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Exotic topological types of Majorana zero modes and their universal quantum manipulation

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From our general index theorem, which characterizes faithfully the topological intrinsic boundary-bulk correspondence of topological superconductors and insulators, we reveal rigorously that four topologically distinct types of Majorana zero modes can emerge at the ends of superconducting wires of various symmetry classes. Moreover, we establish three exotic one-dimensional models that have different types of topological charge of Majorana zero modes and disclose exactly the corresponding topological properties, whose distinct topological essences may be tested experimentally. Moreover, we also address their application in universal quantum manipulation, which is promising for realizing universal topological quantum computation.

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I. INTRODUCTION

Recently, the realization of Majorana fermions (MFs) \cite{1,2}, which are their own antiparticles and usually obey non-Abelian statistics, has attracted a lot of attention both theoretically \cite{3–13} and experimentally \cite{14–17}, because of not only the novel physics but also their potential applications for topological quantum computation \cite{18–24}. In particular, topologically protected Majorana zero modes \cite{25} residing at the ends of one-dimensional topological superconductor (TSC) wires are of great interest, since they are point-like particles topologically stable against disorders and perturbations preserving the symmetries of a corresponding class. The relevant essence was elucidated by Kitaev, i.e., how a nontrivial bulk topological configuration can lead to unpaired Majorana zeroin modes at the two ends of the superconducting wire \cite{3,4}, not only through illustrating a toy model of spinless \textit{p}-wave superconductors, but also, more importantly, by establishing the topology-related theoretical formalism. Inspired by Kitaev’s pioneering work, various theoretical proposals and experimental endeavors have been undertaken for realizing and detecting MFs in one-dimensional (1D) materials \cite{5–10,13–17}, making it very promising to find MFs in 1D TSCs first. However, these proposals are almost all focused on concrete 1D systems with an implicit assumption that only one topological type of MF, like that in the Kitaev model, may exist even for 1D models with different symmetry classes. Here we reveal that four topologically distinct types of Majorana zero modes can actually emerge at the ends of 1D TSCs, based on a faithful quantitative correspondence between the topological charge of Fermi surfaces on the boundary and the topological number in the bulk \cite{26–30}. In particular, from a general index theorem established by us \cite{30}, we construct three exotic 1D models that have different types of topological charge of Majorana zero modes and study rigorously the corresponding topological properties.

Let us first review briefly the bulk-boundary correspondence. We recall that a complete classification was obtained for strong topological insulators (TIs) and TSCs in all eight real Altland-Zirnbauer (AZ) symmetry classes, considering

\begin{equation}
\nu_{L/R}(d-1,i) = \pm N(d,i),
\end{equation}

where $\nu_{L/R}$ denotes the total topological charge of FSs (zero modes) on the the left/right boundary of a given bulk TI (or TSC), corresponding to the $+/-$ sign in Eq. (1), and $N$ is the topological number of the bulk, with $d$ and $i$ denoting respectively the bulk dimension and the symmetry class. It is emphasized that the above general index theorem of Eq. (1) also indicates that the type of topological charge of FSs is the same as that of the bulk topological number. Note that for a $Z$-type TI/TSC, the topological charges of FSs at the left and right boundaries have opposite signs, while for $Z_2$ type, the sign of the topological charge plays no role. For $d = 1$, this general index theorem suggests that the models may have Majorana zero modes (FSs) with different topological origins from that of the Kitaev model in class D, making it possible for us to have a deeper insight into all topological types of Majorana zero modes at the ends of TSC wires, with exotic topological properties and phenomena as well as applications being expected. Models in all symmetry classes can be constructed from a generic form in momentum space, $\mathcal{H} = \sum_{ij} f_j(k) \sigma_i \otimes \tau_j$, where the $f(k)$’s are even or odd functions determined by the required symmetries and $\sigma$ and $\tau$ are Pauli matrices. We shall construct nontrivial models in the other three symmetry classes below, exploring their topological origins and their properties with comparisons to the Kitaev model in class D.

II. DIII MODEL

Let us begin by constructing an intriguing model in class DIII, which has a TRS of negative sign and a PHS of positive
while for the Kitaev model this is in principle impossible. In realizing universal quantum computation with additional spin-orbital couplings to realize nontrivial topology [11,12]. The DIII model may be diagonalized in its spin space under the eigenstates of \( \sigma_z \), consisting of two Kitaev chains with the signs of order parameters being opposite. However, after bosonization, one chain interacts with a gauge field given by the particle density in the other chain [37]. Notably, a topology-preserved quantum simulation of the present DIII model has very recently been proposed in Ref. [38] using experimentally feasible superconducting quantum circuits, with a special gauge structure being realized by a dispersive dynamic modulation approach. According to Table I, it may have a \( Z_2\) -type topological number. From the calculation given in Appendix A, the regime of \(|w| > |\mu|/2\) is identified as the topological phase and the corresponding phase diagram is shown in Fig. 2. The nontrivial topological number implies Majorana zero modes of \( Z_2\) -type topological charge at each end from our general index theorem Eq. (1). So we now examine these Majorana zero modes in detail.

As usual, the Majorana operators can be decomposed as

\[
\gamma^j = e^{i\vartheta/2} a_j + e^{-i\vartheta/2} a_j^\dagger, \\
\gamma^j = (e^{i\vartheta/2} a_j - e^{-i\vartheta/2} a_j^\dagger)/i, 
\]

where \( w, \mu, \) and \( \Delta \) are all real, \( \sigma_i \) and \( \tau_i \) are Pauli matrices, \( \Psi^i = [a_j, a_{-k}(-i\sigma_2)_i] \), and the spin index is implicit. From the expression of \( H_{\text{DIII}}(k) \) in the second equality of Eq. (2), it is seen that the model has a PHS with \( C = \sigma_1 \) and a TRS with \( T = \sigma_2 \) [36], which means that it belongs to class DIII.

We now introduce our DIII model, whose Hamiltonian reads

\[
H_{\text{DIII}} = \sum_j \left[-w(a_j a_{j+1} + a_j^\dagger a_{j+1}^\dagger) - \mu(a_j^\dagger a_j - 1) \right] - \Delta \sum_j (a_{j+1}^\dagger \sigma_3 a_j + a_j^\dagger (-i\sigma_1) a_{j+1}^\dagger) \\
= \int dk \Psi^i_k \left[ (-w \cos k - \mu/2) 1 \otimes \tau_3 \right] - \Delta \sin k \sigma_3 \otimes \tau_3 \Psi_k, 
\]

where \( w, \mu, \) and \( \Delta \) are all real, \( \sigma_i \) and \( \tau_i \) are Pauli matrices, \( \Psi^i_k = [a_j, a_{-k}(-i\sigma_2)_i] \), and the spin index is implicit. From the expression of \( H_{\text{DIII}}(k) \) in the second equality of Eq. (2), it is seen that the model has a PHS with \( C = \sigma_1 \) and a TRS with \( T = \sigma_2 \) [36], which means that it belongs to class DIII. The model may be viewed as a spin-triplet Bogoliubov–de Gennes model, which is different from the existing models utilizing spin-orbital couplings to realize nontrivial topology [11,12].

The DIII model may be diagonalized in its spin space under the eigenstates of \( \sigma_z \), consisting of two Kitaev chains with the signs of order parameters being opposite. However, after bosonization, one chain interacts with a gauge field given by the particle density in the other chain [37]. Notably, a topology-preserved quantum simulation of the present DIII model has very recently been proposed in Ref. [38] using experimentally feasible superconducting quantum circuits, with a special gauge structure being realized by a dispersive dynamic modulation approach. According to Table I, it may have a \( Z_2\) -type topological number. From the calculation given in Appendix A, the regime of \(|w| > |\mu|/2\) is identified as the topological phase and the corresponding phase diagram is shown in Fig. 2. The nontrivial topological number implies Majorana zero modes of \( Z_2\) -type topological charge at each end from our general index theorem Eq. (1). So we now examine these Majorana zero modes in detail.

As usual, the Majorana operators can be decomposed as

\[
\gamma^j = e^{i\vartheta/2} a_j + e^{-i\vartheta/2} a_j^\dagger, \\
\gamma^j = (e^{i\vartheta/2} a_j - e^{-i\vartheta/2} a_j^\dagger)/i, 
\]

where \( \vartheta^a \) with \( a = 1, 2 \) satisfy \( \gamma^\dagger = \gamma \), and \( s \) is the spin index. We point out that \( \vartheta \) in the above decomposition can be chosen arbitrarily, and is physically indistinguishable in our DIII model, in contrast to the \( \vartheta \) in the Kitaev model which is related to the phase of the Cooper-pairing order-parameter. Since the existence of unpaired Majorana zero modes and their features are topologically intrinsic according to the general index theorem Eq. (1), to see the structure of these zero modes it is sufficient to solve the model exactly at one specific point in the topological phase [3,4]. For simplicity, adopting the convention that \( \vartheta = \pi/2 \), let us focus on the case \( w = \Delta \) and \( \mu = 0 \) in the topological phase, where our DIII model (2) is reduced to

\[
H_{\text{DIII}} = \sum_j i w \gamma^j_{j+1} \gamma^j_{j+1, +} + \sum_j -i w \gamma^j_{j-1, -} \gamma^j_{j+1, -}, 
\]

where the \( \pm \) are two eigen spin pairings with respect to \( \sigma_z \), i.e.,

\[
a_{j, +} = \frac{1}{\sqrt{2}} (a_{j, +} + a_{j, -}), \quad a_{j, -} = \frac{1}{\sqrt{2}} (a_{j, +} - a_{j, -}).
\]

It is observed that \( \gamma_{j, +} \) and \( \gamma_{j+1, +}^\dagger \) (with \( \alpha = \pm \)) can pair together to form new electronic operators

\[
\tilde{a}_{j, +} = \frac{1}{2} (\gamma_{j, +}^2 + i \gamma_{j+1, +}^\dagger), \quad \tilde{a}_{j, -} = \frac{1}{2} (\gamma_{j, -}^2 + i \gamma_{j+1, -}^\dagger),
\]

to fully diagonalize the Hamiltonian. The pairing pattern of Majorana operators under the open-boundary condition is
The ground-state space spanned by \(|\bullet\rangle = |\psi_1^+\psi_0^-\rangle\) and \(|\times\rangle = |\psi_1^-\psi_0^+\rangle\) with one Majorana fermion at each end has odd parity, distinguishing it from the other ground states. Because of the orthogonal spin pairings for \(|\bullet\rangle\) and \(|\times\rangle\), the degeneracy may be lifted by coupling the spin degree of the DIII model to an external source, and therefore the space can be regarded as a qubit of which any state is achievable. Let us demonstrate this by coupling all electron spins to a very weak external magnetic field compared with the bulk energy gap, i.e., \(H = \sum_j B \cdot \sigma_j/2\) as a perturbation. After detailed calculations in the electronic representation in Appendix C, we have the low-energy effective results \((\bullet\langle S_z\rangle\bullet) = 1/2, \langle\times|\langle\delta|\times\rangle = -1/2, (\bullet|\langle\delta|\times\rangle = 0, and \langle\times|\langle\delta|\times\rangle = 0\) under the thermodynamic limit, with \(\delta = \sum_j 1/2\sigma_j\). An intuitive picture of this feature is obviously that the MF states are wave packets entering at the ends, with the specific spin orientations being the only degrees that are sensitive to the external magnetic field, irrelevant to the homogeneous bulk state. Thus as the symbols suggest, \(\delta\) may be effectively regarded as a single spin operator acting on the two-level space with \(|\bullet\rangle\) and \(|\times\rangle\) being the two eigenstates of \(\delta\). Thus through a suitable control of \(H(t)\) with \(H(t < 0) = H(t \geq 1) = 0\), an arbitrary state can be created, leading to a universal single-qubit operation. Notably, spatial fluctuations of the above weak field would have no impact on the decoherence of the ground state. The magnetic field response of DIII models without retaining the fermionic parity was addressed in Refs. [11,12], where Rashba-type spin-orbital coupling was utilized to realize nontrivial topological phases. In Ref. [12], a highly anisotropic response to the magnetic field was studied for a DIII model, which confirms the conclusion in our DIII model.

III. BDI MODEL

The Hamiltonian of our BDI model reads
\[
\mathcal{H}_{\text{BDI}} = \sum_j \left( -w a_j^\dagger a_{j+1} + i \Delta a_j a_{j+1} \right) + \text{H.c.} - \mu \left( a_j^\dagger a_j - 1/2 \right) \tag{4}
\]
\[
= \int dk \Psi_k \left[ -\Delta \sin k\tau_1 - (w \cos k + \mu/2)\tau_3 \right] \Psi_k^\dagger
\]

where \(\Delta\) is still real, \(a_j\) are spinless, and therefore \(\Psi_k = (a_{j, a_{j, -1}})\). It is noted that \(\mathcal{H}_{\text{BDI}}(k)\) in the second equality has TRS with \(T = \tau_3\) and PHS with \(C = \tau_2\), corresponding to the class BDI. It is observed that the BDI model may be regarded as a reduced Kitaev model with the phase of the order parameter being fixed; therefore it may be realized by hard-core bosons [38,39]. According to Table 1, the formula for the \(Z\)-type topological number is used in Appendix A, and the resulted phase diagram is plotted in Fig. 2. In topological phases, i.e., where \(|w| > |\mu/2|\), there exist Majorana zero modes at the two ends, noting that now \(N = \pm 1\) are distinguishable, corresponding to different topological phases. The Majorana decompositions adopted are
\[
\gamma_j^1 = e^{i\bar{\gamma}} a_j + e^{-i\bar{\gamma}} a_j^\dagger \quad \gamma_j^2 = (e^{i\bar{\gamma}} a_j - e^{-i\bar{\gamma}} a_j^\dagger)/i.
\]
We investigate the Majorana zero modes for $N = +1$, with the representative point in the topological phase being chosen as $w = \Delta > 0$ and $\mu = 0$, which is exactly solvable. Through fixing $\theta = \pi/2$ in the Majorana decompositions, we reduce the Hamiltonian as

$$
H_{\text{BDI}} = \sum_j i w \gamma_j^2 \gamma_{j+1}^1,
$$

which can be fully diagonalized by using the repaired electronic operator $\tilde{a}_j = \frac{1}{2}(\gamma_j^2 + i \gamma_{j+1}^1)$. It is observed that $\gamma_j^1$ and $\gamma_{j+1}^2$ do not enter the Hamiltonian, serving as Majorana zero modes at the two ends. According to the general index theorem (1), the Z-type topological charges $v_{\ell}[\gamma_{\ell}^1] = +1$ and $v_{\ell}[\gamma_{\ell}^2] = -1$ for the two zero modes can respectively be assigned at the two ends, with the prime indicating that $\theta = \pi/2$ in the Majorana decompositions.

The simple case of the topological phase with $N = -1$ is that of $w = -\Delta > 0$ and $\mu = 0$. We can still simplify the Hamiltonian by using the Majorana decompositions, but in this case fixing $\theta = -\pi/2$. In this phase, similarly $\gamma_{\ell}^1$ and $\gamma_{\ell}^2$ are Majorana zero modes at the two ends with the double prime denoting that $\theta = -\pi/2$ is different from that in the phase $N = +1$. The general index theorem (1) implies that $v_{\ell}[\gamma_{\ell}^1] = -1$ and $v_{\ell}[\gamma_{\ell}^2] = 1$. It is simple to check that $\gamma_{\ell}^{\prime\prime} = \gamma_{\ell}^2$ and $\gamma_{\ell}^{\prime\prime\prime} = -\gamma_{\ell}^1$, which conforms to the general index theorem.

There exists a nontrivial way to realize the topological phase transition through breaking the TRS, an antunitary symmetry, without closing the gap in the bulk, which is essentially different from ordinary phase transitions breaking a unitary continuous symmetry in Landau’s paradigm. We can break the TRS with $T = \tau_3$ to make the system in class D through, replacing $i \Delta$ in Eq. (4) by $|\Delta| w^\theta$. Then $\theta = \pm \pi/2$ correspond to the two topological phases of $N = \pm 1$, respectively, and the two phases can be connected by continuously varying $\theta$ from $\pi/2$ to $-\pi/2$ with $|\Delta|$ fixed, which implies intuitively that the two Majorana zero modes residing respectively at the left and right ends are exchanged. The two ways to realize the phase transition are illustrated in Fig. 3. Furthermore, we point out that during the process of varying $\theta$, the system is protected by a nontrivial $\mathbb{Z}_2$-type topology, while only when $\theta = \pm \pi/2$ is the Z-type topological protection recovered, showing that our BDI model is just the Kitaev model whenever $\Delta$ is complex [3]. To see the distinction of the two phases clearly, it is noted that the ground states of the two phases under open-boundary condition are orthogonal to each other in the thermodynamic limit as is derived in Appendix B; this is expressed as $\langle \Psi_\alpha, 1|\Psi_\beta, -1 \rangle = 0$ with $|\Psi_\alpha, \pm 1 \rangle$ being a generic ground state for $N = \pm 1$ [40], which serves as a refinement of the ground-state orthogonality of the Kitaev model.

**IV. CII Model**

We finally briefly describe our exotic model in class CII, with $2\mathbb{Z}$-type topological number $N = \pm 2$ in its topological phases, as is calculated in Appendix A. The Hamiltonian reads

$$
H_{\text{CII}} = \sum_j (-\Delta a_j^{\dagger} i \sigma_2 a_j + wa_{j+1}^{\dagger} i \sigma_2 a_j^{\dagger}) + \text{H.c.},
$$

$$
= \int d\kappa \Psi_k^{\dagger}(-\Delta \sin \kappa \sigma_2 \otimes \tau_3 + (w \cos \kappa - \mu) \mathbf{I} \otimes \tau_1) \Psi_k,
$$

where $\Delta$ and $w$ are still real, and $\Psi_k$ is the same as that of the DIII model (2). $H_{\text{CII}}(k)$ in the second equality has a TRS with $T = \sigma_2 \otimes \mathbf{I}$ and a PHS with $C = \mathbf{I} \otimes \tau_2$. Although the Hamiltonian takes an exotic spin-pairing form, whose phase diagram is also plotted in Fig. 2, it may be simulated using various artificial systems.

Straightforward calculation using the corresponding Z-type formula shows that this model has topological number $N = \pm 2$ when $|w| > |\mu|/2$ as in Fig. 2, consistent with $2\mathbb{Z}$ in Table I of this paper. To see the form of the topologically protected Majorana zero modes at the two ends, when $w = \Delta > 0$ and $\mu = 0$ corresponding to $N = 2$, we adopt the Majorana decompositions of the DIII model with $\theta = 0$, and simplify the CII model (4) as

$$
H_{\text{CII}} = \sum_j i w \gamma_j^{\prime\prime} \gamma_{j+1}^{\prime\prime\prime} - \sum_j i w \gamma_j^{\prime\prime\prime} \gamma_{j+1}^{\prime\prime},
$$

which may be viewed as two copies of the simplified BDI model. The Hamiltonian can be fully diagonalized by introducing

$$
\tilde{a}_j = \frac{1}{2}(\gamma_j^{\prime\prime} + i \gamma_{j+1}^{\prime\prime\prime}) \quad \tilde{b}_j = \frac{1}{2}(\gamma_j^{\prime\prime\prime} + i \gamma_{j+1}^{\prime\prime}),
$$

which is illustrated in Fig. 4. For the left end, $\gamma_1^{\prime\prime}$ and $\gamma_1^{\prime\prime\prime}$ serve as Majorana zero modes, each having $2\mathbb{Z}$-type topological charge $v_{\ell}[\gamma_{\ell}^{\prime\prime\prime}] = 1$, and accordingly for the right end $v_{\ell}[\gamma_{\ell}^{\prime\prime}] = -1$, which follows the general index theorem of Eq. (1) in this paper. The relevant topological charges are

\[ \sum_{j=1}^{\ell} v_{\ell}[\gamma_{\ell}^{\prime\prime\prime}] = \sum_{j=1}^{\ell} v_{\ell}[\gamma_{\ell}^{\prime\prime}] = \mu_{\ell} = 0 \]

\[ v_{\ell}[\gamma_{\ell}^{\prime\prime\prime}] = v_{\ell}[\gamma_{\ell}^{\prime\prime}] = \gamma_{\ell}^{\prime\prime\prime} = \gamma_{\ell}^{\prime\prime} = -1 \]
of Majorana zero modes can also be assigned for the other topological phase \( N = -2 \). Note that the explanation of the CII model in terms of the general index theorem is entirely parallel to that of the BDI model, since they both belong to the Z group. Although similar to two copies of the BDI model, we wish to indicate that there does not exist a way to connect the two topological phases of the CII model, since breaking either the TRS or PHS makes the topology trivial according to Table 1.

V. SUMMARY

In summary, all topological types of Majorana zero modes at the ends of one-dimensional topological superconductors have been investigated systematically and rigorously in the framework of the general index theorem. Specifically, aside from Kitaev’s model in class D, we have constructed models for the other three classes and solved them exactly at exactly solvable points in their topological phases. Moreover, (i) different topological types of Majorana zero modes have been compared; (ii) the unique properties of each model have been addressed; and (iii) the bulk-boundary correspondence in terms of the general index theorem has explicitly been illustrated for each model. It is anticipated that our exotic results may have applications in universal quantum manipulation, which is promising for realizing universal topological quantum computation.

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APPENDIX A: TOPOLOGICAL NUMBERS

The DIII model is of the \( \mathbb{Z}_2^3 \) topological type, and therefore a two-parameter symmetry-preserving extension of \( \mathcal{H}_{\text{DIII}} \) is made below to calculate its topological number \([29,30]\):

\[
\mathcal{H}_{\text{DIII}}(k,\theta,\phi) = [\mathcal{H}(k) \cos \theta + \sin \theta \mathbf{1} \otimes \tau_2] \cos \phi \\
+ \sin \phi \sigma_1 \otimes \tau_1 \\
= (w \cos k + \mu) \cos \theta \cos \phi \mathbf{1} \otimes \tau_3 \\
+ \sin k \cos \theta \cos \phi \sigma_1 \otimes \tau_1 \\
+ \sin \theta \cos \phi \mathbf{1} \otimes \tau_2 + \sin \phi \sigma_1 \otimes \tau_1,
\]

where the extended parameters \( \theta \) and \( \phi \) both range from \(-\pi/2\) to \(\pi/2\). It can be checked that both TRS and PHS are preserved, if we regard \( \theta \) and \( \phi \) as wave vectors. In the calculation, the following formula has been used:

\[
N_{\text{DIII}} = \frac{1}{48\pi^2} \int_{-\pi}^{\pi} dk \int_{-\pi/2}^{\pi/2} d\theta \int_{-\pi/2}^{\pi/2} d\phi \, e^{i\mu k} \\
\times \text{tr}[\sigma_2 \otimes \tau_1 \mathcal{H}^{-1} \sigma_2 H\mathcal{H}^{-1} \sigma_2 H],
\]

The BDI model and the CII model are both of \( \mathbf{Z} \) type, and therefore their corresponding formulas are \([30]\)

\[
N_{\text{BDI}} = \frac{1}{4\pi i} \int_{-\pi}^{\pi} dk \, \text{tr}[\tau_2 \mathcal{H}^{-1}(k)\sigma_2 \mathcal{H}(k)]
\]

and

\[
N_{\text{CII}} = \frac{1}{4\pi i} \int_{-\pi}^{\pi} dk \, \text{tr}[\sigma_2 \otimes \tau_2 \mathcal{H}^{-1}(k)\sigma_2 \mathcal{H}(k)],
\]

with respect to their chiral symmetries. The results obtained from the above three formulas are illustrated in the phase diagram Fig. 2 in the main text.

APPENDIX B: ORTHOGONALITY OF GROUND STATES OF THE BDI MODEL

We first solve the ground states of the BDI model exactly in the electronic representation when \( w = |\Delta| > 0 \) and \( \mu \) for a generic \( \theta \) and then compare the ground states of \( \theta = \pi/2 \) and \( \theta = -\pi/2 \). The explicit expressions for the two degenerate ground states are

\[
|\psi_0\rangle = \sum_{n=0}^{[N/2]} \sum_{\gamma_1 < \cdots < \gamma_2} e^{-i\pi n \gamma_2} a_{\gamma_1}^\dagger a_{\gamma_2}^\dagger \cdots a_{\gamma_{2n}}^\dagger |0\rangle
\]

and

\[
|\psi_1\rangle = \sum_{n=0}^{[(N-1)/2]} \sum_{\gamma_1 < \cdots < \gamma_{2n+1}} e^{-i\pi(n-1) \gamma_2} a_{\gamma_1}^\dagger a_{\gamma_2}^\dagger \cdots a_{\gamma_{2n+1}}^\dagger |0\rangle,
\]

where \( [r] \) is the integer part of the real number \( r \), \( |\psi_0\rangle \) with even parity has a pair of MFs at the two ends, and \( |\psi_1\rangle \) with odd parity has no MFs. The inner products of the ground states for \( N = \pm 1 \) are computed as

\[
\langle \psi_0, 1 \vert \psi_0, 1 \rangle = \frac{C_N^0 - C^2_N + C^4_N - \cdots}{C_N^0 + C_N^2 + C_N^4 + \cdots} \to 0
\]

and

\[
\langle \psi_1, 1 \vert \psi_1, 1 \rangle = \frac{C_N^1 - C_N^3 + C_N^5 - \cdots}{C_N^1 + C_N^3 + C_N^5 + \cdots} \to 0,
\]

where \( \to \) denotes the thermodynamic limit \( N \to \infty \), and \( C_N^n \) denotes the combination number \( N!/(N-n)!n! \). It is obvious that \( \langle \psi_1 \vert \psi_0 \rangle = 0 \).

APPENDIX C: RESPONSE OF THE DIII MODEL TO AN EXTERNAL MAGNETIC FIELD

Referring to the above expressions for \( |\psi_0\rangle \) and \( |\psi_1\rangle \), the explicit expressions of the four degenerate ground states of the DIII model can also be constructed. Thus every element of the perturbation matrix \( \mathbf{S} \) can be computed directly. Here we
present only the leading steps:

\[ \delta E / B = \langle \psi_0^+ \psi_1^+ | \sum_j \sigma_j^+ | \psi_0^+ \psi_1^- \rangle - \langle \psi_0^+ \psi_1^- | \sum_j \sigma_j^+ | \psi_0^- \psi_1^+ \rangle \]

\[ = \frac{1}{C_L^{2n} C_L^{2n+1}} \left[ \sum_{m=0}^{[L/2]} \sum_{n=0}^{[(L-1)/2]} (-2m + 2n + 1) C_L^{2m} C_L^{2n+1} - \sum_{m=0}^{[L/2]} \sum_{n=0}^{[(L-1)/2]} (-2m + 1 + 2n) C_L^{2m+1} C_L^{2n} \right] \]

\[ = 2 + \frac{4}{C_L^{2m+2n+1}} \sum_{m=0}^{[L/2]} \sum_{n=0}^{[(L-1)/2]} (m - n) C_L^{2m} C_L^{2n+1} \]

In the thermodynamic limit, the second term in the last equality vanishes, and thus we have \( \delta E / B = 2 \). This justifies \( \langle \bullet | \hat{S}_z | \bullet \rangle = 1/2 \) and \( \langle x | \hat{S}_z | x \rangle = -1/2 \), and the other matrix elements can be computed similarly.

[25] Majorana zero modes refer to real operators carrying no energy and Majorana fermions refer to eigenstates of these operators in this paper.
[35] Strictly speaking, the index theorem for 1D Ts/TSCs is not explicitly characterized in Ref. [30], since topological charges for pointlike gapless modes are not formulated in Ref. [29], although it seems to be indicated by the eightfold periodicity addressed there. Thus the present work actually completes the index theorem by explicitly revealing its meaning in 1D Ts/TSCs.
[36] In our convention, the antiunitary operators of TRS and THS are respectively represented as \( \bar{T} = \bar{\kappa} \hat{C} \), where \( \bar{T} \) and \( \bar{\kappa} \) are linear unitary operators, and \( \hat{C} \) denotes the basic antiunitary operator of complex conjugation.
[37] The DIII model may be decomposed as \( H_{DIII} = H_+ + H_- \), with \( H_+ = \sum_{j} (w a_{j+1}^+ a_{j+1} + \Delta a_{j+1} a_{j+1} + H.c.) + \mu (a_{j+1}^+ a_{j+1} - 1) \) and \( H_- = \sum_{j} (w a_{j}^+ a_{j} + \Delta a_{j} a_{j} + H.c.) + \mu (a_{j}^+ a_{j} - 1) \), which may be bosonized as \( H_+ = \sum_{j} (\epsilon_j a_{j+1}^+ b_{j+1} + \Delta \epsilon_j b_{j+1}^+ a_{j+1} + H.c.) + \mu (b_{j+1}^+ b_{j+1} - 1) \) and \( H_- = \sum_{j} (\epsilon_j a_{j}^+ b_{j} + \Delta \epsilon_j b_{j}^+ a_{j} + H.c.) + \mu (b_{j}^+ b_{j} - 1) \).
[40] In principle, we can construct a BDI model with a large topological number \( N \), and because it is of \( Z \) type, there are \( N \) unpaired Majorana operators at each end without entering the Hamiltonian, corresponding to \( 2^N \)-fold ground-state degeneracy. These exotic features provide more possibilities to store and process quantum information, and might be utilized to realize topological quantum computing.