitz
transition. For $\theta > 5^\circ$, the Fermi surface from the $\gamma$ band has the hole-like character. Since the topological aspect only depends on the Fermi surface topology of the $\gamma$-band, the topological number becomes $-1$ (+1) near the surface (in the bulk), which indicates that the topological property may be strongly affected by the surface condition of realistic $\text{Sr}_2\text{RuO}_4$. Therefore no observation of the spontaneous magnetic field in the experimental studies may be attributed to this surface reconstruction in addition to the cancellation due to the spin-polarization [5, 6, 9].

4. Summary and discussion

We have investigated the topological and electronic properties in the chiral $p$-wave superconducting phase by means of the three-band tight-binding model with the ribbon-shaped lattice. We also studied the effect of the RuO$_6$ octahedron along the $c$-axis observed at the surface of $\text{Sr}_2\text{RuO}_4$. While there exist not only charge currents resulting from the time-reversal symmetry breaking in the chiral $p$-wave phase but also spin currents from the $\alpha$-$\beta$ band mainly, the edge states from the $\alpha$-$\beta$ band are not topologically protected. The topological property is attributed to the $\gamma$-band, which is near the Lifshitz transition. Furthermore the small RuO$_6$ octahedron rotation generates a change of the Fermi surface topology, and the topological properties strongly depend on the surface condition of the material.

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