Evolution of Majorona zero-energy edge states in a $T^2 = -1$ symmetry protected 1D topological superconductor with dominant spin-orbit coupling

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We consider a 1D topological superconductor (TSC) constructed by coupling a pair of Kitaev’s Majorana chains with opposite spin configurations. Such a 1D lattice model is known to be protected by a $T^2 = -1$ time-reversal symmetry. Furthermore, we consider a modeled Rashba spin-orbit coupling on such a system of $T^2 = -1$ time-reversal symmetric TSC. The Rashba spin-orbit coupling together with the chemical potential engineered the phase transitions of the edge states in the system and consequently the number of Majorana’s zero-energy edge modes (MZM’s) emerging at the edge of the coupled chains. Correspondingly, the topological nature of the system is described by a phase diagram consisting of three different phases. The three phases are characterized by a topological winding number, $W = 1, 2$ (with one and two MZM’s: topological phases) and $W = 0$ (devoid of any MZM: trivial insulating phase).

An increasing effort in developing the future quantum computer technology has led to full swing research on low-input power integrating circuits. Owing to their conducting edge states, topological insulators are one of those candidates that offer most of all the desirable demands. Ever since it was introduced by Haldane, it has been at the center of condensed matter research. Topological insulators have chiral edge states which essentially do not require any external magnetic field,23 for them to exhibit the quantum Hall effect, thus often called anomalous quantum Hall effect. With no such requirements of an external magnetic field, topological insulators are very much sought after when called upon for a future low-power-consuming integrated circuit application.

One of many premier discoveries in condensed matter physics has been that of the Majorana fermions in a topological superconductor (TSC’s) (a distinct class of superconductors). Majorana fermion is being viewed as a “half-fermion” that obeys non-Abelian statistics. In a TSC, these fermions become localized at the TSC’s edges to form zero-energy bound state modes called Majorana zero modes (MZM’s). Experimental detections of MZM’s are done by transferring topological properties on a conventional superconductor and alternately, by making a contact between a superconductor and a topological insulator. Theoretically, the most accepted model that formulates the MZM’s was proposed by Kitaev. Kitaev proposed a TSC in a 1-dimension chain consisting of an arrangement of spinless electrons with nearest-neighbor hopping energy $t$ and superconducting energy gap $\Delta$. If the chemical potential, $\mu$, is engineered in such a way that $|\mu| \leq 2t$ (with $\Delta \neq 0$), the chain enters a topological phase and hosts unpaired MZM’s at each of its ends.

In this paper, we consider a special class of a 1D TSC protected by the $T^2 = -1$ time-reversal symmetry. The coupling of two Kitaev’s Majorana chains with opposite spin configurations (as shown in Fig. 1) results in this special symmetry-protected topological phase. In such an arrangement, each physical site can be considered to consist of four Majorana modes (see Fig. 1). In this paper, we will show the different conditions on the system parameters (also with the inclusion of spin-orbit coupling effect) by which the chain will enter different topological phases and correspondingly, the phase transitions of the edge states. It is to be noted that the dangling zero-energy Majorana spinons at both ends of the chain become protected by the time-reversal symmetry that reads as

$$
\begin{align}
Td_{l\uparrow}T^{-1} &= -d_{l\downarrow}, & Td_{l\downarrow}T^{-1} &= d_{l\uparrow}, \\
Td_{l\uparrow}T^{-1} &= -d_{l\downarrow}, & Td_{l\downarrow}T^{-1} &= d_{l\uparrow}.
\end{align}
$$

The complex fermionic operators $d_{l\sigma}$ and $d_{l\sigma}^\dagger$ (with $\sigma = \uparrow, \downarrow$ being the spin of the fermion) can be written in terms of the two Majorana operators $\gamma_{l\sigma}$ and $\gamma_{l\sigma}^\dagger$ as

$$
\begin{align}
d_{l\sigma} &= \frac{1}{2}(\gamma_{l\sigma} + i\gamma_{l\sigma}^\dagger), \\
d_{l\sigma}^\dagger &= \frac{1}{2}(\gamma_{l\sigma} - i\gamma_{l\sigma}^\dagger).
\end{align}
$$

![FIG. 1. A time reversal symmetric $T^2 = -1$ protected 1D TSC. A) A coupling of two Majorana chains with opposite spin configurations, emphasising the Rashba spin-orbit couplings. B) The figure depicts the Majorana spinor pair of opposite spins at each ends of the coupled Kitaev’s Majorana chains, $\gamma_{l\uparrow} = \gamma_{l\downarrow}$ and $\gamma_{l\uparrow} = \gamma_{l\downarrow}$ on the left and $\gamma_{l\uparrow} = \gamma_{l\downarrow}$ on the right.](image-url)
Similar to the spinless Majorana fermions, the above Majorana operators $\gamma_{\sigma}^\dagger$ and $\gamma_{\sigma}$ have the anticommutation relations $\{\gamma_{\sigma}^\dagger, \gamma_{\sigma'}\} = 0$ and $\{\gamma_{\sigma}^\dagger, \gamma_{\sigma'}^\dagger\} = 2\delta_{\sigma\sigma'} \delta_{\sigma\sigma'}$. From Eq. (1), it is easy to see that the time-reversal symmetry has a projective representation of $T^2 = -1$ for the fermion parity odd basis and $T^2 = 1$ for fermion parity the even basis. To construct a total symmetry group for this system of spin-full fermions we need four group elements $\{I, T, T^2, T^3\}$ with $T^2 = 1$, which is a $\mathbb{Z}_4$ group, an extension of the $\mathbb{Z}_2$ fermion parity symmetry group.

For analyzing the bulk spectrum, we write down the fermionic operator $d_{j,\sigma}$ in Eq. (3) as

$$d_{j,\sigma} = \frac{1}{\sqrt{N}} \sum_k d_{k,\sigma} e^{ikj}$$

where we have taken a unit lattice constant and the momentum, $k'$ is restricted within the first Brillouin zone, i.e. $k \in [-\pi, \pi]$. Using the above equation for the fermionic operator, the Hamiltonian in Equation (3), can now be written as

$$H = -\mu \sum_{s,k} d_{k,\sigma}^\dagger d_{k,\sigma} + \sum_{s\neq s',k} [-t e^{ik} d_{s,\sigma}^\dagger d_{s',\sigma} + \Delta e^{-ik} d_{s,\sigma}^\dagger d_{s',\sigma} - (\alpha_z - \alpha e^{ik}) d_{s,\sigma}^\dagger d_{s',\sigma'} + \text{h. c.}].$$

FIG. 2. (a): Band diagram of the first 7 bands (counting from the first edge state) for a total number of sites $N = 40$. The two edge states are shown in solid red color and dashed blue color. The MZM’s in regimes I and II are localized towards the end of the chain at $j = 1$ and $j = N$ indicating that the MZM’s are contributions from those states at the two edges of the chain. In regime III, the wave-function of the two edge states has significant contributions from those sites at the bulk of the chain.

$$H = \psi_{k,\uparrow,\downarrow}^\dagger H(k) \psi_{k,\uparrow,\downarrow}$$

$$= \begin{pmatrix}
    d_{k,\uparrow}^\dagger & d_{k,\downarrow}^\dagger & d_{-k,\uparrow} & d_{-k,\downarrow}
\end{pmatrix}
\begin{pmatrix}
    -\mu - 2t \cos k & -\alpha_z + 2\alpha \cos k & 2i\Delta \sin k & 0 \\
    -\alpha_z + 2\alpha \cos k & -\mu - 2t \cos k & 0 & 2i\Delta \sin k \\
    2i\Delta \sin k & 0 & \mu + 2t \cos k & \alpha_z - 2\alpha \cos k \\
    0 & 2i\Delta \sin k & \alpha_z - 2\alpha \cos k & \mu + 2t \cos k
\end{pmatrix}
\begin{pmatrix}
    d_{k,\uparrow} \\
    d_{k,\downarrow} \\
    d_{-k,\uparrow} \\
    d_{-k,\downarrow}
\end{pmatrix}, \quad (6)$$
The $4 \times 4$ Bogoliubov-de Gennes (BdG) Hamiltonian, $\mathcal{H}(k)$ is easily diagonalized to yield a 4-band energy spectrum given by

$$E_\alpha^\lambda(k) = s\sqrt{(\mu + 2t \cos k)^2 + (\mu + 2\lambda \cos k)^2 + (\mu - \lambda_2)\cos k + 8\lambda t \cos^2 k + 4\Delta^2 \sin^2 k - 2(\mu^2 + 2\alpha_2(\alpha + \lambda t) \cos k)}.$$ 

Here, $s, \lambda = \pm$. In the limit of $\mu \to 0$ and $\alpha_2 \to 0$, the above result reduced to a system of two Kitaev chains that hosted two degenerated unpaired MZM’s when $|\mu| < 2|t|$.[3] As expected, the BdG Hamiltonian in Eq. (6) should exhibit a time-reversal symmetry $T^2\mathcal{H}^*(k)(T^{-1})^2 = \mathcal{H}(-k)$, with $T = \sigma_z \otimes \sigma_z$. Also, it has an electron-hole symmetry $\xi\mathcal{H}^*(k)\xi^{-1} = -\mathcal{H}(-k)$, with $\xi = \sigma_x \otimes \sigma_0$. Here $(\sigma_0, \sigma_x, \sigma_y)$ are the Pauli’s matrices. To reduce the BdG Hamiltonian into an off-diagonal matrix block, we introduce a unitary operator, ‘$U$’, defined as

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} \sigma_x & \sigma_x \\ -\sigma_y & \sigma_y \end{pmatrix}.$$ 

On doing the unitary transformation $U^\dagger \mathcal{H}(k)U$, we obtained a transformed BdG Hamiltonian

$$U^\dagger \mathcal{H}(k)U = \begin{pmatrix} \mathcal{O} & Q(k) \\ Q^\dagger(k) & \mathcal{O} \end{pmatrix}.$$ 

Here $\mathcal{O}$ is a $2 \times 2$ null matrix and $Q(k)$ is given by

$$Q(k) = i(\mu + 2t \cos k)\sigma_z - 2\Delta \sin k\sigma_z + (\alpha_2 - 2\alpha \cos k)\sigma_y.$$ 

We note that $\det[\mathcal{H}(k)] = \det[Q(k)] \cdot \det[Q^\dagger(k)]$. For a band closing condition, $\det[\mathcal{H}(k)] = 0$. We, thus, arrive at the two conditions for closing the gap which are given as:

$$(\mu - \alpha_2 + 2(t + \alpha) \cos k)^2 + 4\Delta^2 \sin^2 k = 0$$

$$(\mu + \alpha_2 + 2(t - \alpha) \cos k)^2 + 4\Delta^2 \sin^2 k = 0.$$ 

The above two conditions basically mark the boundaries for the appearance of the spin-up and spin-down MZM’s, respectively. Similar to the case of a single Majorana Kitaev’s chain,[20][21] we now have an appearance of a gap closing at $k = 0$, and $k = \pm \pi$, when the superconducting gap $\Delta \neq 0$ and the remaining parameters set to $\mu = \alpha_2 = -2(t \pm \alpha)$ and $\mu = \alpha_2 = 2(t \pm \alpha)$, respectively. The system of two Majorana Kitaev’s chains enters any of the topological phases when the different parameters dictate the conditions $\Delta \neq 0$ and $|\mu \mp \alpha_2| < 2|t \pm \alpha|$. In order to understand the characterization of the different topological phases, we calculate the winding number for the BdG Hamiltonian in Eq. (6)[3][5][11]

$$W = \text{Im} \int_0^{\pi} \frac{d}{dk} \ln[\det(Q(k))].$$ 

We show the variation of this number as a function of $\mu$ and $\alpha$ in Figure. 3(a), for the cases of $\alpha_2 = 1.5t$. The boundaries separating the different topological phases are determined by the equation $|\mu \mp \alpha_2| = \pm 2|t \pm \alpha|$ obtained by the gap closing conditions in Eq. (11). The winding number gives the number of MZM’s at each edge of the chain

$$\text{No’s of MZM’s} = \begin{cases} 2, & \text{if } W = 2 \\ 1, & \text{if } W = 1 \\ 0, & \text{if } W = 0 \end{cases}$$

To demonstrate the different topological phases we plot the band diagram as a function of the chemical potential for different strengths of the two types of spin-orbit couplings in Fig. 3(b & c)]]. For better understanding, the bands coming from the two edge states are shown in dashed-blue and solid-red colors. In the band diagram shown in section Fig. 3(b), the Zeeman type spin-orbit coupling is set to zero. In this case, two MZM’s appear for $\mu/t \leq 1$ at the end of the chain, thereafter, one of those modes starts to undergo a phase transition.
to an insulating state on increasing the chemical potential. On further increasing of the chemical potential, the system enters the trivial insulating phase (when both the two edge states have been transitioned to their insulating states). In Fig. [3 (c)], we plot the band diagram with the spin-orbit coupling parameters set to \(\alpha_z = 1.5t\), and \(\alpha = 0.5t\). One of the states (indicated by red color) enters a topological phase only in the range \(0.5t \leq \mu \leq 1.5t\) and remains insulating for \(\mu\) not in this range. Whereas there is only one phase transition from the other edge state (shown in dashed blue color) in the range \(0 \leq \mu/t \leq 3\).

In conclusion, we have studied the phase transitions of the edge states in a Rashba spin-orbit coupling dominated 1D topological superconductor (TSC). The 1D TSC we considered is protected by a \(T^2 = -1\) time-reversal symmetry and is constructed by coupling a pair of Kitaev’s Majorana chains with opposite spin configurations. The Rashba spin-orbit coupling is capable of engineering the phase transitions of the edge states, subsequently, the number of MZM’s at the edge of the 1D system. Depending on the strength of the Rashba spin-orbit coupling and the chemical potential, the system identified two topological phases (with topological winding number, \(W = 1\) and \(2\)) and a trivial insulating phase (with a topological winding number \(W = 0\)). The two topological phases are characterized by one (for \(W = 1\)) and two (for \(W = 2\)) MZM’s at the edge of the two coupled Kitaev’s Majorana chains.

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