Spontaneous spin polarization at the edge of the chiral superconducting states in a spin Hall metal

Tsuyoshi Imazu and Jun Goryo
Department of Mathematics and Physics, Hirosaki University, Hirosaki 036-8561, Japan
E-mail: jungoryo@hirosaki-u.ac.jp

Abstract. We discuss the chiral superconducting state in a square lattice system with an intrinsic spin-orbit coupling causing the spin Hall effect. We estimate the spontaneous spin polarization \( \langle m_i \rangle \) at the \( i \)-th site and its sum \( M = \sum_i \langle m_i \rangle \) in ribbons. In the zigzag ribbon, we see \( \langle m_i \rangle \neq 0 \) near the edge. The energy spectra of the chiral edge states show the spin splitting and then we have non-zero \( M \). Moreover, we find that \( M \) is enhanced significantly at a topological phase transition point, where the energy gap is closing. We also have non-zero \( \langle m_i \rangle \) near the edge of the straight ribbon, but in contrast, there is no spin splitting in the spectra and \( M \) vanishes.

1. Introduction
The chiral superconductor is the topological superconducting state with broken time-reversal symmetry supporting the chiral edge state at the sample boundary and has been keeping a lot of attention. The role of the spin-orbit coupling in a superconductor has also been studied intensively, and its relation to the chiral edge state is the central issue of this paper. In this point of view, Imai, Wakabayashi and Sigrist argued the spontaneous spin polarization due to the chiral edge states in the model of the chiral superconductor \( \text{Sr}_2\text{RuO}_4 \) [1]. The same mechanism was also examined in the ordered honeycomb network superconductor \( \text{SrPtAs} \), which is a potential candidate for the chiral \( d \)-wave superconductor[2, 3, 4, 5]. Both systems possess the spin-orbit coupling which gives in the normal state the spin-dependent Aharonov-Bohm phase to an electron and causes the spin Hall effect.

To gain the insight into this intriguing phenomena, it would be important to examine a minimal model intensively. We then utilize the simple model on the square lattice proposed by Bernevig, Hughes and Zhang (BHZ) to discuss the quantum spin Hall insulator in the HgTe quantum wells [6, 7].

2. The chiral p-wave pairing in the BHZ metal
In the BHZ model we have four electron fields on a cite \( r \); \( \psi_{s\uparrow}(r), \psi_{p\downarrow}(r), \) and \( \psi_{p\uparrow}(r) \), where \( p_{\pm} = p_x \pm ip_y \). We consider the metallic state by shifting the Fermi level and introduce the chiral p-wave order parameter. The mean field Hamiltonian is

\[
H = H_{\text{BHZ}} + H_\Delta,
\]

\[
H_{\text{BHZ}} = \sum_{r, \sigma = \pm} \sum_{\delta = \pm e_x, \pm e_y} \left\{ -t_{ss} \psi_{s\sigma}^\dagger (r + \delta) \psi_{s\sigma} (r) + t_{pp} \psi_{p\sigma}^\dagger (r + \delta) \psi_{p\sigma} (r) \right\}
\]
arises near the edge, whereas its sum \( \langle N \rangle \) in Figure 3. We have Fermi surfaces shown in Figure 1(b), and \( \Delta = 1 \).

The topology of the chiral to an electron hopping along a certain closed path and causes the spin Hall effect. The term \(-t_{sp} e^{i\delta \sigma} \psi_{sp}^\dagger(r + \delta)\psi_{ps\sigma}(r) - t_{sp} e^{-i\delta \sigma} \psi_{ps\sigma}^\dagger(r + \delta)\psi_{sp\sigma}(r)\),

\[
H_\Delta = \frac{1}{2} \sum_{\sigma = \pm} \sum_{\delta = \pm e_x, \pm e_y} \left\{ \Delta e^{i\delta \sigma} \psi_{sp\sigma}^\dagger(r + \delta)\psi_{sp\sigma}(r) + \Delta e^{i\delta \sigma} \psi_{ps\sigma}^\dagger(r + \delta)\psi_{ps\sigma}(r) + h.c. \right\},
\]

where the up (down) spin is denoted by + (−), \( \sigma = -\sigma \), and \( \theta_{\delta} = \theta_{-\delta} + \pi = 0, \pi/2 \) for \( \delta = e_x, e_y \). The term \( t_{sp} \) is the spin-orbit coupling, which gives the spin-dependent Aharonov-Bohm phase to an electron hopping along a certain closed path and causes the spin Hall effect.

We may diagonalize \( H_{\text{BHZ}} \) by the Fourier transformation in the bulk, and 3D plots of the energy bands and Fermi surfaces are given in Figures 1(a) and 1(b). The topology of the chiral \( p \)-wave state is characterized by the Chern integer \( N_{\text{Ch}} \) [8, 9], which counts the phase winding of the \( k \)-space gap functions around the Fermi surface and gives the number of the topologically protected chiral edge states in a finite-size system.

**Figure 1.** (a): 3D plots of the energy bands of \( H_{\text{BHZ}} \) with parameters \( t_{ss} = t_{pp} = 1.0, t_{sp} = 0.1 \), \( \mu = -1.5, \delta \mu = 1.0 \). Each sheet has two-fold degeneracy with respect to spin. (b): Fermi surfaces of \( H_{\text{BHZ}} \) with parameters \( t_{ss} = t_{pp} = 1.0, t_{sp} = 0.1, \mu = -1.5, \delta \mu = 1.0 \). Purple dots and integers show the zeros of the \( k \)-space chiral \( p \)-wave gap function \( \Delta(\sin k_x + i \sin k_y) \) and their contributions to the Chern integer \( N_{\text{Ch}} \) including the spin degrees of freedom. In this case, \( N_{\text{Ch}} = 4 \).

### 3. Spontaneous spin polarization at the edge

Besides the spontaneous charge current, we would have the spin current and therefore spin at the edge due to the spin orbit coupling [1, 5]. In this paper, we focus on the spin polarization in our model and discuss its enhancement.

We examine straight and zigzag ribbons (see Figure 2), and obtain the energy spectra and spin polarization (local moment) at the \( i \)-th site in the unit cell \( (i = 1, ..., N) \)

\[
\langle m_i \rangle = \sum_{\sigma = \pm} \sum_{k} \sigma \left( \langle \psi_{ik\sigma}^\dagger \psi_{ik\sigma} \rangle + \langle \psi_{ik\sigma}^\dagger \psi_{ik\sigma} \rangle \right),
\]

where \( \langle \ldots \rangle \) denotes the expectation value in the superconducting ground state and \( k \) wave number. We verify that \( \langle m_i \rangle \) would be zero in the absence of the spin-orbit coupling \( t_{sp} \).

We then use the parameters \( t_{ss} = t_{pp} = 1.0, t_{sp} = 0.1, \mu = -1.5, \delta \mu = 1.0 \), which give the bulk Fermi surfaces shown in Figure 1(b), and \( \Delta = 1.0 \) and \( N = 100 \). The results are summarized in Figure 3. We have \( N_{\text{Ch}} = 4 \) and four chiral states at each edge. In the straight ribbon, all edge spectra are degenerate with respect to spin degrees of freedom. The spin polarization \( \langle m_i \rangle \) arises near the edge, whereas its sum

\[
M = \sum_{i=1}^{N} \langle m_i \rangle
\]
vanishes completely. On the other hand, in the zigzag case the degeneracy is lifted for the edge spectra with respect to spin. We thus have a difference between the total occupation numbers for up and down spin and $M \neq 0$ besides the spin polarization near the edge.

We then examine the $\mu$ dependence of $M$. The result is summarized in Figure 4. We see a sharp enhancement slightly below $\mu = -1$, where the topological phase transition occurs and $\mathcal{N}_{Ch}$ shows a jump from $+4$ to $0$ with increasing $\mu$. This enhancement comes from the fact that the split edge spectra become almost flat when the gaps at $k = \pm \pi$ become tiny, and we have a large difference between the occupation numbers of up and down spin.

![Figure 2. (a) The straight and (b) zigzag ribbons we have examined.](image)

![Figure 3. The energy spectra in (a) the straight and (d) zigzag ribbons (b) and (e) are magnifications for (a) around $k = 0$ and (e) around $k = -0.5$, respectively, and the spin polarization $\langle m_i \rangle$ in the left half of (c) the straight and (f) the zigzag ones. Each result is symmetric in the right half. Note that the spectra in (b) do not but that in (e) show the spin splitting; Orange and green lines in (e) show the spectra of chiral edge states with up and down spin. The spectra in (b) are two-fold degenerate.](image)

4. Summary and discussion
We discuss the chiral $p$-wave pairing in the BHZ spin Hall metal and estimate the spin polarization $\langle m_i \rangle$ in Eq. (2) and its sum $M$ in Eq. (3) in the ribbon geometries. The result depends on the shape of the ribbon significantly. We have $\langle m_i \rangle$ around the edge but no $M$ in the straight ribbon. In the zigzag ribbon, on the other hand, we have both since the energy
In the straight edge, the spectrum are completely degenerate with respect to spin. The spin expectation value in the superconducting ground state.

In this paper, we estimate the spin polarization in our model and discuss its enhancement.

We examine straight and zigzag ribbons and obtain the energy spectrum and spin polarization by Imai, Wakabayashi and Sigrist in the model for the chiral superconductor Sr$_2$RuO$_4$ -wave superconductor.

The same issue has been pointed out also in Ref. [5].

We use the parameters $\Delta_{pp}=1$, $\Delta_{ss}=0.25$, $\delta_{ip}=1$, where we have $N_{Ch}=0$ and the edge state is absent.

spectra of the chiral edge states show spin splitting. $M$ is significantly enhanced at the vicinity of a topological phase transition (gap closing) point, since the spin-split edge spectra become almost flat.

We would discuss elsewhere the relation between the ribbon geometry and the spin splitting in the edge spectra [10].

**Figure 4.** The $\mu$ dependence of $M$. We see a sharp peak slightly below $\mu = -1$, where we have the topological phase transition (gap closing) at $k = \pm \pi$. $M$ vanishes suddenly when $\mu > -1$, since $N_{Ch} = 0$ and the edge state is absent.

This work was supported by JSPS KAKENHI Grant Number JP20K03826.

**Acknowledgment**

This work was supported by JSPS KAKENHI Grant Number JP20K03826.

**References**

[1] Imai Y, Wakabayashi K, and Sigrist M, 2011 J. Phys. Soc. Jpn. 80 055002.
[2] Nishikubo Y, et al. 2013 Phys. Rev. B 87 180500(R).
[3] Bisbas P K, et al. 2013 Phys. Rev. B 87 180500(R).
[4] Fischer M H, et al. 2014 Phys. Rev. B 89 020509(R).
[5] Goryo J, Imai Y, Rui W B, Schnyder A P, and Sigrist M, 2017 Phys. Rev. B 96 140502(R).
[6] Bernevig B A, Hughes H L, and Zhang S -C, 2006 Science 314 1757.
[7] König M, et al. 2007 Science 317 766.
[8] Thouless D J, Kohmoto M, Nightingale M P, and den Nijs M, 1982 Phys. Rev. Lett. 49 405.
[9] Kohmoto M, 1985 Ann. Phys. (N. Y.) 160 355.
[10] The same issue has been pointed out also in Ref. [5].