Chiral Majorana fermion edge states in a heterostructure of superconductor and semiconductor with spin-orbit coupling

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Abstract. We study low-energy excitations in a device, consisting of spin-orbit coupling semiconductor, \textit{s}-wave superconductor and ferromagnetic insulator. A vortex in the device generates zero-energy Majorana Fermions at both the edge of a finite sample and the vortex core. In this work, we identify the chirality of edge excitation states, and investigate how it is affected by Zeeman field and spin-orbit coupling. We prove the commutation relation of total angular momentum with Bogoliubov-de Gennes (BdG) Hamiltonian. With the help of the relation, we get analytically the angular part of the solution to the BdG equation for a circular sample. We perform numerical simulations to evaluate the radial part of wave-function, and derive distribution of Majorana fermion state and energy dispersion for low-energy excitations.

1. Introduction

Majorana Fermions (MFs) are particles with an intriguing property that they are their own anti-particles [1]. It is predicted theoretically that MFs obey non-Abelian statistics [2], which have potential applications in constructing topological quantum computers [3]. With such a promising future, MFs are searched among numerous systems. However, there is no firm evidence that MFs can be elementary particles up until now. It’s more likely to have them as quasi-particle excitations in condensed matter systems. Many potential MF hosts have been proposed, including spinless \textit{p}-wave superconductors [4], Pfaffian $\nu = 5/2$ fractional quantum Hall state [5] and \textit{p}-wave superfluid of cold atoms [6]. Recently, there is a surge of discussions on realizing MFs in heterostructures, such as the surface state of a topological insulator with proximity-induced \textit{s}-wave superconductivity [7], spin-orbit coupled semiconductor sandwiched by \textit{s}-wave superconductor and ferromagnetic insulator (S/SM/FI) [8]. In these devices, the \textit{p}-wave pairing is superseded by the interplay between proximity-induced \textit{s}-wave superconductivity and spin-orbit coupling. One advantage that they offer is a relatively easier experimental accessibility.

In a finite S/SM/FI device, it has been shown that MFs appear as zero-energy excitations in the presence of vortex, one at the sample edge while the other bounded by vortex core [10]. Although there are numerous theoretical studies on the existence of MFs, not much attention has been paid to detailed properties of the MF at the edge, which is capable of being manipulated efficiently and follows non-Abelian statistics for braiding process [11]. In this
sense, more complete understanding of the MFs is indispensable before one can make use of them. In the present work, we study the chirality and the spin direction of the MF at the edge and their dependence on Zeeman field and spin-orbit coupling. The total angular momentum for quasi-particles is proved to be a conserved quantity. Based on this, we get analytically the angular part of the solution to the Bogoliubov-de Gennes (BdG) equation. We solve the radial part numerically for several low-energy excitation states in a finite circular sample. With the full numerical wave-functions, we are able to study the distribution of MF state and the energy dispersion for low-energy excitations.

2. Bogoliubov-de Gennes equation and solution

We start from the Hamiltonian of a semiconductor with sizable Rashba-type spin-orbit coupling in proximity to a ferromagnetic insulator

\[
H_0 = \int d\vec{r} \hat{c}^\dagger(\vec{r}) \left[ \frac{\vec{p}^2}{2m^*} - \mu + \alpha_R (\vec{\sigma} \times \vec{p}) \cdot \hat{z} + V_z \hat{\sigma}_z \right] \hat{c}(\vec{r}),
\]

where \(m^*, \mu, \alpha_R\) and \(V_z\) are effective electron mass, chemical potential, Rashba spin-orbit coupling strength and Zeeman field respectively, \(c = (\hat{c}_\uparrow \hat{c}_\downarrow)^T\) is electron annihilation operator, \(\vec{\sigma} = (\hat{\sigma}_x \hat{\sigma}_y \hat{\sigma}_z)\) are Pauli matrices.

The proximity-induced s-wave superconductivity is described by

\[
H_{SC} = \int d\vec{r} \left[ \Delta(\vec{r}) \hat{c}^\dagger_\uparrow \hat{c}^\dagger_\downarrow + h.c. \right],
\]

where \(\Delta(\vec{r})\) is the effective s-wave pairing potential. Therefore, the total Hamiltonian is \(H = H_0 + H_{SC}\). The system behaves effectively as a 2D spinless \(p_x + ip_y\) superconductor for \(\sqrt{\Delta^2 + \mu^2} < V_z\) [8, 9], which gives rise to MFs.

With respect to \(H\), we can write down the BdG equation

\[
\begin{pmatrix}
H_0 & \Delta \\
\Delta^\dagger & -\hat{\sigma}_y H_0^\dagger \hat{\sigma}_y
\end{pmatrix} \Psi(\vec{r}) = E \Psi(\vec{r}),
\]

with the Nambu spinor \(\Psi(\vec{r}) = [u_\uparrow(\vec{r}), u_\downarrow(\vec{r}), v_\downarrow(\vec{r}), -v_\uparrow(\vec{r})]^T\). Provided \(\Psi\) is an eigenstate of the BdG equation with eigenenergy \(E\), we always have another eigenstate \(\Xi \Psi\) with eigenenergy \(-E\), where \(\Xi\) is the particle-hole transformation operator.

In the presence of \(n\) vortices, the induced s-wave pairing potential is \(\Delta = \tilde{\Delta}_0(\vec{r}) e^{in\theta}\). The matrix form of the total Hamiltonian \(H\) in polar coordinates is given by

\[
H = \left( -\frac{\hbar^2}{2m^*} \nabla^2 - \mu \right) \tau_z + V_z \sigma_z + \frac{\alpha}{2} (\sigma_+ p_- - \sigma_- p_+) \tau_z + \tilde{\Delta}_0 [\cos(n\theta) \tau_x + \sin(n\theta) \tau_y],
\]

where \(\tau_x, \tau_y, \tau_z\) are 4 \(\times\) 4 unitary matrices in the particle space with their explicit representations given by Eq.(A.3) in Appendix, and \(\sigma_\pm\) and \(p_\pm\) are defined as \(\sigma_x \pm i\sigma_y\) and \(p_x \pm ip_y\) respectively.

Total angular momentum \(J_z\) defined by [10]

\[
J_z = L_z + \frac{\hbar}{2} (\sigma_z - n\tau_z),
\]

where \(L_z, \sigma_z\) are orbit and spin angular momentum operators respectively, can be proven to commute with the total Hamiltonian \(H\) (see Appendix for detailed proof). Due to the
commutation relation, the eigenfunction of $H$, denoted by $\Psi(r, \theta)$ in polar coordinates, can be written in terms of eigenfunction of $J_z$ with additional radial part. Since

$$J_z \psi(\theta) = \left[ L_z + \frac{\hbar}{2}(\sigma_z - n\tau_z) \right] \psi(\theta) = m_J \hbar \psi(\theta)$$

for eigenvalue $m_J \hbar$ and corresponding eigenstate $\psi(\theta)$ of operator $J_z$, we have

$$L_z \psi(\theta) = -i\hbar \frac{\partial}{\partial \theta} \psi(\theta) = \left( m_J \hbar - \frac{\hbar \sigma_z}{2} + \frac{n\hbar \tau_z}{2} \right) \psi(\theta).$$

We can then compose the eigenstate of the BdG Hamiltonian

$$\Psi(r, \theta) = \begin{pmatrix} u_{\theta, m_J}(r)e^{i(m_J + \frac{n+1}{2})\theta} \\ u_{\theta, m_J}(r)e^{i(m_J + \frac{n+1}{2})\theta} \\ v_{\theta, m_J}(r)e^{i(m_J - \frac{n+1}{2})\theta} \\ -v_{\theta, m_J}(r)e^{i(m_J - \frac{n+1}{2})\theta} \end{pmatrix},$$

where $(u_{\theta, m_J}(r), u_{\theta, m_J}(r), v_{\theta, m_J}(r), -v_{\theta, m_J}(r))^T$ is the radial part of $\Psi(r, \theta)$. Analyzing the radial part of $\Psi(r, \theta)$, one can derive the condition for the existence of MFs [10]. However, physical quantities of edge states in finite systems are not accessible analytically. Therefore, we rely on numerical solutions to the BdG equation to study the distribution of MF state and the energy dispersion of low-energy excitations.

3. Low-energy excitations at the sample edge

We now solve the BdG equation numerically by employing tight binding model [11]

$$\hat{H} = -t_0 \sum_{l, \sigma} \hat{c}_l^\dagger \hat{c}_{l+\delta_0} e^{i\sigma} - t_{\alpha} \sum_{l, \sigma} \hat{c}_l^\dagger \hat{c}_{l+\delta_0} e^{-i\sigma} + \sum_{l} V_z \left( \hat{c}_l^\dagger \hat{c}_{l+1} - \hat{c}_l^\dagger \hat{c}_{l+1} \right)$$

$$+ it_{\alpha} \sum_{l, \delta} \left( \hat{c}_{l+\delta_0}^\dagger \sigma_y \hat{c}_l - \hat{c}_{l+\delta_0}^\dagger \sigma_y \hat{c}_l + h.c. \right) + \sum_{l} \left( \Delta \hat{c}_l^\dagger \hat{c}_l^\dagger + h.c. \right),$$

where $t_0 = \hbar^2 / 2m^* a^2$ and $t_{\alpha} = \alpha \hbar R / 2a$ are hopping rates with respect to spin-reservation and spin-flipping between nearest neighbors; $a$ is the grid spacing; $l$ are two dimensional mesh indices. The radius of the circular sample we take is $75a$, which leads the dimension of the Hamiltonian matrix to the order of $10^5$. The discretized Hamiltonian $\hat{H}$ is diagonalizable by applying the numerical technique provided in [12].

For a circular sample (see Fig.1(a)), where one vortex is induced at the center with pairing potential $\Delta(r) = \Delta_0[1 - \exp((-r/s)^2)]e^{i\theta}$ ($s = 4a$), we find a zero-energy MF state at the sample edge, as shown in Fig.1(b). The chirality of the MF is clockwise for $V_z > 0$, and the in-plane spin component of the MF points away from the center of circle with additionally $\alpha > 0$, as shown in Fig. 2. The chirality and the in-plane spin component depend on the Zeeman field and the spin-orbit coupling in the way summarized in Table 1.

By diagonalizing the Hamiltonian $\hat{H}$, we are able to calculate the energy and the total angular momentum $\langle J_z \rangle$ of quasi-particles at the edge of a finite circular sample. As shown in Fig. 3, the excitation energy and the total angular momentum are in linear relationship with slope $-E_0$ for $V_z > 0$, where $E_0$ is the excitation gap between the first excitation state with finite positive energy and the zero-energy MF state, and the sign of the slope can be changed by turning the Zeeman field to the opposite direction.
Figure 1. (a) Heterostructure of s-wave superconductor with a vortex, spin-orbit coupled semiconductor and ferromagnetic insulator. (b) Distribution of the MF at the sample edge. Results are obtained in a sample with radius 75a for $\Delta_0 = 0.5t_0$, $V_z = 0.8t_0$, $\mu = 0$ and $\alpha = 0.9$, which satisfy the relation $V_z > \sqrt{\mu^2 + \Delta^2}$.

Figure 2. Chirality (black arrow) and in-plane spin component (blue arrow) of the MF at the edge. The parameters used are the same as those given in Fig. 1.

Table 1. Chirality and in-plane spin component of the MF as function of Zeeman field and spin-orbit coupling

| $V_z$ | $\alpha$ | Chirality     | In-plane spin component |
|-------|----------|---------------|-------------------------|
| +     | +        | clockwise     | away from center        |
| +     | -        | clockwise     | towards center          |
| -     | +        | anticlockwise | towards center          |
| -     | -        | anticlockwise | away from center        |

Figure 3. Energy dispersion relation of the edge states for both $V_z > 0$ and $V_z < 0$. $E_0 = 1.55 \times 10^{-2}t_0$ for parameters given in Fig. 1.

4. Conclusion
We have studied the edge states in a finite sample of circular shape. The commutation relation between the total angular momentum and the full Hamiltonian has been proven. Based on the relation, the angular part of the solution to the Bogoliubov-de Gennes equation has been derived analytically. For the radial part, we solve the Bogoliubov-de Gennes equation numerically. With the full solutions, we have derived the energy dispersion of low-energy excitations at the edge. We have revealed the dependence of the chirality and the in-plane spin component of the MF on the Zeeman field and the spin-orbit coupling.
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Appendix
In this Appendix, we prove the commutation relation between the total angular momentum $J_z$ and the Bogoliubov-de Gennes (BdG) Hamiltonian $H$. Let’s define $\sigma_+ = \sigma^\dagger = \sigma_x + i\sigma_y$, $p_+ = p_x + ip_y = e^{i\theta}(-i\partial_r + \frac{\tau}{r}\partial_\phi)$ and $p_- = p_x - ip_y = e^{-i\theta}(-i\partial_r - \frac{\tau}{r}\partial_\phi)$. The matrix $\sigma_x, \sigma_y$ and $\sigma_z$ are given by

$$
\sigma_x = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.
$$

(A.1)

After substituting $\vec{p}$ in Eq.(3) by $p_\pm$, we can form the full BdG Hamiltonian in polar coordinates

$$
H_{BdG} = \int d^2r \left( -\frac{\hbar^2}{2m^*} \nabla^2 - \mu \right) (c_\uparrow^\dagger c_\downarrow + c_\downarrow^\dagger c_\uparrow - c_\uparrow^\dagger c_\uparrow - c_\downarrow^\dagger c_\downarrow + V_z (c_\uparrow^\dagger c_\uparrow - c_\downarrow^\dagger c_\downarrow + c_\downarrow^\dagger c_\uparrow + c_\uparrow^\dagger c_\downarrow)) + i\alpha \left( p_- c_\uparrow^\dagger c_\downarrow + V_z (c_\downarrow^\dagger c_\uparrow - c_\downarrow^\dagger c_\downarrow + c_\downarrow^\dagger c_\uparrow + c_\uparrow^\dagger c_\downarrow) + \tilde{\Delta}_0 \left( e^{i\theta} c_\downarrow^\dagger c_\uparrow + e^{-i\theta} c_\uparrow^\dagger c_\uparrow - e^{i\theta} c_\downarrow^\dagger c_\downarrow - e^{-i\theta} c_\uparrow^\dagger c_\downarrow \right) \right).$$

(A.2)

By defining unitary matrix $\tau_x, \tau_y$ and $\tau_z$ in the particle space as

$$
\tau_x = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad \tau_y = \begin{pmatrix} 0 & 0 & i & 0 \\ 0 & 0 & 0 & i \\ -i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix}, \quad \tau_z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix},
$$

(A.3)

we have the matrix form of full Hamiltonian in Nambu space

$$
H_{BdG} = \left( -\frac{\hbar^2}{2m^*} \nabla^2 - \mu \right) \tau_z + V_z \sigma_z + i\alpha \frac{\tau}{2} (\sigma_+ p_- - \sigma_- p_+) \tau_z + \tilde{\Delta}_0 \left\{ \cos(n\theta) \tau_z + \sin(n\theta) \tau_y \right\}.
$$

(A.4)

Let $\tau_+ = \frac{\tau_x + i\tau_y}{2}$ and $\tau_- = \frac{\tau_x - i\tau_y}{2}$, the following basic commutation relations are established.

$$
[\sigma_a, \sigma_b] = 2i\varepsilon_{abc} \sigma_c; \quad [\tau_a, \tau_b] = -2i\varepsilon_{abc} \tau_c; \quad [\sigma_z, \sigma_+] = 2\sigma_+; \quad [\tau_z, \tau_+] = -2\tau_+; \quad [\sigma_z, \sigma_-] = -2\sigma_-; \quad [\tau_z, \tau_-] = 2\tau_-; \quad [\sigma_z, \tau_+] = 0; \quad [\tau_z, \sigma_+] = 0; \quad [\tau_z, \tau_+] = 0.
$$

(A.5)

$$
[L_z, p_-] = [xp_y - yp_x, p_x - ip_y] = [x, p_x]\hbar y + i[y, p_y]p_x = i\hbar p_y - \hbar p_x = -h p_-; \quad [L_z, p_+] = [xp_y - yp_x, p_x + ip_y] = [x, p_x]\hbar y - i[y, p_y]p_x = i\hbar p_y + \hbar p_x = h p_+.
$$

(A.6)

The first two terms in Eq.(A.4) remain invariant under rotation. Therefore, we have

$$
\left[ J_z, \left( -\frac{\hbar^2}{2m^*} \nabla^2 - \mu \right) \tau_z + V_z \sigma_z \right] = 0.
$$

(A.7)

Considering the spin-orbit coupling part in Eq.(A.4), we have

$$
[J_z, \sigma_+ p_-] = [L_z, \sigma_+ p_-] + \frac{\hbar}{2} [\sigma_z - n\tau_z, \sigma_+ p_-] = [L_z, \sigma_+ p_-] + \frac{\hbar}{2} \{[\sigma_z, \sigma_+] p_- + \sigma_+ [\sigma_z, p_-] + \frac{\hbar}{2} [n\tau_z, \sigma_+ p_-] - \frac{\hbar}{2} [n\tau_z, \sigma_+ p_-] \} = -\hbar \sigma_+ p_- + \hbar \sigma_+ p_- = 0.
$$

(A.10)
Similarly, \([J_z, \sigma_- p_+] = 0\). Thus,

\[
\left[J_z, \frac{\alpha}{2} (\sigma_+ p_- - \sigma_- p_+) \tau_z \right] = 0.
\]

(A.13)

As for the superconducting part \((e^{-in\theta} \tau_+ + e^{in\theta} \tau_-)\) in Eq.(A.4), we have

\[
\left[J_z, e^{-in\theta} \tau_+ \right] = \left[L_z, e^{-in\theta} \tau_+ \right] + \frac{\hbar}{2} \left[\sigma_z - n \tau_z, e^{-in\theta} \tau_+ \right]
\]

(A.14)

\[
= \left[L_z, e^{-in\theta} \tau_+ \right] + e^{-in\theta} \left[L_z, \tau_+ \right] + \frac{\hbar e^{-in\theta}}{2} \left[\sigma_z, \tau_+ \right] - \frac{n \hbar}{2} e^{-in\theta} \cdot (-2 \tau_+)
\]

(A.15)

\[
= [-i\hbar \partial_\theta, e^{-in\theta} \tau_+] + 0 + 0 + n \hbar e^{-in\theta} \tau_+
\]

(A.16)

\[
= -n \hbar e^{-in\theta} \tau_+ + n \hbar e^{-in\theta} \tau_+ = 0.
\]

(A.17)

Similarly, \([J_z, e^{in\theta} \tau_-] = 0\). Therefore, We get

\[
\left[J_z, \tilde{\Delta}_0 \{\cos(n\theta) \tau_x + \sin(n\theta) \tau_y \} \right] = 0.
\]

(A.18)

Thus, the BdG Hamiltonian \(H\) commutes with the total angular momentum \(J_z\)

\[
[J_z, H] = 0.
\]

(A.19)

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