Correspondence of topological classification between quantum graph extra dimension and topological matter

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In this paper, we study five-dimensional Dirac fermions of which the extra-dimension is compactified on quantum graphs. We find that there is a nontrivial correspondence between matrices specifying boundary conditions at the vertex of the quantum graphs and zero-dimensional Hamiltonians in gapped free-fermion systems. Based on the correspondence, we provide a complete topological classification of the boundary conditions in terms of noninteracting fermionic topological phases. The ten symmetry classes of topological phases are fully identified in the language of five-dimensional Dirac fermions, and topological numbers of the boundary conditions are given. In analogy with the bulk-boundary correspondence in noninteracting fermionic topological phases, the boundary condition topological numbers predict four-dimensional massless fermions localized at the vertex of the quantum graphs and thus govern the low energy physics in four dimensions.

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I. INTRODUCTION

A quantum graph is a one-dimensional (1D) graph that consists of edges and vertices connected to each other with differential operators defined on each edge like Fig. 1 (see [1,2] for a review of the quantum graph). The quantum graph describes quantum mechanics on a 1D graph and has been paid attention to since we can obtain attractive physics caused by the degrees of freedom in boundary conditions for wave functions imposed at vertices from the requirement of current conservation. The graph has been applied to the wide range of research areas, e.g. scattering theory on 1D graphs [3–6], quantum chaos [7–9], anyons [10–12], supersymmetric quantum mechanics [13–15], Berry's phases [16–19], extra-dimensional models [20–30] and so on.

Here we focus on applying quantum graphs to the extra space of 5D fermions, that is, 5D fermions with the extra space given by the quantum graph. In the previous paper [31], three of the present authors and collaborators revealed that 5D fermions on quantum graphs could naturally solve the problems of the fermion generation, namely the fermion mass hierarchy and the origin of the CP-violating phase in the standard model. However, the possible 4D effective theories remained unclear because the parameter space of the boundary conditions was huge. Thus, the next step is a systematic investigation of the boundary conditions. A hint to this step is that we obtained 4D chiral zero modes localized at the vertex depending on the topological structure of the parameter space of the boundary conditions. This reminds us of topological insulators and superconductors, where gapless states appear on the boundaries by the topology in bulk from the bulk-boundary correspondence. These topological matters are classified into ten symmetry classes by the presence or absence of time-reversal, particle-hole, and chiral symmetries [32–34].

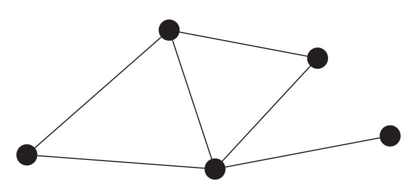

FIG. 1. Quantum graph consisting of five vertices and six edges.

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In this paper, we perform a topological classification of the boundary conditions for 5D Dirac fermions on quantum graphs. The boundary conditions are classified into ten symmetry classes by considering time reversal, charge conjugation, and extra spatial symmetries in 5D Dirac fermions. Surprisingly, the classification of the boundary conditions has a complete correspondence to the topological classification of $0 + 1$D gapped free-fermion systems: A Hermitian matrix that specifies the boundary conditions of quantum graphs corresponds to a zero-dimensional Hamiltonian for topological insulators and superconductors. In addition, symmetry classes of the boundary conditions coincide with those in the topological matter side. This means that the restrictions for the boundary conditions by the symmetries of 5D fermions are the same as those for zero-dimensional Hamiltonians with the Altland-Zirnbauder symmetries. Furthermore, we obtain the topological numbers $\mathbb{Z}, \mathbb{Z}_2, 2\mathbb{Z}$ for each symmetry class of the boundary conditions in the same manner as those of topological insulators and superconductors. Importantly, these numbers predict the number of 4D massless fields localized at the vertex of quantum graphs, i.e. the $\mathbb{Z}$ and $2\mathbb{Z}$ indices are equal to the number of Kaluza-Klein (KK) chiral zero modes, and the $\mathbb{Z}_2$ index coincides with the parity of the number of Dirac zero modes. These zero modes would be regarded as gapless boundary states of topological phases. A similar relation between boundary conditions and $1 + 1$D symmetry-protected topological (SPT) phases [35] or $1 + 2$D SPT phases [36] has been known in the boundary conformal field theories. In this paper, we reveal for the first time the relation between the boundary conditions on quantum graphs and $1 + 0$d SPT phases.

This paper is organized as follows: In the next section, we briefly review 5D Dirac fermions on quantum graphs. Quantum graphs provide the most general 1D extra compactified spaces. In particular, we consider the so-called rose graph where any edge of the graph forms a loop that begins and ends at a common vertex, as shown in Fig. 2. This choice does not lose the generality because the rose graph can generate an arbitrary graph with the same number of edges by imposing suitable boundary conditions for wave functions at the vertex. See Fig. 3.[1] In Sec. III, we classify allowed boundary conditions in the rose graph subject to symmetries of 5D fermions and obtain ten symmetry classes. Then we relate them to Hamiltonians and symmetries in the gapped free-fermion systems. In Sec. IV, we investigate the topological number of the boundary conditions in each symmetry class and the number of KK zero modes. Section V is devoted to summary and discussion.

[1] For example, if we impose the Dirichlet boundary condition on all edges of a rose graph, wave functions on different edges are independent of each other. Thus, this boundary condition decomposes the rose graph into isolated edges with the Dirichlet boundary conditions at both ends. The other graphs can also be obtained by suitable boundary conditions. Thus, we can collectively investigate any 1D extra space with N edges by using a single rose graph with N edges.

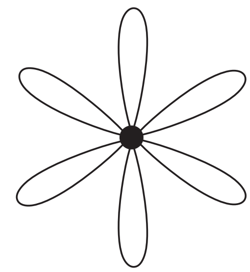

FIG. 2. Rose graph consisting of one vertex and six loops.

II. 5D DIRAC FERMION ON QUANTUM GRAPH

In this section, we briefly review the properties of a 5D Dirac fermion on a quantum graph given in the previous paper [31]. As discussed in Sec. I, we take the extra space as the rose graph which consists of one vertex and N loops with the length $L_a (a = 1, \ldots, N)$ shown in Fig. 4. We consider a KK decomposition of the 5D field and derive boundary conditions that the field should satisfy at the vertex in the graph. We also discuss how the degeneracy of 4D chiral zero-modes depend on the boundary conditions and show that it corresponds to the topological invariant so-called Witten index.

A. Setup

Let us consider the 5D Dirac action

$$S = \int d^4x \sum_{a=1}^{N} \int_{L_{a-1}}^{L_a} dy \bar{\Psi}(x,y)[i\gamma^\mu \partial_\mu + i\gamma^y \partial_y + M]\Psi(x,y), \tag{2.1}$$

where x^μs' $(\mu = 0,1,2,3)$ are the coordinates of the 4D Minkowski space-time and y is the coordinate on the rose graph. $\Psi(x,y)$ is a four-component 5D Dirac spinor and the Dirac conjugate $\bar{\Psi}$ is defined by $\bar{\Psi} = \Psi^\dagger \gamma^0$. γ^μs' $(\mu = 0,1,2,3)$ are 4×4 gamma matrices that satisfy the Clifford algebra

$$\{\gamma^\mu, \gamma^\nu\} = -2\eta^{\mu\nu}, \qquad \eta^{\mu\nu} = \mathrm{diag}(-,+,+,+), \tag{2.2}$$

and γ^y is taken to be $\gamma^y = -i\gamma^5 (\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3)$ with 4D chiral matrix γ^5. The hermiticity of the gamma matrices is given by

$$(\gamma^0)^\dagger = \gamma^0, \quad (\gamma^i)^\dagger = -\gamma^i (i = 1,2,3), \quad (\gamma^y)^\dagger = -\gamma^y. \tag{2.3}$$

The parameter M in the action (2.1) is the bulk mass of the 5D Dirac fermion.

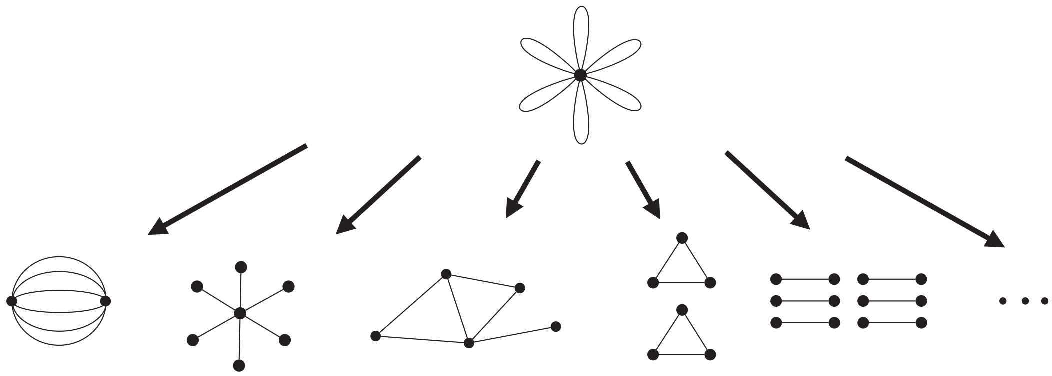

FIG. 3. Decompositions of the rose graph with six edges.

It should be noted that the model in Eq. (2.1) can realize the domain wall fermion used in the lattice gauge theory [37] as a special case. The domain wall configuration is obtained by a circular rose graph consisting of two edges and two vertices, where the bulk mass has an opposite sign on the two edges. Each vertex of this graph supports a 4D chiral fermion, of which chirality is opposite to each other on the two vertices. In the long length limit of the edges, the two 4D chiral fermions are decoupled to each other, so a chiral theory is realized effectively. Because rose graphs allow configurations other than the domain wall, our quantum graph approach is more general than that of the domain wall fermions.

The action principle $\delta S = 0$ gives the 5D Dirac equation

$$[i\gamma^{\mu}\partial_{\mu} + i\gamma^{y}\partial_{y} + M]\Psi(x, y) = 0, \tag{2.4}$$

and also the condition for the surface term

$$\sum_{a=1}^{N} [\bar{\Psi}(x, y)\gamma^{y}\delta\Psi(x, y)]_{y=L_{a-1}+\varepsilon}^{y=L_{a}-\varepsilon} = 0, \tag{2.5}$$

where ε is an infinitesimal positive constant. This condition can be regarded as the conservation of the current for y-direction. As we will see in the next section, Eq. (2.5) leads to boundary conditions that the field $\Psi(x, y)$ should obey at the boundaries $y = L_0 + \varepsilon, L_1 \pm \varepsilon, \ldots, L_{N-1} \pm \varepsilon, L_N - \varepsilon$.[2]

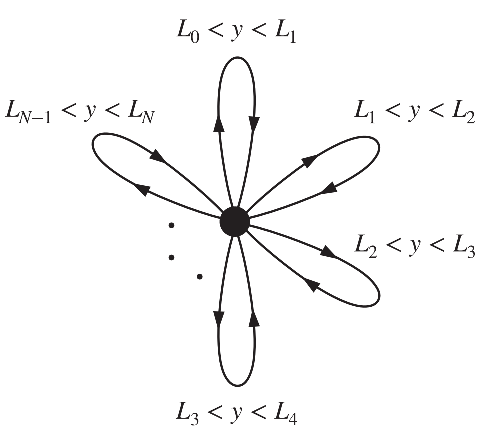

FIG. 4. Rose graph consisting of one vertex and N loops.

If the extra dimension is compact, a higher dimensional field can be decomposed into 4D fields with x-dependence and Kaluza–Klein (KK) mode functions with discrete eigenvalues on an extra space. Here, we decompose $\Psi(x, y)$ into 4D chiral fields $\psi^{(i)}_{\mathrm{R/L},n}(x)$ and KK mode functions $f^{(i)}_{n}(y)$, $g^{(i)}_{n}(y)$ as follows:

$$\Psi(x, y) = \sum_{i}\sum_{n} [\psi^{(i)}_{\mathrm{R},n}(x) f^{(i)}_{n}(y) + \psi^{(i)}_{\mathrm{L},n}(x) g^{(i)}_{n}(y)], \tag{2.6}$$

where the index n indicates the nth level of the KK modes and i denotes the index that distinguishes the degeneracy of the nth KK modes (if it exists). The mode functions $f^{(i)}_{n}(y)$ and $g^{(i)}_{n}(y)$ are assumed to form a complete set, respectively, and satisfy the orthonormality relations

$$\sum_{a=1}^{N} \int_{L_{a-1}}^{L_a} dy f^{(i)*}_{n}(y) f^{(j)}_{m}(y) = \delta_{nm}\delta^{ij}, \tag{2.7}$$

$$\sum_{a=1}^{N} \int_{L_{a-1}}^{L_a} dy g^{(i)*}_{n}(y) g^{(j)}_{m}(y) = \delta_{nm}\delta^{ij}. \tag{2.8}$$

We also require that the 4D fields $\psi^{(i)}_{\mathrm{R/L},n}$ are mass eigenstates with masses m_n and the following 4D action can be obtained by substituting the decomposition (2.6) into the 5D action Eq. (2.1):

[2]If we impose boundary conditions such that partial summations of the terms in the left hand side of Eq. (2.5) vanish independently, the rose graph is decomposed into graphs correspond to the partial summations, as discussed in Sec. I.

$$S = \int d^4x \Big\{ \sum_i \bar{\psi}^{(i)}_{\mathrm{R},0}(x) i\gamma^\mu \partial_\mu \psi^{(i)}_{\mathrm{R},0}(x) + \sum_j \bar{\psi}^{(j)}_{\mathrm{L},0}(x) i\gamma^\mu \partial_\mu \psi^{(j)}_{\mathrm{L},0}(x) + \sum_i \sum_{n\neq 0} \bar{\psi}^{(i)}_n(x)(i\gamma^\mu\partial_\mu + m_n)\psi^{(i)}_n(x) \Big\}, \tag{2.9}$$

where $\psi^{(i)}_n(x) \equiv \psi^{(i)}_{\mathrm{R},n}(x) + \psi^{(i)}_{\mathrm{L},n}(x)$ for $n \neq 0$, and $\psi^{(i)}_{\mathrm{R/L},0}(x)$ denote the 4D chiral massless spinors with $m_0 = 0$. Then the mode functions $f^{(i)}_n(y)$ and $g^{(i)}_n(y)$ should satisfy the relation

$$(\partial_y + M) f^{(i)}_n(y) = m_n g^{(i)}_n(y), \tag{2.10}$$

$$(-\partial_y + M) g^{(i)}_n(y) = m_n f^{(i)}_n(y). \tag{2.11}$$

It follows that $f^{(i)}_n$ and $g^{(i)}_n$ are given by the eigenfunctions of the equations

$$(-\partial_y^2 + M^2) f^{(i)}_n(y) = m_n^2 f^{(i)}_n(y), \tag{2.12}$$

$$(-\partial_y^2 + M^2) g^{(i)}_n(y) = m_n^2 g^{(i)}_n(y), \tag{2.13}$$

and the 4D masses m_n are determined by solving these equations with allowed boundary conditions.

B. Boundary conditions

Then, let us derive the allowed boundary conditions. From the decomposition (2.6) of $\Psi(x,y)$ [and also $\delta\Psi(x,y)$] and the independence of the fields $\psi^{(i)}_{\mathrm{R/L},n}(x)$ and $\delta\psi^{(i)}_{\mathrm{R/L},n}(x)$, Eq. (2.5) can be written as

$$\vec{F}^{(i)\dagger}_n \vec{G}^{(j)}_m = \vec{G}^{(j)\dagger}_m \vec{F}^{(i)}_n = 0 \quad \text{for} \quad \forall\ n, m, i, j, \tag{2.14}$$

where $\vec{F}^{(i)}_n$ and $\vec{G}^{(j)}_m$ are $2N$-dimensional complex vectors defined by

$$\vec{F}^{(i)}_n \equiv \begin{pmatrix} f^{(i)}_n(L_0+\varepsilon) \\ f^{(i)}_n(L_1-\varepsilon) \\ f^{(i)}_n(L_1+\varepsilon) \\ f^{(i)}_n(L_2-\varepsilon) \\ \vdots \\ f^{(i)}_n(L_{a-1}+\varepsilon) \\ f^{(i)}_n(L_a-\varepsilon) \\ \vdots \\ f^{(i)}_n(L_{N-1}+\varepsilon) \\ f^{(i)}_n(L_N-\varepsilon) \end{pmatrix}, \qquad \vec{G}^{(j)}_m \equiv \begin{pmatrix} g^{(j)}_m(L_0+\varepsilon) \\ -g^{(j)}_m(L_1-\varepsilon) \\ g^{(j)}_m(L_1+\varepsilon) \\ -g^{(j)}_m(L_2-\varepsilon) \\ \vdots \\ g^{(j)}_m(L_{a-1}+\varepsilon) \\ -g^{(j)}_m(L_a-\varepsilon) \\ \vdots \\ g^{(j)}_m(L_{N-1}+\varepsilon) \\ -g^{(j)}_m(L_N-\varepsilon) \end{pmatrix}. \tag{2.15}$$

These vectors consist of values of the mode function at the boundaries $y = L_0+\varepsilon, L_1\pm\varepsilon, \ldots, L_{N-1}\pm\varepsilon, L_N-\varepsilon$. Here, we call $\vec{F}^{(i)}_n$ and $\vec{G}^{(j)}_m$ boundary vectors. The condition (2.14) means that the vector space spanned by $\{\vec{F}^{(i)}_n\}$ is orthogonal to the one by $\{\vec{G}^{(j)}_m\}$.

Now, to solve the Eqs. (2.12) and (2.13) and determine the mass eigenvalues m_n, we want to obtain $4N$ constraints in total, since the graph has $2N$ boundaries $y = L_0 + \varepsilon, L_1\pm\varepsilon, \ldots, L_{N-1}\pm\varepsilon, L_N-\varepsilon$ for $f^{(i)}_n$ and $g^{(j)}_m$. However, the relations (2.10) and (2.11) imply that the massive mode functions $f^{(i)}_n$ and $g^{(j)}_m$ are related with each other (except for the zero mode functions which obey the first differential equations). Thus, we should require that the condition (2.14) provides $2N$ constraints in total, otherwise the system is undetermined or overdetermined.[3] It follows from this observation that Eq. (2.14) is replaced by the boundary conditions

$$(1_{2N} - U_{\mathrm{B}})\vec{F}^{(i)}_n = 0, \tag{2.16}$$

$$(1_{2N} + U_{\mathrm{B}})\vec{G}^{(j)}_m = 0, \tag{2.17}$$

where U_{B} is a $2N\times 2N$ Hermitian unitary matrix

$$U_{\mathrm{B}}^2 = 1_{2N}, \qquad U_{\mathrm{B}}^\dagger = U_{\mathrm{B}}. \tag{2.18}$$

We can find that $(1_{2N} \mp U_{\mathrm{B}})/2$ in Eqs. (2.16) and (2.17) correspond to the projection matrices which map the $2N$-dimensional complex vector space into the ones spanned by $\{\vec{F}^{(i)}_n\}$ and $\{\vec{G}^{(j)}_m\}$, respectively. Thus, we conclude that a

[3]For example, if we impose $4N$ constraints with the condition that $f^{(i)}_n$ and $g^{(j)}_m$ equal to 0 at each boundary, there are no solutions for (2.12) and (2.13) since the mode functions should satisfy both the Dirichlet and Neumann boundary conditions from the relations (2.10) and (2.11).

Hermitian unitary matrix $U_{\rm B}$ specifies a 5D Dirac theory on a rose graph depicted in Fig. 4.

We can classify the matrix $U_{\rm B}$ into $2N+1$ types by the number of the eigenvalues $+1$ (or -1). We call the case with k negative eigenvalues the type $(2N-k, k)$ boundary condition (BC) ($k = 0, 1, \ldots, 2N$). The matrix $U_{\rm B}$ in this type can be represented as

$$\mathrm{Type}(2N-k,k): \quad U_{\rm B} = V \left(\begin{array}{ccc|ccc} +1 & & 0 & & & \\ & \ddots & & & 0 & \\ 0 & & +1 & & & \\ \hline & & & -1 & & 0 \\ & 0 & & & \ddots & \\ & & & 0 & & -1 \end{array}\right) V^\dagger \quad (0 \le k \le 2N) \tag{2.19}$$
$$\underbrace{\qquad\qquad}_{2N-k}\underbrace{\qquad\qquad}_{k}$$

with a $2N \times 2N$ unitary matrix V. Therefore the parameter space of the type $(2N-k, k)$ BC is given by the complex Grassmaniann

$$\frac{U(2N)}{U(2N-k) \times U(k)}. \tag{2.20}$$

Since continuous deformations of V do not change the numbers of positive and negative eigenvalues in $U_{\rm B}$, the different types of boundary conditions cannot be connected continuously.

For later convenience, we write the $2N \times 2N$ unitary matrix V as

$$V = (\vec{u}_1, \vec{u}_2, \cdots, \vec{u}_{2N}), \tag{2.21}$$

where $\vec{u}_r (r = 1, 2, \ldots, 2N)$ are $2N$-dimensional orthonormal complex vectors which satisfy $\vec{u}_r^\dagger \vec{u}_s = \delta_{rs} (r, s = 1, 2, \ldots, 2N)$. Then, the matrix $U_{\rm B}$ for the type $(2N-k, k)$ BC can be expressed by

$$U_{\rm B} = \sum_{r=1}^{2N-k} \vec{u}_r \vec{u}_r^\dagger - \sum_{r=2N-k+1}^{2N} \vec{u}_r \vec{u}_r^\dagger \tag{2.22}$$

and the boundary conditions (2.16) and (2.17) are of the form

$$\vec{u}_r^\dagger \vec{F}_n^{(i)} = 0 \quad \text{for } r = 2N-k+1, \ldots, 2N, \tag{2.23}$$

$$\vec{u}_r^\dagger \vec{G}_m^{(j)} = 0 \quad \text{for } r = 1, \ldots, 2N-k. \tag{2.24}$$

C. Zero-mode degeneracy

One of the features of the quantum graph is that the mode functions can be degenerate due to the boundary conditions. In our model, this degeneracy can be regarded as the number of four dimensional fields with degenerate masses. In particular, the degeneracy of zero mode solutions plays important roles to classify the boundary conditions. Then, we focus on the zero mode solutions $f_0^{(i)}(y)$ and $g_0^{(j)}(y)$, which obey the equations [see Eqs. (2.10) and (2.11)]

$$(\partial_y + M) f_0^{(i)}(y) = 0, \tag{2.25}$$

$$(-\partial_y + M) g_0^{(j)}(y) = 0. \tag{2.26}$$

The mode functions $f_0^{(i)}(y)$ and $g_0^{(j)}(y)$ on the rose graph can be discontinuous at the vertex and written into the form of exponentially localized functions:

$$f_0^{(i)}(y) = \sum_{a=1}^{N} \theta(y - L_{a-1}) \theta(L_a - y) F_a^{(i)} C_a e^{-My}, \tag{2.27}$$

$$g_0^{(j)}(y) = \sum_{a=1}^{N} \theta(y - L_{a-1}) \theta(L_a - y) G_a^{(i)} C'_a e^{+My}, \tag{2.28}$$

where $\theta(y)$ denotes the Heaviside step function and the complex constants $F_a^{(i)}, G_a^{(j)} \in \mathbb{C} (a = 1, \ldots, N)$ are determined by the boundary conditions. Here we also introduced the constants

$$C_a = \sqrt{\frac{1}{e^{-2M(L_{a-1}-\varepsilon)} + e^{-2M(L_a+\varepsilon)}}},$$
$$C'_a = \sqrt{\frac{1}{e^{2M(L_{a-1}-\varepsilon)} + e^{2M(L_a+\varepsilon)}}}, \tag{2.29}$$

for later convenience.

We can see that the number of linearly independent solutions $f_0^{(i)}(y)(g_0^{(j)}(y))$ corresponds to the number of linearly independent N-dimensional complex vectors $\boldsymbol{F}^{(i)} \equiv (F_1^{(i)}, F_2^{(i)}, \ldots, F_N^{(i)})^\top$ $(\boldsymbol{G}^{(j)} \equiv (G_1^{(j)}, G_2^{(j)}, \ldots, G_N^{(j)})^\top)$. Then, let us discuss the vectors $\boldsymbol{F}^{(i)}$ and $\boldsymbol{G}^{(j)}$ under the type $(2N-k, k)$ BC. For this purpose, we introduce orthonormal $2N$-dimensional vectors $\vec{\mathcal{F}}_a$ and $\vec{\mathcal{G}}_a (a = 1, \ldots, N)$

$$\vec{\mathcal{F}}_a \equiv C_a(\underbrace{0,\ldots,0}_{2(a-1)}, e^{-M(L_{a-1}+\varepsilon)}, e^{-M(L_a-\varepsilon)}, 0, \ldots, 0)^\top, \quad (2.30)$$

$$\vec{\mathcal{G}}_a \equiv C'_a(\underbrace{0,\ldots,0}_{2(a-1)}, e^{M(L_{a-1}+\varepsilon)}, -e^{M(L_a-\varepsilon)}, 0, \ldots, 0)^\top, \quad (2.31)$$

which form a complete set in the $2N$-dimensional complex vector space. Here the constants C_a and C'_a are the same as Eq. (2.29).

Then the boundary vectors $\vec{F}_0^{(i)}$, $\vec{G}_0^{(j)}$ in Eq. (2.15) for $n = 0$ and the $2N$-dimensional complex vectors $u_p (p = 1, \ldots, 2N)$ in Eq. (2.21) can be decomposed by $\vec{\mathcal{F}}_a$ and $\vec{\mathcal{G}}_a (a = 1, \ldots, N)$ as follows:

$$\vec{F}_0^{(i)} = \sum_{a=1}^{N} F_a^{(i)} \vec{\mathcal{F}}_a, \qquad \vec{G}_0^{(j)} = \sum_{a=1}^{N} G_a^{(j)} \vec{\mathcal{G}}_a, \quad (2.32)$$

$$\vec{u}_r = \sum_{a=1}^{N} \alpha_{r,a} \vec{\mathcal{F}}_a + \sum_{a=1}^{N} \beta_{r,a} \vec{\mathcal{G}}_a \qquad (r = 1, 2, \ldots, 2N), \quad (2.33)$$

where $\alpha_{r,a}$ and $\beta_{r,a}$ are complex constants and satisfy

$$\sum_{a=1}^{N} (\alpha_{r,a}^* \alpha_{s,a} + \beta_{r,a}^* \beta_{s,a}) = \delta_{rs} \qquad (r, s = 1, 2, \ldots, 2N) \quad (2.34)$$

from the orthonormal relations for $\vec{u}_r$. From the boundary conditions (2.23) and (2.24) for $n = 0$, we obtain the conditions that $\boldsymbol{F}^{(i)}$ and $\boldsymbol{G}^{(j)}$ are orthogonal to the vector $\boldsymbol{\alpha}_q \equiv (\alpha_{q,1}, \alpha_{q,2}, \ldots, \alpha_{q,N})^\top$ $(q = 2N-k+1, \ldots, 2N)$ and $\boldsymbol{\beta}_p \equiv (\beta_{p,1}, \beta_{p,2}, \ldots, \beta_{p,N})^\top (p = 1, \ldots, 2N-k)$, respectively:

$$\boldsymbol{\alpha}_q^\dagger \boldsymbol{F}^{(i)} = 0 \qquad (q = 2N-k+1, \ldots, 2N), \quad (2.35)$$

$$\boldsymbol{\beta}_p^\dagger \boldsymbol{G}^{(j)} = 0 \qquad (p = 1, 2, \ldots, 2N-k). \quad (2.36)$$

Let us suppose that the number of the linearly independent vectors for $\boldsymbol{\alpha}_q (q = 2N-k+1, \ldots, 2N)$ is ℓ. Then the number of the linearly independent vectors for $\boldsymbol{\beta}_q (q = 2N-k+1, \ldots, 2N)$, $\boldsymbol{\alpha}_p$ and $\boldsymbol{\beta}_p (p = 1, \ldots, 2N-k)$ are $k-\ell, N-\ell$ and $N-k+\ell$, respectively, because of the independence of $\vec{u}_p (p = 1, \ldots, 2N-k)$ and $\vec{u}_q (q = 2N-k+1, \ldots, 2N)$. Therefore the range of ℓ is restricted to $0 \le \ell \le k$ for the case of $k = 0, \ldots, N$ and $k-N \le \ell \le N$ for the case of $k = N, \ldots, 2N$. If the number of the linearly independent vectors for $\boldsymbol{\alpha}_q (q = 2N-k+1, \ldots, 2N)$ and $\boldsymbol{\beta}_p (p = 1, \ldots, 2N-k)$ are ℓ and $N-k+\ell$, respectively, we can find that there exist $N-\ell$ linearly independent solutions for $\boldsymbol{F}^{(i)} (i = 1, \ldots, N-\ell)$ and $k-\ell$ linearly independent solutions for $\boldsymbol{G}^{(j)} (j = 1, \ldots, k-\ell)$ from Eqs. (2.35) and (2.36). Therefore, for the type $(2N-k, k)$ BC, we can conclude that the degeneracy of zero mode $f_0^{(i)}(y)$ is given by $N_{f_0} = N-\ell$, and that of zero mode $g_0^{(i)}(y)$ is given by $N_{g_0} = k-\ell$. The degeneracies N_{f_0} and N_{g_0} for each boundary condition are described in Table I.

TABLE I. The number of the zero mode solutions of $f_0^{(i)}(y)$ and $g_0^{(j)}(y)$ for the type $(2N-k, k)$ BC. ℓ denotes the maximal number of the linearly independent vectors $\boldsymbol{\alpha}_q (q = 2N-k+1, \ldots, 2N)$ in Eq. (2.33). N_{f_0} (N_{g_0}) is the number of the zero mode solutions of $f_0^{(i)}(y)$ ($g_0^{(j)}(y)$). We can find that $N_{f_0} - N_{g_0}$ is independent of ℓ, though both of N_{f_0} and N_{g_0} depend of ℓ.

k	ℓ	N_{f_0}	N_{g_0}	$\Delta_{\mathrm{W}} = N_{f_0} - N_{g_0}$
$0 \le k \le N$	0	N	k	$N-k$
	1	$N-1$	$k-1$	$N-k$
	$\vdots$	$\vdots$	$\vdots$	$\vdots$
	k	$N-k$	0	$N-k$
$N \le k \le 2N$	$k-N$	$2N-k$	N	$N-k$
	$k-N+1$	$2N-k-1$	$N-1$	$N-k$
	$\vdots$	$\vdots$	$\vdots$	$\vdots$
	N	0	$k-N$	$N-k$

We also comment about phenomenological aspects of this model. In the case of the type $(2N-k, k)$ BC, there are $|N-k|$ massless chiral fields in the 4D effective theory since pairs of left and right-handed chiral zero modes can form massless Dirac spinors (and these may become massive through quantum corrections if we introduce interactions). Therefore, we can obtain three generations of chiral fermions for the type $(N-3, N+3)$ and $(N+3, N-3)$ BCs. Since the zero mode functions are exponentially localized at some boundaries, overlap integrals of the mode functions can easily produce hierarchical masses and also the flavor mixing if we introduce the 5D Yukawa interactions. Moreover, complex parameters in the matrix U_{B} generally give the genuine complex zero mode functions and this would result in the *CP* violating phase in the CKM (Cabibbo-Kobayashi-Maskawa) matrix. Therefore, we can find that this model has the desired properties to explain the fermion flavor structure in the standard model from the viewpoint of higher dimensional theories.

D. Witten index

We can notice that the difference $N_{f_0} - N_{g_0} (= N - k)$ is independent of ℓ. This implies that the number of chiral zero modes is invariant under continuous deformations of the boundary conditions, since the type $(2N - k,\, k)$ BC is not continuously connected to the type $(2N - k', k')$ one with $k \neq k'$ (although ℓ can be changed by those deformations). This topological property is related to a hidden structure of the supersymmetric quantum mechanics in this model.

If we introduce the two-component functions constructed from the mode functions

$$\Phi^{(i)}_{n,+}(y) = \begin{pmatrix} f^{(i)}_n(y) \\ 0 \end{pmatrix}, \quad \Phi^{(i)}_{n,-}(y) = \begin{pmatrix} 0 \\ g^{(i)}_n(y) \end{pmatrix} \tag{2.37}$$

and also the Hermitian operators H, Q and $(-1)^F$ defined by

$$H = \begin{pmatrix} -\partial_y^2 + M & 0 \\ 0 & -\partial_y^2 + M \end{pmatrix}, \qquad Q = \begin{pmatrix} 0 & -\partial_y + M \\ \partial_y + M & 0 \end{pmatrix}, \qquad (-1)^F = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2.38}$$

we can find that these satisfy the supersymmetric relations

$$H = Q^2, \qquad \{Q, (-1)^F\} = 0, \qquad [H, (-1)^F] = 0, \tag{2.39}$$

$$H\Phi^{(i)}_{n,\pm}(y) = m_n^2 \Phi^{(i)}_{n,\pm}(y), \qquad Q\Phi^{(i)}_{n,\pm}(y) = m_n \Phi^{(i)}_{n,\mp}(y), \qquad (-1)^F \Phi^{(i)}_{n,\pm}(y) = \pm\Phi^{(i)}_{n,\pm}(y). \tag{2.40}$$

Then we can regard the operators H, Q, $(-1)^F$ and the functions $\Phi^{(i)}_{n,\pm}(y)$ as the Hamiltonian, supercharge, fermion number operator, and bosonic and fermionic states in the supersymmetric quantum mechanics, respectively. In the supersymmetric quantum mechanics, it is known that there is a topological invariant which is called the Witten index $\Delta_{\rm W}$. This index is defined by the difference of the number of the zero energy states with the eigenvalue $(-1)^F = +1$ and with $(-1)^F = -1$. The topological property of this index is due to the fact that nonzero energy states with $(-1)^F = +1$ and $(-1)^F = -1$ should be paired with each other by the supercharge Q, and can move to or from zero energy states together. In our model, this index corresponds to

$$\Delta_{\rm W} = N_{f_0} - N_{g_0} = N - k, \tag{2.41}$$

and then the number of chiral zero modes becomes a topological invariant. We will see that this index plays important roles for the topological classification of the boundary conditions with symmetries in Sec. IV.

III. TENFOLD CLASSIFICATION OF BOUNDARY CONDITIONS WITH SYMMETRIES

So far, we have not considered symmetries except for the 4D Lorentz invariance. It should be emphasized that even if the 5D Dirac equation or action is invariant under some transformations, our model does not necessarily have those symmetries since transformed fields may not always satisfy the boundary conditions. Therefore, in order for our model to have the symmetries, additional restrictions should be on the boundary conditions at the vertex.

Here, we introduce the time-reversal and charge conjugation symmetries combined with some extra-spatial symmetries and show that the boundary matrix $U_{\rm B}$ can be classified into ten classes by those symmetries. We reveal these classes correspond to the ones in the classification of SPT phases of zero-dimensional noninteracting gapped fermions with the Altland-Zirnbauer (AZ) symmetries, which gives the tenfold classification of topological insulators and superconductors. In this section, we will discuss the correspondence between the boundary matrix $U_{\rm B}$ and the zero-dimensional Hamiltonian for the gapped free-fermion system, and also show that the symmetries in our model provide the restrictions for $U_{\rm B}$ identical to the ones for the Hamiltonian from the AZ symmetries. The correspondence of topological properties will be given in Sec. IV.

A. Topological classification of gapped free-fermion system

The topological insulators and superconductors of fully gapped free-fermion systems are topologically classified with AZ symmetries which denote three nonspatial discrete symmetries: time-reversal symmetry (TRS), particle-hole symmetry (PHS) and chiral symmetry (CS), i.e. a single-particle Hamiltonian is classified with the presence or absence of the following symmetries:

$$\text{TRS}:\ TH(\mathbf{k})T^{-1} = H(-\mathbf{k}) \qquad (T^2 = \pm 1), \tag{3.1}$$

TABLE II. Tenfold classification of topological insulators and superconductors. The class A, AIII, AI, BDI, $\cdots$ represent the ten AZ symmetry classes of the Hamiltonian. The signs $+1$ in the chiral symmetry Γ and ± 1 in the time-reversal T and the particle-hole C mean the presence of those symmetries and also they denote the squares of corresponding symmetries, while 0 indicates the absence of the symmetries. d is the spatial dimension of the system and V_d denotes the classifying space in each class for the d dimensional space given in Table III. $\mathbb{Z}$, $\mathbb{Z}_2$, $2\mathbb{Z}$ and 0 in the other entries mean the presence or absence of nontrivial topological insulators or superconductors. The class A and AIII are called the complex AZ symmetry classes and have twofold periodicity, while the other classes are referred to the real AZ symmetry classes and have eightfold periodicity. These periodicities are known as the Bott periodicity, which are related to the structure of the K-theory and Clifford algebra.

Class	T	C	Γ	V_d	$\pi_0(V_0)$	$\pi_0(V_1)$	$\pi_0(V_2)$	$\pi_0(V_3)$	$\pi_0(V_4)$	$\pi_0(V_5)$	$\pi_0(V_6)$	$\pi_0(V_7)$
A	0	0	0	C_{0+d}	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AIII	0	0	1	C_{1+d}	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AI	$+1$	0	0	R_{0+d}	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
BDI	$+1$	$+1$	1	R_{1+d}	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
D	0	$+1$	0	R_{2+d}	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0
DIII	-1	$+1$	1	R_{3+d}	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$
AII	-1	0	0	R_{4+d}	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
CII	-1	-1	1	R_{5+d}	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
C	0	-1	0	R_{6+d}	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
CI	$+1$	-1	1	R_{7+d}	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$

$$\text{PHS}:\ CH(\mathbf{k})C^{-1} = -H(-\mathbf{k}) \qquad (C^2 = \pm 1), \tag{3.2}$$

$$\text{CS}:\ \Gamma H(\mathbf{k})\Gamma^{-1} = -H(\mathbf{k}) \qquad (\Gamma^2 = 1), \tag{3.3}$$

where $H(\mathbf{k})$ is the Hamiltonian in the momentum space with the momentum $\mathbf{k}$ and we assume that there are no nontrivial unitary symmetries which commute with the Hamiltonian. If there are such symmetries, we take the Hamiltonian as a block diagonal form and treat each irreducible block as the Hamiltonian H in (3.1)–(3.3). The TRS and PHS are the antiunitary transformations whose squares should be $+1$ or -1. The CS is the unitary transformation and can be given by the product $\Gamma = TC$ up to a phase. Here we take the CS as its square to be $+1$. This symmetry is always present when both the TRS and PHS are present, although the CS can be symmetry alone even if the TRS and PHS are absent. It should be noted that we can assume there are single TRS, PHS, and CS. For example, if there are two TRS such as T_1 and T_2, we can consider the unitary symmetry T_1T_2 which commutes with the Hamiltonian. Then the Hamiltonian can be taken to the block diagonal form and T_1 and T_2 are trivially related in each irreducible block, which is regarded as H in (3.1)–(3.3).

It is known that we can obtain total ten symmetry classes with topological numbers as shown in Table II [32–34]. These ten symmetry classes were originally introduced by A. Altland and M. R. Zirnbauer and are therefore called AZ symmetry classes [38,39]. The topological numbers $\mathbb{Z}$, $\mathbb{Z}_2$ and $2\mathbb{Z}$ in Table II indicate the presence of nontrivial topological insulators or superconductors. This topological classification is obtained by classifying symmetry-allowed mass terms in the Dirac Hamiltonian and the topological numbers correspond to the 0th homotopy groups of the classifying spaces, which is the parameter space of the symmetry-allowed mass terms with taking the limit of an infinite number of energy bands. See Table III. These topological numbers characterize whether Hamiltonians can continuously deform to each other or not without closing a mass gap or breaking the symmetries. When they belong to the same symmetry class and have the same topological number, they can be continuously deformed to each other. One of the significant features of the topological

TABLE III. Classifying spaces and 0-th homotopy groups. The integers p and q are related to the number of empty bands and occupied bands, respectively. Here, taking the limit of p means that there are an infinite number of empty bands and we focus on the stable classification which is independent of the addition of empty bands. From the viewpoint of the K-theory, this limit results from the property of the so-called stable equivalence.

ℓ mod 2	Complex classifying space C_ℓ	$\pi_0(C_\ell)$
$\ell = 0$	$C_0 = \bigcup_q \lim_{p\to\infty} \frac{U(p+q)}{U(p)\times U(q)}$	$\mathbb{Z}$
$\ell = 1$	$C_1 = \lim_{p\to\infty} U(p)$	0

ℓ mod 8	Real classifying space R_ℓ	$\pi_0(R_\ell)$
$\ell = 0$	$R_0 = \bigcup_q \lim_{p\to\infty} \frac{O(p+q)}{O(p)\times O(q)}$	$\mathbb{Z}$
$\ell = 1$	$R_1 = \lim_{p\to\infty} O(p)$	$\mathbb{Z}_2$
$\ell = 2$	$R_2 = \lim_{p\to\infty} \frac{O(2p)}{U(p)}$	$\mathbb{Z}_2$
$\ell = 3$	$R_3 = \lim_{p\to\infty} \frac{U(2p)}{Sp(p)}$	0
$\ell = 4$	$R_4 = \cup_q \lim_{p\to\infty} \frac{Sp(p+q)}{Sp(p)\times Sp(q)}$	$2\mathbb{Z}$
$\ell = 5$	$R_5 = \lim_{p\to\infty} Sp(p)$	0
$\ell = 6$	$R_6 = \lim_{p\to\infty} \frac{Sp(p)}{U(p)}$	0
$\ell = 7$	$R_7 = \lim_{p\to\infty} \frac{U(p)}{O(p)}$	0

insulators and superconductors is that if there are boundaries in the system and the bulk Hamiltonians in each side have different topological numbers, topologically protected gapless states appear on the boundaries. This is well known as the bulk-boundary correspondence.

B. Correspondence to zero-dimensional Hamiltonian

Let us focus on the zero-dimensional Hamiltonian. In this case, the Hamiltonian has no momentum dependence. Therefore it consists of only a mass term and is given by a constant Hermitian matrix. As long as the mass gap does not close and symmetries are restored, the topological structure does not change. Then we can discuss the topological classification by deforming the Hamiltonian to the following normalized form without closing the gap:

$$H^2 = 1, \qquad H^\dagger = H. \tag{3.4}$$

This Hamiltonian is called a flattened Hamiltonian and has eigenvalues ± 1. We can aware that this condition is the same as Eq. (2.18) and there is a correspondence between the flattened Hamiltonian and the boundary matrix U_{B}. Then, it is expected that the classification of the zero-dimensional topological insulators and superconductors can be applied to that of the boundary conditions in our model.

To show the correspondence of the classification, we need symmetries which correspond to the TRS and PHS in the zero-dimensional gapped free Hamiltonian. In the following subsections, we introduce the time-reversal and charge conjugation symmetries combined with some extra-spatial symmetries in our model and show that these provide restrictions for the boundary matrix U_{B} consistent with the conditions (3.1)–(3.3).

C. Transformations in the y-direction

First of all, we introduce transformations that act only in the extra dimensional direction, i.e. y-direction. These transformations will be used later when we construct the symmetries corresponding to the AZ symmetry classes. For convenience, we will label the edge $L_{a-1} < y < L_a$ on the rose graph as

$$D_a = \{y | L_{a-1} < y < L_a\}, \quad a = 1, 2, \ldots, N. \tag{3.5}$$

1. Permutation S_y

We introduce a permutation S_y that exchanges the a-edge to the $(N/2 + a)$-edge $(a = 1, \ldots, N/2)$. This permutation is well defined when the a-edge and the $(N/2 + a)$-edge have the same length

$$L_a - L_{a-1} = L_{a+N/2} - L_{a-1+N/2} \qquad (a = 1, 2, \ldots, N/2) \tag{3.6}$$

and the number of edges N is even. This transformation can be also regarded as the translation of the a-edge to the $(N/2 + a)$-edge. The mode functions $\varphi(y) = \{f_n^{(i)}(y)$ or $g_n^{(i)}(y)\}$ on D_a are transformed as

$$(S_y\varphi)(y) = \begin{cases} \varphi(y + L_{a-1+N/2} - L_{a-1}) & (y \in D_a, a = 1, 2, \ldots, N/2), \\ \varphi(y + L_{a-1-N/2} - L_{a-1}), & (y \in D_a, a = N/2 + 1, \ldots, N). \end{cases} \tag{3.7}$$

Figure 5 is a diagram of the transformation S_y.

Under the permutation S_y, the boundary vectors $\vec{F}_n^{(i)}$ and $\vec{G}_m^{(j)}$ transform as follows:

$$\vec{F}_n^{(i)} \xrightarrow{S_y} \begin{pmatrix} f_n^{(i)}(L_{N/2} + \varepsilon) \\ f_n^{(i)}(L_{N/2+1} - \varepsilon) \\ \vdots \\ f_n^{(i)}(L_{N-1} + \varepsilon) \\ f_n^{(i)}(L_N - \varepsilon) \\ \hline f_n^{(i)}(L_0 + \varepsilon) \\ f_n^{(i)}(L_1 - \varepsilon) \\ \vdots \\ f_n^{(i)}(L_{N/2-1} + \varepsilon) \\ f_n^{(i)}(L_{N/2} - \varepsilon) \end{pmatrix} = \begin{pmatrix} 0 & 1_N \\ 1_N & 0 \end{pmatrix} \begin{pmatrix} f_n^{(i)}(L_0 + \varepsilon) \\ f_n^{(i)}(L_1 - \varepsilon) \\ \vdots \\ f_n^{(i)}(L_{N/2-1} + \varepsilon) \\ f_n^{(i)}(L_{N/2} - \varepsilon) \\ \hline f_n^{(i)}(L_{N/2} + \varepsilon) \\ f_n^{(i)}(L_{N/2+1} - \varepsilon) \\ \vdots \\ f_n^{(i)}(L_{N-1} + \varepsilon) \\ f_n^{(i)}(L_N - \varepsilon) \end{pmatrix} = (\sigma_1 \otimes 1_N)\vec{F}_n^{(i)}, \tag{3.8}$$

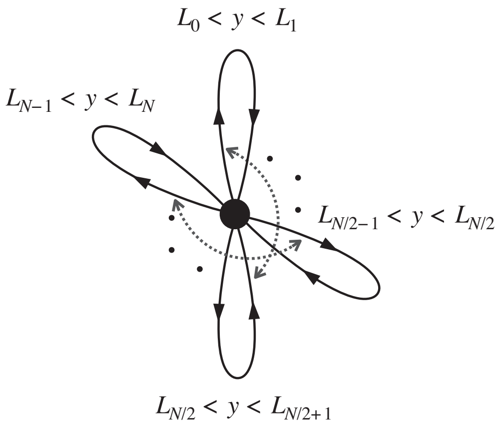

FIG. 5. Permutation S_y that exchanges the ath edge for the $(N/2+a)$th edge $(a = 1, \ldots, N/2)$.

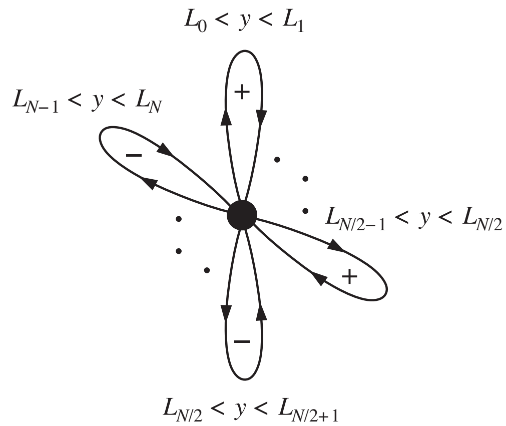

FIG. 6. Half-reflection R_y that multiplies the mode functions on $D_a(a = N/2+1, \ldots, 2N)$ by −1.

$$\vec{G}_m^{(j)} \xrightarrow{S_y} \begin{pmatrix} g_m^{(j)}(L_{N/2}+\varepsilon) \\ -g_m^{(j)}(L_{N/2+1}-\varepsilon) \\ \vdots \\ g_m^{(j)}(L_{N-1}+\varepsilon) \\ -g_m^{(j)}(L_N-\varepsilon) \\ \hline g_m^{(j)}(L_0+\varepsilon) \\ -g_m^{(j)}(L_1-\varepsilon) \\ \vdots \\ g_m^{(j)}(L_{N/2-1}+\varepsilon) \\ -g_m^{(j)}(L_{N/2}-\varepsilon) \end{pmatrix} = \begin{pmatrix} 0 & 1_N \\ 1_N & 0 \end{pmatrix} \begin{pmatrix} g_m^{(j)}(L_0+\varepsilon) \\ -g_m^{(j)}(L_1-\varepsilon) \\ \vdots \\ g_m^{(j)}(L_{N/2-1}+\varepsilon) \\ -g_m^{(j)}(L_{N/2}-\varepsilon) \\ \hline g_m^{(j)}(L_{N/2}+\varepsilon) \\ -g_m^{(j)}(L_{N/2+1}-\varepsilon) \\ \vdots \\ g_m^{(j)}(L_{N-1}+\varepsilon) \\ -g_m^{(j)}(L_N-\varepsilon) \end{pmatrix} = (\sigma_1 \otimes 1_N)\vec{G}_m^{(j)}. \tag{3.9}$$

2. Half-reflection R_y

Next, we consider a transformation R_y that multiplies the mode function on $D_a(a = N/2+1, \ldots, 2N)$ by −1. This is called the half-reflection conversion because only signs of the mode functions on the half sections $D_a(a = N/2+1, \ldots, 2N)$ are flipped as if they were reflected in a mirror. This transformation is well defined when the quantum graph has even edges. It should be emphasized that the transformation R_y on the mode functions does not change the mass eigenvalues. Figure 6 is a diagram of half-reflection R_y.

The mode functions $\varphi(y) = \{f_n^{(i)}(y) \,\mathrm{or}\, g_n^{(i)}(y)\}$ on $D_a(a = 1, 2, \ldots, N)$ are transformed as

$$(R_y\varphi)(y) = \begin{cases} \varphi(y) & (y \in D_a, a = 1, 2, \ldots, N/2), \\ -\varphi(y) & (y \in D_a, a = N/2+1, \ldots, N). \end{cases} \tag{3.10}$$

Then, this half-reflection R_y acts on the boundary vectors $\vec{F}_n^{(i)}$ and $\vec{G}_m^{(j)}$ as

$$\vec{F}_n^{(i)} \xrightarrow{R_y} (\sigma_3 \otimes 1_N)\vec{F}_n^{(i)}, \tag{3.11}$$

$$\vec{G}_m^{(j)} \xrightarrow{R_y} (\sigma_3 \otimes 1_N)\vec{G}_m^{(j)}. \tag{3.12}$$

3. Composite transformation $Q_y = -iR_yS_y$

Furthermore, we can consider the transformation Q_y which is given by the product of S_y and R_y

$$Q_y = -iR_yS_y, \tag{3.13}$$

where we suppose that S_y acts on the mode function first, and then R_y acts on it.[4]

The mode functions $\varphi(y) = \{f_n^{(i)}(y) \,\mathrm{or}\, g_n^{(i)}(y)\}$ on $D_a(a = 1, 2, \ldots, N)$ are transformed as

[4]It is worth noting that operators Q_y, R_y and S_y form the $SU(2)$ algebra and that the operators $(\mathcal{O}_1, \mathcal{O}_2, \mathcal{O}_3) = (Q_y, R_y, S_y)$ satisfy the following relations:

$$\{\mathcal{O}_i, \mathcal{O}_j\} = 2\delta_{ij}, \qquad [\mathcal{O}_i, \mathcal{O}_j] = 2i\varepsilon_{ijk}\mathcal{O}_k \qquad (i, j = 1, 2, 3).$$

$$(Q_y\varphi)(y) = \begin{cases} -i\varphi(y + L_{a-1+N/2} - L_{a-1}) & (y \in D_a, a = 1, \ldots, N/2), \\ i\varphi(y + L_{a-1-N/2} - L_{a-1}) & (y \in D_a, a = N/2+1, \ldots, N), \end{cases} \tag{3.14}$$

and the transformation for the boundary vectors $\vec{F}_n^{(i)}$ and $\vec{G}_m^{(j)}$ are given as

$$\vec{F}_n^{(i)} \xrightarrow{Q_y} (\sigma_2 \otimes 1_N)\vec{F}_n^{(i)}, \tag{3.15}$$

$$\vec{G}_m^{(j)} \xrightarrow{Q_y} (\sigma_2 \otimes 1_N)\vec{G}_m^{(j)}. \tag{3.16}$$

4. Parity in the y-direction P_y

Finally, we introduce the parity P_y that inverts the coordinates in each edge described in Fig. 7. The transformation for the mode functions $\varphi(y) = \{f_n^{(i)}(y)$ or $g_n^{(i)}(y)\}$ on $D_a (a = 1, 2, \ldots, N)$ is given by

$$(P_y\varphi)(y) = \varphi(L_a - y + L_{a-1}) \qquad y \in D_a (a = 1, \ldots, N), \tag{3.17}$$

and the boundary vectors transform as

$$\vec{F}_n^{(i)} \xrightarrow{P_y} (1_N \otimes \sigma_1)\vec{F}_n^{(i)}, \tag{3.18}$$

$$\vec{G}_m^{(j)} \xrightarrow{P_y} -(1_N \otimes \sigma_1)\vec{G}_m^{(j)}. \tag{3.19}$$

D. Correspondence to time-reversal symmetries

Here we define the two types of time-reversal symmetries in the 5D spacetime, the one of which is combined with the extra-spatial transformation Q_y. These time-reversal symmetries lead to the restrictions for the boundary matrix U_{B}. We show that these restrictions correspond to the condition of the TRS (3.1) in the AZ symmetry classes.

1. Time-reversal $\mathcal{T}_+$

First, we consider the ordinary time-reversal transformation $\mathcal{T}_+$ for the 5D Dirac fermion

$$\Psi(x, y) \xrightarrow{\mathcal{T}_+} \Psi^{\mathcal{T}_+}(x, y) = U_T \Psi^*(-x^0, x^i, y), \tag{3.20}$$

where U_T is defined as a 4×4 unitary matrix that satisfies the following relation:[5]

$$U_T(\gamma^A)^* U_T^{-1} = \begin{cases} \gamma^0 & (A = 0), \\ -\gamma^i & (A = i = 1, 2, 3), \\ -\gamma^y & (A = y). \end{cases} \tag{3.21}$$

Although the 5D Dirac equation is invariant under this transformation, we should further require that the boundary conditions (2.16) and (2.17) hold even after the transformation (3.20) in order that $\mathcal{T}_+$ becomes a symmetry in our model.

Then, let us substitute the KK decomposition (2.6) into (3.20) to derive the restrictions for U_{B}:

$$\begin{aligned} &\sum_i \sum_n [\psi_{\mathrm{R},n}^{(i)}(x) f_n^{(i)}(y) + \psi_{\mathrm{L},n}^{(i)}(x) g_n^{(i)}(y)] \\ &\xrightarrow{\mathcal{T}_+} \sum_i \sum_n U_T \psi_{\mathrm{R},n}^{(i)*}(-x^0, x^i) f_n^{(i)*}(y) \\ &\quad + \sum_i \sum_n U_T \psi_{\mathrm{L},n}^{(i)*}(-x^0, x^i) g_n^{(i)*}(y). \end{aligned} \tag{3.22}$$

Taking account of the chirality in four dimensions, we obtain the transformations for the 4D fields $\psi_{\mathrm{R/L},n}^{(i)}$ and the mode functions $f_n^{(i)}$, $g_n^{(i)}$ as

$$\psi_{\mathrm{R/L},n}^{(i)}(x) \xrightarrow{\mathcal{T}_+} U_T \psi_{\mathrm{R/L},n}^{(i)*}(-x^0, x^i), \qquad f_n^{(i)}(y) \xrightarrow{\mathcal{T}_+} f_n^{(i)*}(y),$$
$$g_n^{(i)}(y) \xrightarrow{\mathcal{T}_+} g_n^{(i)*}(y). \tag{3.23}$$

The 4D part follows the usual 4D Dirac equation and gives no restrictions. On the other hand, the following additional relations must hold for the transformation of the mode functions:

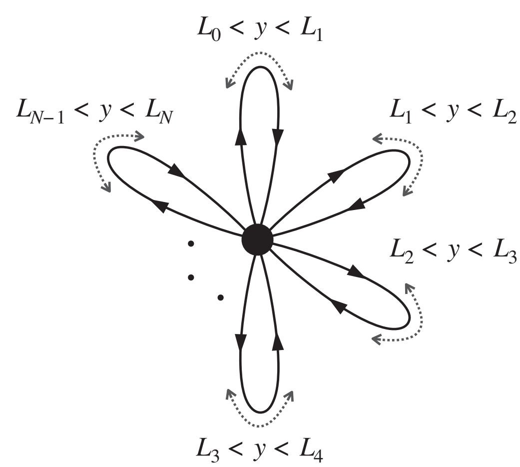

FIG. 7. Parity in the y-direction P_y that inverts the coordinates in each edge.

[5]In the chiral representation $\gamma^0 = \sigma_1 \otimes 1_2$, $\gamma^i = -i\sigma_2 \otimes \sigma_i$, $\gamma^y = -i\sigma_3 \otimes 1_2$, the matrix U_T is given by $U_T = \gamma^1\gamma^3$ up to a phase.

$$(1_{2N} - U_{\rm B})\vec{F}_n^{(i)*} = 0, \quad (3.24)$$

$$(1_{2N} + U_{\rm B})\vec{G}_m^{(j)*} = 0. \quad (3.25)$$

Comparing these relations with the complex conjugate of the original boundary conditions (2.16) and (2.17), we obtain the restriction

$$T_+ U_{\rm B} T_+^{-1} = U_{\rm B}, \qquad T_+ \equiv \mathcal{K}, \quad (3.26)$$

where $\mathcal{K}$ is a complex conjugate operator that acts like $\mathcal{K} z \mathcal{K}^{-1} = z^*$ on the complex number z. Since T_+ is antiunitary and satisfies

$$T_+^2 = 1, \quad (3.27)$$

Eq. (3.26) implies that T_+ corresponds to the TRS with $T^2 = 1$ in the AZ symmetry classes.

2. Time-reversal $\mathcal{T}_-$

Next, let us consider a symmetry which leads to the restriction corresponds to the TRS with $T^2 = -1$ in the AZ symmetry classes. Here we introduce a transformation that combines Q_y with the transformation of $\mathcal{T}_+$

$$\Psi(x,y) \xrightarrow{\mathcal{T}_-} \Psi^{\mathcal{T}_-}(x,y) = Q_y U_T \Psi^*(-x^0, x^i, y), \quad (3.28)$$

where U_T is defined by Eq. (3.21). The only difference from the case of $\mathcal{T}_+$ is that the transformation Q_y is included and we will see that this plays the role to flip the sign of the square (3.27). Q_y does not affect the 5D Dirac equation described on each edge and then the 5D Dirac equation is also invariant for the transformation (3.28). However, the transformed field should satisfy the same boundary condition as the original one in order for $\mathcal{T}_-$ to be a symmetry.

If we compare the 4D chirality in the same way, we obtain the transformation $\mathcal{T}_+$ for the 4D fields and the mode functions as

$$\psi_{{\rm R/L},n}^{(i)}(x) \xrightarrow{\mathcal{T}_-} U_T \psi_{{\rm R/L},n}^{(i)*}(-x^0, x^i), \qquad f_n^{(i)}(y) \xrightarrow{\mathcal{T}_-} Q_y f_n^{(i)*}(y),$$
$$g_n^{(i)}(y) \xrightarrow{\mathcal{T}_-} Q_y g_n^{(i)*}(y). \quad (3.29)$$

Then, in order for our model to have the time-reversal symmetry $\mathcal{T}_-$, we find that the relations

$$(1_{2N} - U_{\rm B})(\sigma_2 \otimes 1_N)\vec{F}_n^{(i)*} = 0, \quad (3.30)$$

$$(1_{2N} + U_{\rm B})(\sigma_2 \otimes 1_N)\vec{G}_m^{(j)*} = 0 \quad (3.31)$$

must hold from Eqs. (3.15) and (3.16).

Comparing these relations with the complex conjugate of the original boundary condition (2.16) and (2.17), we obtain the restriction

$$T_- U_{\rm B} T_-^{-1} = U_{\rm B}, \qquad T_- \equiv (i\sigma_2 \otimes 1_N)\mathcal{K}. \quad (3.32)$$

T_- is antiunitary and its square is

$$T_-^2 = -1. \quad (3.33)$$

Therefore Eq. (3.32) implies T_- corresponds to the TRS with $T^2 = -1$ in the AZ symmetry classes.

E. Correspondence to particle-hole symmetries

We consider two types of charge conjugations with extra-spatial transformations similar to the time-reversal symmetries and show those provide the restrictions for $U_{\rm B}$. They correspond to the PHS (3.2) in the AZ symmetry classes.

1. Charge conjugation $\mathcal{C}_-$

First, we introduce a transformation defined by the 4D charge conjugation with the parity P_y in the extra space which is consistent with the 4D Lorentz symmetry in our model:

$$\Psi(x,y) \xrightarrow{\mathcal{C}_-} \Psi^{\mathcal{C}_-}(x,y) = P_y U_C \bar{\Psi}^\top(x,y), \quad (3.34)$$

where U_C is the usual 4D charge conjugation matrix defined by[6]

$$U_C(\gamma^\mu)^\top U_C^{-1} = -\gamma^\mu, \qquad U_C^\top = -U_C. \quad (3.35)$$

From the above relation between U_C and γ^μ, the gamma matrix $\gamma^y(= -i\gamma^5)$ satisfies

$$U_C(\gamma^y)^\top U_C^{-1} = \gamma^y. \quad (3.36)$$

In this paper, we refer to this transformation as the charge conjugation $\mathcal{C}_-$. While the 5D Dirac equation is not invariant by only the 4D charge conjugation due to the sign of the right-hand side in Eq. (3.36), it is invariant by $\mathcal{C}_-$ since this transformation additionally includes the parity P_y.[7]

[6]In the chiral representation $\gamma^0 = \sigma_1 \otimes 1_2$, $\gamma^i = -i\sigma_2 \otimes \sigma_i$, $\gamma^y = -i\sigma_3 \otimes 1_2$, the matrix U_C is given by $U_C = \gamma^0\gamma^2$ up to a phase.

[7]Although we focus on the $\mathcal{C}_-$ symmetry in this paper, we can also consider a 5D charge conjugation without the parity which is given by

$$\Psi(x,y) \to U_{C'}\bar{\Psi}^\top(x,y), \qquad U_{C'}^\top = -U_{C'},$$
$$U_{C'}(\gamma^A)^\top U_{C'}^{-1} = +\gamma^A \qquad (A = 0, \ldots, 3, y).$$

The bulk mass should vanish under this symmetry unlike the case of $\mathcal{C}_-$. See [40] for detail.

In addition to the invariance of the 5D Dirac equation, the field after the transformation should satisfy the boundary condition in order for $\mathcal{C}_-$ to be a symmetry. By substituting the KK decomposition (2.6) into (3.34) and comparing the chirality in four dimensions, we obtain the transformation $\mathcal{C}_-$ for the 4D fields and the mode functions as

$$\psi^{(i)}_{\mathrm{R/L},n}(x) \xrightarrow{\mathcal{C}_-} U_C \overline{\psi^{(i)}_{\mathrm{L/R},n}}^{\top}(x), \qquad f^{(i)}_n(y) \xrightarrow{\mathcal{C}_-} P_y g^{(i)*}_n(y),$$
$$g^{(i)}_n(y) \xrightarrow{\mathcal{C}_-} P_y f^{(i)*}_n(y). \tag{3.37}$$

The mode functions $f^{(i)}_n$ and $g^{(i)}_n$ are interchanged because of the change of the 4D chirality. Therefore, if there exist zero mode functions $f^{(i)}_0$, zero modes $g^{(i)}_0$ should also exist and we can take it as

$$g^{(i)}_0(y) = P_y f^{(i)*}_0(y). \tag{3.38}$$

For massive modes ($n \neq 0$), since the relations between $f^{(i)}_n(y)$ and $g^{(i)}_n(y)$ are already fixed by Eqs. (2.10) and (2.11), $P_y g^{(i)*}_n(y)(P_y f^{(i)*}_n(y))$ is given by linear combinations of $f^{(i)}_n(y)(g^{(i)}_n(y))$.

The transformation for the boundary vectors $\vec{F}^{(i)}_n$ and $\vec{G}^{(j)}_m$ are

$$\vec{F}^{(i)}_n \xrightarrow{\mathcal{C}_-} -(1_N \otimes i\sigma_2)\vec{G}^{(i)*}_n, \tag{3.39}$$

$$\vec{G}^{(j)}_m \xrightarrow{\mathcal{C}_-} (1_N \otimes i\sigma_2)\vec{F}^{(j)*}_m, \tag{3.40}$$

and the following relations must hold:

$$(1_{2N} - U_{\mathrm{B}})(1_N \otimes i\sigma_2)\vec{G}^{(i)*}_n = 0, \tag{3.41}$$

$$(1_{2N} + U_{\mathrm{B}})(1_N \otimes i\sigma_2)\vec{F}^{(j)*}_m = 0. \tag{3.42}$$

From the original boundary conditions (2.16) and (2.17), the above relations give the restriction for U_{B}

$$C_- U_{\mathrm{B}} C_-^{-1} = -U_{\mathrm{B}}, \qquad C_- \equiv (1_N \otimes i\sigma_2)\mathcal{K}. \tag{3.43}$$

Here C_- is antiunitary and satisfies

$$C_-^2 = -1. \tag{3.44}$$

Then we can find that C_- corresponds to the PHS with $C^2 = -1$ in the AZ symmetry classes.

2. Charge conjugation $\mathcal{C}_+$

Next, we consider the transformation $\mathcal{C}_+$ which consists of the charge conjugation $\mathcal{C}_-$ with the transformation Q_y

$$\Psi(x,y) \xrightarrow{\mathcal{C}_+} \Psi^{\mathcal{C}_+}(x,y) = Q_y P_y U_C \bar{\Psi}^{\top}(x,y), \tag{3.45}$$

where U_C is defined by Eq. (3.35). The 5D Dirac equation is also invariant by this transformation.

Then let us consider the restriction for U_{B} in order for $\mathcal{C}_+$ to be a symmetry. The transformation for the 4D fields and the mode functions are given by

$$\psi^{(i)}_{\mathrm{R/L},n}(x) \xrightarrow{\mathcal{C}_+} U_C \overline{\psi^{(i)}_{\mathrm{L/R},n}}^{\top}(x), \qquad f^{(i)}_n(y) \xrightarrow{\mathcal{C}_+} Q_y P_y g^{(i)*}_n(y),$$
$$g^{(i)}_n(y) \xrightarrow{\mathcal{C}_+} Q_y P_y f^{(i)*}_n(y). \tag{3.46}$$

Then the boundary vectors $\vec{F}^{(i)}_n$ and $\vec{G}^{(j)}_m$ are transformed as

$$\vec{F}^{(i)}_n \xrightarrow{\mathcal{C}_+} -(\sigma_2 \otimes 1_{N/2} \otimes i\sigma_2)\vec{G}^{(i)*}_n, \tag{3.47}$$

$$\vec{G}^{(j)}_m \xrightarrow{\mathcal{C}_+} (\sigma_2 \otimes 1_{N/2} \otimes i\sigma_2)\vec{F}^{(j)*}_m. \tag{3.48}$$

Therefore the following relations must hold:

$$(1_{2N} - U_{\mathrm{B}})(\sigma_2 \otimes 1_{N/2} \otimes i\sigma_2)\vec{G}^{(i)*}_n = 0, \tag{3.49}$$

$$(1_{2N} + U_{\mathrm{B}})(\sigma_2 \otimes 1_{N/2} \otimes i\sigma_2)\vec{F}^{(j)*}_m = 0. \tag{3.50}$$

Comparing these relations with the original boundary conditions (2.16) and (2.17), we obtain the restriction

$$C_+ U_{\mathrm{B}} C_+^{-1} = -U_{\mathrm{B}}, \qquad C_+ \equiv (i\sigma_2 \otimes 1_{N/2} \otimes i\sigma_2)\mathcal{K}. \tag{3.51}$$

C_+ is antiunitary and its square is

$$C_+^2 = +1. \tag{3.52}$$

Therefore C_+ corresponds to the PHS with $C^2 = +1$ in the AZ symmetry classes.

F. Correspondence to chiral symmetry

Finally, let us discuss the symmetries which are obtained by the product of the time-reversal and charge conjugation transformations discussed above. We show that these symmetries lead to restrictions for U_{B} and correspond to the CS (3.3) in the AZ symmetry classes.

1. Chiral symmetry Γ_+

We introduce the transformation of the product $\mathcal{T}_+\mathcal{C}_+$ or $\mathcal{T}_-\mathcal{C}_-$. From Eqs. (3.20), (3.45) or (3.28), (3.34), the transformation properties of $\Psi(x,y)$ are given by

$$\Psi(x,y) \xrightarrow{\mathcal{T}_+\mathcal{C}_+} -Q_y P_y U_T U_C^* \gamma^0 \Psi(-x^0, x^i, y), \tag{3.53}$$

$$\Psi(x,y) \xrightarrow{\mathcal{T}_-\mathcal{C}_-} +Q_y P_y U_T U_C^* \gamma^0 \Psi(-x^0, x^i, y). \tag{3.54}$$

Thus, these transformations are equivalent up to the sign. Comparing the chirality in four dimensions, we obtain the transformations for the 4D fields and the mode functions as

$$\psi^{(i)}_{\mathrm{R/L},n}(x) \xrightarrow{\mathcal{T}_\pm\mathcal{C}_\pm} U_T U_C^* \gamma^0 \psi^{(i)}_{\mathrm{L/R},n}(-x^0, x^i), \quad (3.55)$$

$$f^{(i)}_n(y) \xrightarrow{\mathcal{T}_\pm\mathcal{C}_\pm} \mp Q_y P_y g^{(i)}_n(y), \qquad g^{(i)}_n(y) \xrightarrow{\mathcal{T}_\pm\mathcal{C}_\pm} \mp Q_y P_y f^{(i)}_n(y). \quad (3.56)$$

Therefore, the boundary vectors $\vec{F}^{(i)}_n$ and $\vec{G}^{(j)}_m$ are transformed as

$$\vec{F}^{(i)}_n \xrightarrow{\mathcal{T}_\pm\mathcal{C}_\pm} \pm (\sigma_2 \otimes 1_{N/2} \otimes i\sigma_2) \vec{G}^{(i)}_n, \quad (3.57)$$

$$\vec{G}^{(j)}_m \xrightarrow{\mathcal{T}_\pm\mathcal{C}_\pm} \mp (\sigma_2 \otimes 1_{N/2} \otimes i\sigma_2) \vec{F}^{(j)}_m. \quad (3.58)$$

These indicate that the relations

$$(1_{2N} - U_\mathrm{B})(\sigma_2 \otimes 1_{N/2} \otimes i\sigma_2) \vec{G}^{(i)}_n = 0, \quad (3.59)$$

$$(1_{2N} + U_\mathrm{B})(\sigma_2 \otimes 1_{N/2} \otimes i\sigma_2) \vec{F}^{(i)}_n = 0 \quad (3.60)$$

must hold in order for $\mathcal{T}_\pm\mathcal{C}_\pm$ to be a symmetry. We then obtain the restriction for U_B

$$\Gamma_+ U_\mathrm{B} \Gamma_+^{-1} = -U_\mathrm{B}, \qquad \Gamma_+ \equiv i\sigma_2 \otimes 1_{N/2} \otimes i\sigma_2. \quad (3.61)$$

Γ_+ is unitary and we can find that Γ_+ corresponds to the CS in the AZ symmetry classes. In terms of operators that act on U_B, we can confirm the relation

$$\Gamma_+ = T_\pm C_\pm. \quad (3.62)$$

2. *Chiral symmetry* Γ_-

We can consider the another transformation of the product $\mathcal{T}_+\mathcal{C}_-$ or equivalently $\mathcal{T}_-\mathcal{C}_+$

$$\Psi(x, y) \xrightarrow{\mathcal{T}_\pm\mathcal{C}_\mp} \pm P_y U_T U_C^* \gamma^0 \Psi(-x^0, x^i, y). \quad (3.63)$$

The transformation for the 4D fields and the mode functions are then given by

$$\psi^{(i)}_{\mathrm{R/L},n}(x) \xrightarrow{\mathcal{T}_\pm\mathcal{C}_\mp} U_T U_C^* \gamma^0 \psi^{(i)}_{\mathrm{L/R},n}(-x^0, x^i), \quad (3.64)$$

$$f^{(i)}_n(y) \xrightarrow{\mathcal{T}_\pm\mathcal{C}_\mp} \pm (P_y g^{(i)}_n)(y), \qquad g^{(i)}_n(y) \xrightarrow{\mathcal{T}_\pm\mathcal{C}_\mp} \pm (P_y f^{(i)}_n)(y). \quad (3.65)$$

Therefore, the boundary vectors $\vec{F}^{(i)}_n$ and $\vec{G}^{(j)}_m$ are transformed as

$$\vec{F}^{(i)}_n \xrightarrow{\mathcal{T}_\pm\mathcal{C}_\mp} \mp (1_N \otimes i\sigma_2) \vec{G}^{(i)}_n, \quad (3.66)$$

$$\vec{G}^{(j)}_m \xrightarrow{\mathcal{T}_\pm\mathcal{C}_\mp} \pm (1_N \otimes i\sigma_2) \vec{F}^{(j)}_m, \quad (3.67)$$

and the following relations should be satisfied in order for $\mathcal{T}_\pm\mathcal{C}_\mp$ to be a symmetry:

$$(1_{2N} - U_\mathrm{B})(1_N \otimes i\sigma_2) \vec{G}^{(i)}_n = 0, \quad (3.68)$$

$$(1_{2N} + U_\mathrm{B})(1_N \otimes i\sigma_2) \vec{F}^{(i)}_n = 0. \quad (3.69)$$

These relations yield the restriction for U_B

$$\Gamma_- U_\mathrm{B} \Gamma_-^{-1} = -U_\mathrm{B}, \qquad \Gamma_- \equiv 1_N \otimes \sigma_2. \quad (3.70)$$

Γ_- is unitary and we can find that Γ_- corresponds to the chiral symmetry in the AZ symmetry classes. We can also confirm that Γ_- can be given by

$$\Gamma_- = \mp i T_\pm C_\mp. \quad (3.71)$$

G. Summary of correspondence to AZ symmetry class

In this section, we considered the time-reversal and the charge conjugation with the extra-spatial transformations in our model and it was revealed that these symmetries provide the restrictions for the boundary matrix U_B as shown in Table IV. These correspond to the TRS, PHS and CS in the AZ symmetry classes. The matrix U_B corresponds to the zero-dimensional Hamiltonian H in (3.1)–(3.3) and therefore we can classify U_B into ten symmetry classes as in Table II for the $d = 0$ case.

It should be noted that we assume only one of the same type symmetries such as $\mathcal{T}_+$ and $\mathcal{T}_-$ can be present so far. If both symmetries are present, Q_y also becomes the symmetry independently since Q_y can be given by their product. In this case, we consider the identification of the $(a + N/2)$-edge to a-edge $(a = 1, \ldots, N/2)$ by the symmetry Q_y with the eigenvalues $Q_y = +1$ or $Q_y = -1$, and then classify the boundary conditions of this reduced system. This identification effectively reduces the rose graph with N edges to the one with $N/2$ edges like the S^1 is reduced to the interval by the $\mathbb{Z}_2$ orbifold, and the same type symmetries such as $\mathcal{T}_+$ and $\mathcal{T}_-$ are trivially related with each other after the identification. The symmetry Q_y requires that U_B commutes with $\sigma_2 \otimes 1_N$ from Eqs. (3.15) and (3.16), and the matrix U_B can be written as

$$U_B = \frac{1_2 + \sigma_2}{2} \otimes u_{\mathrm{B}+} + \frac{1_2 - \sigma_2}{2} \otimes u_{\mathrm{B}-}, \quad (3.72)$$

where $u_{\mathrm{B}\pm}$ are $N \times N$ Hermitian unitary matrices. This $u_{\mathrm{B}+}(u_{\mathrm{B}-})$ specifies the boundary condition for the reduced rose graph with $N/2$ edges with $Q_y = +1 (Q_y = -1)$ and

TABLE IV. The transformations in our model and the correspondence to the AZ symmetries.

AZ symmetry	Transformation for $\Psi(x,y)$	Restriction for U_{B}
Time-reversal ($T^2=+1$)	$\Psi(x,y)\xrightarrow{\mathcal{T}_+}U_T\mathcal{K}\Psi(-x^0,x^i,y)$	$T_+U_{\mathrm{B}}T_+^{-1}=U_{\mathrm{B}}$ $T_+=\mathcal{K}$
Time-reversal ($T^2=-1$)	$\Psi(x,y)\xrightarrow{\mathcal{T}_-}Q_yU_T\mathcal{K}\Psi(-x^0,x^i,y)$	$T_-U_{\mathrm{B}}T_-^{-1}=U_{\mathrm{B}}$ $T_-=(i\sigma_2\otimes 1_N)\mathcal{K}$
Particle-hole ($C^2=+1$)	$\Psi(x,y)\xrightarrow{\mathcal{C}_+}Q_yP_yU_C\bar{\Psi}^\top(x,y)$	$C_+U_{\mathrm{B}}C_+^{-1}=-U_{\mathrm{B}}$ $C_+=(i\sigma_2\otimes 1_{N/2}\otimes i\sigma_2)\mathcal{K}$
Particle-hole ($C^2=-1$)	$\Psi(x,y)\xrightarrow{\mathcal{C}_-}P_yU_C\bar{\Psi}^\top(x,y)$	$C_-U_{\mathrm{B}}C_-^{-1}=-U_{\mathrm{B}}$ $C_-=(1_N\otimes i\sigma_2)\mathcal{K}$
Chiral	$\Psi(x,y)\xrightarrow{\mathcal{T}_\pm\mathcal{C}_\pm}\mp Q_yP_yU_TU_C^*\gamma^0\Psi(-x^0,x^i,y)$	$\Gamma_+U_{\mathrm{B}}\Gamma_+^{-1}=-U_{\mathrm{B}}$ $\Gamma_+=i\sigma_2\otimes 1_{N/2}\otimes i\sigma_2$
Chiral	$\Psi(x,y)\xrightarrow{\mathcal{T}_\pm\mathcal{C}_\mp}\pm P_yU_TU_C^*\gamma^0\Psi(-x^0,x^i,y)$	$\Gamma_-U_{\mathrm{B}}\Gamma_-^{-1}=-U_{\mathrm{B}}$ $\Gamma_-=1_N\otimes\sigma_2$

corresponds to the irreducible blocks in the Hamiltonian for the gapped free-fermion system discussed in Sec. III A.

IV. INDEX AND ZERO MODES IN EACH SYMMETRY CLASS

From the correspondence of the boundary conditions in our model and the zero-dimensional gapped free-fermion system, we can obtain the nontrivial topological numbers $\mathbb{Z},\mathbb{Z}_2$ and $2\mathbb{Z}$ for the boundary conditions in each symmetry class as well as the topological insulators and superconductors in Table II for the $d=0$ case. In the topological matter side, the topological numbers specify the number of gapless states which appear on boundaries. Then, the question is what do these topological numbers physically mean in our model?

In this section, we will reveal that these topological numbers correspond to the numbers of zero modes localized at the vertex in our model as summarized in Table V. The topological numbers $\mathbb{Z}$ and $2\mathbb{Z}$ are related to the Witten index, which describes the number of chiral zero modes given in Sec. II D. By considering a sufficiently large number of the edges N, this number can take any integer values in the class A and AI and also any multiple of two in the class AII. The large N limit corresponds to taking an

TABLE V. Tenfold classification of the boundary conditions in our model. The sign ± 1 in the column of T and C denote the presence of $T_\pm$ and $C_\pm$, respectively and also 1 in Γ indicates the presence of the chiral symmetry Γ_+ or Γ_-, while 0 means the absence of corresponding symmetries. We also describe the Witten index for the type $(2N-k,k)$ BC in each symmetry class, which is equivalent to the number of the chiral zero modes in our model. In addition, $\mathbb{Z}_2$ in the column of the $\mathbb{Z}_2$ index indicates that the number of massless 4D Dirac fields in module 2 is topologically nontrivial, while 0 means topologically trivial and the number of massless 4D Dirac fields can be zero by continuous deformations of parameters. These correspond to the topological numbers in Table II for the $d=0$ case.

Class	T	C	Γ	Classifying space of U_{B}	Δ_{W} for type $(2N-k,k)$ BC	$\mathbb{Z}_2$ index
A	0	0	0	$C_0=\bigcup_{k=0}^{2N}\frac{U(2N)}{U(2N-k)\times U(k)}$	$N-k$	0
AIII	0	0	1	$C_1=U(N)$	0	0
AI	+1	0	0	$R_0=\bigcup_{k=0}^{2N}\frac{O(2N)}{O(2N-k)\times O(k)}$	$N-k$	0
BDI	+1	+1	1	$R_1=O(N)$	0	$\mathbb{Z}_2$
D	0	+1	0	$R_2=\frac{O(2N)}{U(N)}$	0	$\mathbb{Z}_2$
DIII	−1	+1	1	$R_3=\frac{U(N)}{U(N/2)}$	0	0
AII	−1	0	0	$R_4=\bigcup_{k=0}^{2N}\frac{Sp(N)}{Sp((2N-k)/2)\times Sp(k/2)}$	$N-k$ (N,k: even)	0
CII	−1	−1	1	$R_5=Sp(N/2)$	0	0
C	0	−1	0	$R_6=\frac{Sp(N)}{U(N)}$	0	0
CI	+1	−1	1	$R_7=\frac{U(N)}{O(N)}$	0	0

infinite number of bands in the zero-dimensional Hamiltonian. In addition, the topological number $\mathbb{Z}_2$ in the class BDI and D corresponds to the number of Dirac zero modes in module 2. Here we call it $\mathbb{Z}_2$ index. We will see that the $\mathbb{Z}_2$ index becomes topological invariant due to the additional degeneracy of the massive modes by the symmetry $\mathcal{C}_+$. We also investigate the classifying spaces of U_B in our model, which are the parameter spaces of U_B restricted by symmetry conditions, and show they are identical to the ones in the gapped free-fermion system.

A. Witten index and classifying spaces

Here, let us discuss the Witten index and the classifying space for each symmetry class in our model, and show the correspondence to the topological numbers $\mathbb{Z}$, $2\mathbb{Z}$ and the classifying spaces in the gapped free-fermion system. The $\mathbb{Z}_2$ index will be discussed in the next subsection.

1. Class A

Since the class A has no symmetries, there are no additional conditions for U_B. Therefore, U_B is diagonalized as follows (see Section II B):

$$U_\mathrm{B} = V\begin{pmatrix} 1_{2N-k} & 0 \\ 0 & -1_k \end{pmatrix}V^\dagger, \qquad V \in U(2N) \quad (k = 0, 1, \ldots, 2N). \tag{4.1}$$

The Witten index is determined by the number of the eigenvalues ± 1 of U_B, and is given by

$$\Delta_\mathrm{W} = N - k \ (k = 0, 1, \ldots, 2N). \tag{4.2}$$

By considering a sufficiently large N, the Witten index can take any integer and this corresponds to the topological number $\mathbb{Z}$.

In addition, the parameter space of U_B in the type $(2N - k, k)$ BC is $U(2N)/(U(2N-k)\times U(k))$ from the matrix V. Then we can obtain the classifying space of U_B as

$$C_0 = \bigcup_{k=0}^{2N} \frac{U(2N)}{U(2N-k)\times U(k)}. \tag{4.3}$$

This is also identical to the one for the zero-dimensional Hamiltonian in the gapped free-fermion system.

2. Class AIII

The class AIII has only the CS with the unitarity operator Γ for U_B which denotes Γ_+ or Γ_- given in Sec. III. This operator satisfies

$$\{U_\mathrm{B}, \Gamma\} = 0, \qquad \Gamma^2 = 1_{2N}. \tag{4.4}$$

This implies that the boundary vectors of the zero mode functions with the chiral operator $\Gamma\vec{F}_0^{(i)}(\Gamma\vec{G}_0^{(j)})$ satisfy the boundary condition of $\vec{G}_0^{(j)}(\vec{F}_0^{(i)})$. Therefore, if the CS is present, $\vec{F}_0^{(i)}$ and $\vec{G}_0^{(j)}$ have the same degrees of degeneracy, i.e. the equal degrees of freedom for i and j. For this reason, U_B should be diagonalized as

$$U_\mathrm{B} = V\begin{pmatrix} 1_N & 0 \\ 0 & -1_N \end{pmatrix}V^\dagger, \qquad V \in U(2N) \tag{4.5}$$

and the Witten index is given by

$$\Delta_\mathrm{W} = 0. \tag{4.6}$$

Γ can be taken to the diagonal form of $\tilde{\Gamma} = \sigma_3 \otimes 1_N$ by an appropriate basis change such as

$$U_\mathrm{B} \to \tilde{U}_\mathrm{B} = \tilde{V}^\dagger U_\mathrm{B}\tilde{V}, \tag{4.7}$$

$$\Gamma \to \tilde{\Gamma} = \tilde{V}^\dagger\Gamma\tilde{V}, \tag{4.8}$$

$$\vec{F}_n^{(i)} \to \tilde{V}^\dagger\vec{F}_n^{(i)}, \tag{4.9}$$

$$\vec{G}_m^{(j)} \to \tilde{V}^\dagger\vec{G}_m^{(j)}, \quad \tilde{V} \in U(2N). \tag{4.10}$$

In this basis, $\tilde{U}_\mathrm{B}$ is written as

$$\tilde{U}_\mathrm{B} = \begin{pmatrix} 0 & u_\mathrm{B} \\ u_\mathrm{B}^\dagger & 0 \end{pmatrix}, \qquad u_\mathrm{B} \in U(N) \tag{4.11}$$

from Eq. (4.4) and the conditions $U_\mathrm{B}^2 = 1_{2N}$ and $U_\mathrm{B}^\dagger = U_\mathrm{B}$. Therefore the parameter space of U_B is specified by u_B and then the classifying space is

$$C_1 = U(N). \tag{4.12}$$

3. Class AI

The class AI has the $\mathcal{T}_+$ symmetry and the additional condition for U_B is

$$T_+U_\mathrm{B}T_+^{-1} = U_\mathrm{B}, \qquad T_+ = \mathcal{K}. \tag{4.13}$$

This requires that U_B is a real matrix. Then U_B can be written as

$$U_\mathrm{B} = R\begin{pmatrix} 1_{2N-k} & 0 \\ 0 & -1_k \end{pmatrix}R^\top, \qquad R \in O(2N) \quad (k = 0, 1, \ldots, 2N). \tag{4.14}$$

Therefore, the Witten index and the classifying space are given by

$$\Delta_\mathrm{W} = N - k \qquad (k = 0, 1, \ldots, 2N), \tag{4.15}$$

$$R_0 = \bigcup_{k=0}^{2N} \frac{O(2N)}{O(2N-k)\times O(k)}, \tag{4.16}$$

respectively. The difference between the class A and AI is that U_{B} is a real matrix in this class. Therefore the mode functions can be taken to be real since the complex conjugation of the mode functions also satisfy the boundary condition and become solutions of Eqs. (2.12) and (2.13) with the same mass eigenvalues.

4. Class BDI

The class BDI has the three symmetries $\mathcal{T}_+, \mathcal{C}_+$, and $\mathcal{T}_+\mathcal{C}_+$. Then U_{B} satisfies

$$T_+U_{\mathrm{B}}T_+^{-1} = U_{\mathrm{B}}, \qquad T_+ = \mathcal{K}, \tag{4.17}$$

$$C_+U_{\mathrm{B}}C_+^{-1} = -U_{\mathrm{B}}, \qquad C_+ = (i\sigma_2\otimes 1_{N/2}\otimes i\sigma_2)\mathcal{K}, \tag{4.18}$$

$$\Gamma_+U_{\mathrm{B}}\Gamma_+^{-1} = -U_{\mathrm{B}}, \qquad \Gamma_+ = i\sigma_2\otimes 1_{N/2}\otimes i\sigma_2. \tag{4.19}$$

From the same discussion in the class AIII, the degeneracy of $\vec{F}_0^{(i)}$ and $\vec{G}_0^{(j)}$ are equal to each other due to Γ_+ and the Witten index becomes

$$\Delta_{\mathrm{W}} = 0. \tag{4.20}$$

Then let us discuss the classifying space. Here we focus on the operators T_+ and Γ_+ due to the relation $\Gamma_+ = T_+C_+$. Since Γ_+ is the real symmetric matrix, this can be diagonalized by a real orthogonal matrix. When we consider a basis change such that

$$\tilde{\Gamma}_+ = \tilde{V}^\top\Gamma_+\tilde{V} = \sigma_3\otimes 1_N, \tag{4.21}$$

$$\tilde{T}_+ = \tilde{V}^\top T_+\tilde{V} = \mathcal{K} \tag{4.22}$$

with the real orthogonal matrix $\tilde{V}$

$$\tilde{V} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1_N & 1_{N/2}\otimes\sigma_1 \\ -1_{N/2}\otimes i\sigma_2 & 1_{N/2}\otimes\sigma_3 \end{pmatrix}. \tag{4.23}$$

$\tilde{U}_{\mathrm{B}} = \tilde{V}^\top U_{\mathrm{B}}\tilde{V}$ is given by a real matrix and restricted to the form

$$\tilde{U}_{\mathrm{B}} = \begin{pmatrix} 0 & u_{\mathrm{B}} \\ u_{\mathrm{B}}^\top & 0 \end{pmatrix}, \qquad u_{\mathrm{B}}\in O(N) \tag{4.24}$$

by the conditions (4.17), (4.19) and $U_{\mathrm{B}}^\dagger = U_{\mathrm{B}}^\top$ and $U_{\mathrm{B}}^\dagger = U_{\mathrm{B}}$. Then we can see that the classifying space of U_{B} is given by

$$R_1 = O(N). \tag{4.25}$$

5. Class D

Since the class D has the $\mathcal{C}_+$ symmetry, the condition for U_{B} is

$$C_+U_{\mathrm{B}}C_+^{-1} = -U_{\mathrm{B}}, \qquad C_+ = (i\sigma_2\otimes 1_{N/2}\otimes i\sigma_2)\mathcal{K}. \tag{4.26}$$

First, let us diagonalize C_+ as

$$\tilde{C}_+ = \tilde{V}^\dagger C_+\tilde{V} = \mathcal{K}, \tag{4.27}$$

where

$$\tilde{V} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1_N & 1_{N/2}\otimes i\sigma_1 \\ -1_{N/2}\otimes i\sigma_2 & 1_{N/2}\otimes i\sigma_3 \end{pmatrix}. \tag{4.28}$$

In this basis, the condition $U_{\mathrm{B}}^\dagger = U_{\mathrm{B}}$ and Eqs. (4.26) and (4.27) imply that $\tilde{U}_{\mathrm{B}} = \tilde{V}^\dagger U_{\mathrm{B}}\tilde{V}$ can be of the form

$$\tilde{U}_{\mathrm{B}} = iA, \qquad A^\top = -A, \tag{4.29}$$

where A is a $2N\times 2N$ antisymmetric real matrix. Since any pure imaginary antisymmetric matrix has the same number of positive and negative eigenvalues, the Witten index is

$$\Delta_{\mathrm{W}} = 0. \tag{4.30}$$

Next, let us consider the classifying space in this class. In general, using a real orthogonal matrix R, we can bring the real antisymmetric matrix A into a block off-diagonal form:

$$A = R\begin{pmatrix} 0 & 1_N \\ -1_N & 0 \end{pmatrix}R^\top, \qquad R\in O(2N). \tag{4.31}$$

If there is a matrix R' which satisfies

$$R'\begin{pmatrix} 0 & 1_N \\ -1_N & 0 \end{pmatrix}R'^\top = \begin{pmatrix} 0 & 1_N \\ -1_N & 0 \end{pmatrix}, \qquad R'\in SO(2N), \tag{4.32}$$

the replacement $R\to RR'$ does not change the matrix A. Therefore the classifying space is given by the coset space, which is $O(2N)$ divided by the parameter space of R'. We mention that R' should have the determinant $\det R' = +1$ since this matrix also belongs to the symplectic group.[8] We can write R' as

[8]From the properties of the Pfaffian, we obtain

$$\mathrm{Pf}\left(R'\begin{pmatrix} 0 & 1_N \\ -1_N & 0 \end{pmatrix}R'^\top\right) = \det(R')\cdot\mathrm{Pf}\begin{pmatrix} 0 & 1_N \\ -1_N & 0 \end{pmatrix}.$$

Substituting Eq. (4.32) into the left-hand side of the above equation, we see that $\det R' = +1$.

$$R' = \exp\{1_2 \otimes X_0 + \sigma_2 \otimes X_2\}, \tag{4.33}$$

where X_0 is an antisymmetric real matrix and X_2 is a symmetric pure imaginary matrix. Since σ_2 can be diagonalized by the unitary matrix

$$G_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}, \qquad G_2^\dagger G_2 = G_2 G_2^\dagger = 1_2, \tag{4.34}$$

R' is given by

$$\begin{aligned} R' &= (G_2^\dagger \otimes 1_N)\exp\{1_2 \otimes X_0 + \sigma_3 \otimes X_2\}(G_2 \otimes 1_N) \\ &= (G_2^\dagger \otimes 1_N)\begin{pmatrix} \exp(X_0 + X_2) & 0 \\ 0 & \exp(X_0 - X_2) \end{pmatrix}(G_2 \otimes 1_N) \\ &\equiv (G_2^\dagger \otimes 1_N)\begin{pmatrix} r & 0 \\ 0 & r^* \end{pmatrix}(G_2 \otimes 1_N) \qquad (r \equiv \exp(X_0 + X_2)). \end{aligned} \tag{4.35}$$

Here r is a unitary matrix because it satisfies $r^\dagger r = 1_N$. Therefore, it turns out that R' is specified by an element of $U(N)$. Then the classifying space of U_{B} is

$$R_2 = \frac{O(2N)}{U(N)}. \tag{4.36}$$

6. Class DIII

The class DIII has the three symmetries $\mathcal{T}_-$, $\mathcal{C}_+$, and $\mathcal{T}_-\mathcal{C}_+$. Then U_{B} satisfies

$$T_- U_{\mathrm{B}} T_-^{-1} = U_{\mathrm{B}}, \qquad T_- = (i\sigma_2 \otimes 1_N)\mathcal{K}, \tag{4.37}$$

$$C_+ U_{\mathrm{B}} C_+^{-1} = -U_{\mathrm{B}}, \qquad C_+ = (i\sigma_2 \otimes 1_{N/2} \otimes i\sigma_2)\mathcal{K}, \tag{4.38}$$

$$\Gamma_- U_{\mathrm{B}} \Gamma_-^{-1} = -U_{\mathrm{B}}, \qquad \Gamma_- = 1_N \otimes \sigma_2. \tag{4.39}$$

Since the CS is present, the Witten index in this class should be zero, i.e.

$$\Delta_{\mathrm{W}} = 0. \tag{4.40}$$

T_- and Γ_- are anticommutative and we can take the basis

$$\tilde{\Gamma}_- = \tilde{V}^\dagger \Gamma_- \tilde{V} = \sigma_3 \otimes 1_N, \tag{4.41}$$

$$\begin{aligned} \tilde{T}_- &= \tilde{V}^\dagger T_- \tilde{V} = (\sigma_1 \otimes i\sigma_2 \otimes 1_{N/2})\mathcal{K} \\ &= \begin{pmatrix} 0 & (i\sigma_2 \otimes 1_{N/2})\mathcal{K} \\ (i\sigma_2 \otimes 1_{N/2})\mathcal{K} & 0 \end{pmatrix} \end{aligned} \tag{4.42}$$

by the unitary matrix $\tilde{V}$

$$\tilde{V} = W_{N\leftrightarrow 2}\frac{1}{\sqrt{2}}\begin{pmatrix} 1_N & 1_N \\ i1_N & -i1_N \end{pmatrix}. \tag{4.43}$$

Here we define the real orthogonal matrix $W_{n_a\leftrightarrow n_b}$ which exchanges the order of the direct product of an $n_a \times n_a$ matrix A and an $n_b \times n_b$ matrix B such that

$$W_{n_a\leftrightarrow n_b}^\top (A \otimes B) W_{n_a\leftrightarrow n_b} = B \otimes A, \tag{4.44}$$

$$W_{n_a\leftrightarrow n_b} = \sum_{i,\alpha} (\vec{e}_i \otimes \vec{E}_\alpha)(\vec{E}_\alpha^\top \otimes \vec{e}_i^\top), \tag{4.45}$$

$$\vec{e}_i^\top = (\underbrace{0, \ldots, 0}_{i-1}, 1, 0, \ldots, 0)^\top, \tag{4.46}$$

$$\vec{E}_\alpha^\top = (\underbrace{0, \ldots, 0}_{\alpha-1}, 1, 0, \ldots, 0)^\top \qquad (i = 1, \ldots, n_a,\ \alpha = 1, \ldots, n_b). \tag{4.47}$$

In this basis, $\tilde{U}_{\mathrm{B}} = \tilde{V}^\dagger U_{\mathrm{B}} \tilde{V}$ is restricted to the block off-diagonalized form

$$\tilde{U}_{\mathrm{B}} = \begin{pmatrix} 0 & u_{\mathrm{B}} \\ u_{\mathrm{B}}^\dagger & 0 \end{pmatrix}, \qquad u_{\mathrm{B}} u_{\mathrm{B}}^\dagger = 1_N,$$
$$(\sigma_2 \otimes 1_{N/2}) u_{\mathrm{B}}^\top (\sigma_2 \otimes 1_{N/2}) = u_{\mathrm{B}}. \tag{4.48}$$

Since u_{B} is a unitary matrix, it can be diagonalized as

$$u_{\mathrm{B}} = v^\dagger u_{\mathrm{d}} v, \quad u_{\mathrm{d}} = \begin{pmatrix} e^{i\alpha_1} & & 0 \\ & \ddots & \\ 0 & & e^{i\alpha_N} \end{pmatrix}, \quad v \in U(N),$$
$$\alpha_i \in \mathbb{R} \quad (i = 1, \ldots, N). \tag{4.49}$$

Substituting the first equation in (4.49) into the third equation in (4.48) with $J_y \equiv \sigma_2 \otimes 1_{N/2}$, we can get the relation

$$(vJ_y v^\top) u_{\mathrm{d}} = u_{\mathrm{d}} (vJ_y v^\top), \tag{4.50}$$

or equivalently

$$(vJ_yv^\top)_{ij}(u_\mathrm{d})_{jj} = (u_\mathrm{d})_{ii}(vJ_yv^\top)_{ij} \qquad (i,j=1,\ldots,N), \tag{4.51}$$

where i, j denote the indices of the matrix elements and are not summed up. This implies that $(u_\mathrm{d})_{ii} = (u_\mathrm{d})_{jj}$ if $(vJ_yv^\top)_{ij} \neq 0$. Then, by dividing both sides of the above equation by $u_\mathrm{d}^{1/2}$, we can also obtain the following relation:

$$(vJ_yv^\top)_{ij}\sqrt{(u_\mathrm{d})_{jj}} = \sqrt{(u_\mathrm{d})_{ii}}(vJ_yv^\top)_{ij}. \tag{4.52}$$

This relation is also trivially satisfied in the case of $(vJ_yv^\top)_{ij} = 0$. With this relation, u_B can be rewritten as

$$u_\mathrm{B} = w^\top J_y w J_y, \qquad w \equiv v^\top u_\mathrm{d}^{1/2} v^*. \tag{4.53}$$

By definition, w is an $N\times N$ unitary matrix. This w specifies the parameter space of u_B. We can find that u_B is invariant by the transformation

$$w \to gw \qquad (g^\dagger g = 1_N,\ g^\top J_y g = J_y). \tag{4.54}$$

Since g is an element of the symplectic group $Sp(N/2)$, the classifying space of U_B is given by

$$R_3 = \frac{U(N)}{Sp(N/2)}. \tag{4.55}$$

7. Class AII

The class AII has the $\mathcal{T}_-$ symmetry. The additional condition for U_B is

$$T_- U_\mathrm{B} T_-^{-1} = U_\mathrm{B}, \qquad T_- = (i\sigma_2 \otimes 1_N)\mathcal{K}. \tag{4.56}$$

Let $\vec{F}^{(i)}$ and $\vec{G}^{(j)}$ $(i,j=1,2,\ldots)$ are orthonormal eigenvectors with $U_\mathrm{B} = +1$ and $U_\mathrm{B} = -1$, respectively. From the above condition, the vectors $\vec{F}^{(i)}$ and $T_-\vec{F}^{(i)}$ (with the same index i) have the same eigenvalues $U_\mathrm{B} = +1$, and they are orthogonal to each other from the direct calculation. If we have a boundary vector $\vec{F}^{(j)} (i \neq j)$ which is orthogonal with $\vec{F}^{(i)}$ and $T_-\vec{F}^{(i)}$, $T_-\vec{F}^{(j)}$ is also orthogonal with them. Therefore, the number of the eigenvalue $U_\mathrm{B} = +1$ is even in this class. The same is true for the case of $\vec{G}^{(j)}$ and $T_-\vec{G}^{(j)}$, and the number of the eigenvalue $U_\mathrm{B} = -1$ is also even. Then, in the type $(2N-k, k)$ BC, the number k should be even. It should be noted that N is also even for the Q_y transformation in $\mathcal{T}_-$ to be well defined. Thus, the Witten index in this class is given by an even number:

$$\Delta_\mathrm{W} = N - k \qquad (k = 0,2,4,\ldots,N, N\colon \text{even}). \tag{4.57}$$

This corresponds to the topological number $2\mathbb{Z}$.

For the type $(2N-k, k)$ BC, we can rewrite U_B as

$$U_\mathrm{B} = V \begin{pmatrix} 1_{(2N-k)/2} & & & 0 \\ & -1_{k/2} & & \\ & & 1_{(2N-k)/2} & \\ 0 & & & -1_{k/2} \end{pmatrix} V^\dagger, \tag{4.58}$$

where the $2N\times 2N$ matrix V is a unitary matrix defined by

$$V = \left(\vec{F}^{(1)},\ldots,\vec{F}^{(\frac{2N-k}{2})},\vec{G}^{(1)},\ldots,\vec{G}^{(\frac{k}{2})},-T_-\vec{F}^{(1)},\ldots,-T_-\vec{F}^{(\frac{2N-k}{2})},-T_-\vec{G}^{(1)},\ldots,-T_-\vec{G}^{(\frac{k}{2})}\right). \tag{4.59}$$

This matrix is of the form

$$V = \begin{pmatrix} A & -B^* \\ B & A^* \end{pmatrix} \tag{4.60}$$

with $N\times N$ matrices A and B. Since V is a unitarity matrix, A and B must satisfy

$$A^\dagger A + B^\dagger B = 1_N, \tag{4.61}$$

$$-B^\top A + A^\top B = 0, \tag{4.62}$$

$$AA^\dagger + B^* B^\top = 1_N, \tag{4.63}$$

$$BA^\dagger - A^* B^\top = 0. \tag{4.64}$$

Then V satisfies

$$V^\top \begin{pmatrix} 0 & 1_N \\ -1_N & 0 \end{pmatrix} V = \begin{pmatrix} 0 & 1_N \\ -1_N & 0 \end{pmatrix}. \tag{4.65}$$

This implies that the matrix V is an element of the symplectic group $Sp(N)$. However there is redundancy left in this V. Let

$$g_i = \begin{pmatrix} A_i & -B_i^* \\ B_i & A_i^* \end{pmatrix} \tag{4.66}$$

be an element of $Sp(i)$ and we consider the matrix g which belongs to $Sp((2N-k)/2) \times Sp(k/2)$ such as

$$g = \begin{pmatrix} A_{(2N-k)/2} & 0 & -B^*_{(2N-k)/2} & 0 \\ 0 & A_{k/2} & 0 & -B^*_{k/2} \\ B_{(2N-k)/2} & 0 & A^*_{(2N-k)/2} & 0 \\ 0 & B_{k/2} & 0 & A^*_{k/2} \end{pmatrix}. \tag{4.67}$$

We find that U_B is invariant by the replacement $V \to Vg$. Therefore, the classifying space of U_B is given by the coset space

$$R_4 = \bigcup_{k=0}^{N} \frac{Sp(N)}{Sp((2N-k)/2) \times Sp(k/2)} \quad (N,k\text{:even}). \tag{4.68}$$

8. Class CII

The class CII has the three symmetries, $\mathcal{T}_-$, $\mathcal{C}_-$, and $\mathcal{T}_-\mathcal{C}_-$. Then U_B satisfies

$$T_- U_\mathrm{B} T_-^{-1} = U_\mathrm{B}, \qquad T_- = (i\sigma_2 \otimes 1_N)\mathcal{K}, \tag{4.69}$$

$$C_- U_\mathrm{B} C_-^{-1} = -U_\mathrm{B}, \qquad C_- = (1_N \otimes i\sigma_2)\mathcal{K}, \tag{4.70}$$

$$\Gamma_+ U_\mathrm{B} \Gamma_+^{-1} = -U_\mathrm{B}, \qquad \Gamma_+ = i\sigma_2 \otimes 1_{N/2} \otimes i\sigma_2. \tag{4.71}$$

Since the CS is present, the Witten index in the class CII is

$$\Delta_\mathrm{W} = 0. \tag{4.72}$$

When we take the basis

$$\tilde{\Gamma}_+ = \tilde{V}^\top \Gamma_+ \tilde{V} = \sigma_3 \otimes 1_N, \tag{4.73}$$

$$\begin{aligned} \tilde{T}_- &= \tilde{V}^\top T_- \tilde{V} = (1_2 \otimes i\sigma_2 \otimes 1_{N/2})\mathcal{K} \\ &= \begin{pmatrix} i\sigma_2 \otimes 1_{N/2} & 0 \\ 0 & i\sigma_2 \otimes 1_{N/2} \end{pmatrix}\mathcal{K}, \end{aligned} \tag{4.74}$$

$$\tilde{V} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1_{N/2} \otimes \sigma_3 & -1_{N/2} \otimes i\sigma_2 \\ 1_{N/2} \otimes \sigma_1 & 1_N \end{pmatrix} (1_2 \otimes W_{N/2\leftrightarrow 2}) \tag{4.75}$$

using the matrix $W_{N/2\leftrightarrow 2}$ defined by (4.45), $\tilde{U}_\mathrm{B} = \tilde{V}^\top U_\mathrm{B} \tilde{V}$ is of the form

$$\tilde{U}_\mathrm{B} = \begin{pmatrix} 0 & u_\mathrm{B} \\ u_\mathrm{B}^\dagger & 0 \end{pmatrix} \tag{4.76}$$

with the conditions

$$u_\mathrm{B}^\dagger u_\mathrm{B} = 1_N, \qquad u_\mathrm{B}^\top (\sigma_2 \otimes 1_{N/2}) u_\mathrm{B} = \sigma_2 \otimes 1_{N/2}. \tag{4.77}$$

This means that the matrix u_B is an element of the symplectic group $Sp(N/2)$. Therefore, the classifying space of U_B is given by

$$R_5 = Sp(N/2). \tag{4.78}$$

9. Class C

The class C has the $\mathcal{C}_-$ symmetry with the condition

$$C_- U_\mathrm{B} C_-^{-1} = -U_\mathrm{B}, \qquad C_- = (1_N \otimes i\sigma_2)\mathcal{K}. \tag{4.79}$$

Let $\vec{F}^{(i)} (i = 1, 2, \ldots)$ are orthonormal eigenvectors with $U_\mathrm{B} = +1$. Then we can find that $C_- \vec{F}^{(i)}$ has the opposite eigenvalue $U_\mathrm{B} = -1$ from the above condition. Therefore U_B has the same number of positive and negative eigenvalues, and the Witten index in this class is given by

$$\Delta_\mathrm{W} = 0. \tag{4.80}$$

Let us consider the basis change such as

$$\tilde{C}_- = \tilde{V}^\top C_- \tilde{V} = (i\sigma_2 \otimes 1_N)\mathcal{K}, \qquad \tilde{V} = W_{N\leftrightarrow 2}, \tag{4.81}$$

where $W_{N\leftrightarrow 2}$ is defined by (4.45). In this basis, we diagonalize the matrix $\tilde{U}_\mathrm{B} (= \tilde{V}^\top U_\mathrm{B} \tilde{V})$ as

$$\tilde{U}_\mathrm{B} = V \begin{pmatrix} 1_N & 0 \\ 0 & -1_N \end{pmatrix} V^\dagger, \tag{4.82}$$

where V is a $2N \times 2N$ unitary matrix which specifies the parameter space of U_B. By using the redundancy of V, the matrix can be given as follows:

$$V = (\tilde{V}\vec{F}^{(1)}, \ldots, \tilde{V}\vec{F}^{(N)}, -\tilde{C}_-\tilde{V}\vec{F}^{(1)}, \ldots, -\tilde{C}_-\tilde{V}\vec{F}^{(N)}). \tag{4.83}$$

From Eq. (4.81), V is of the form

$$V = \begin{pmatrix} A & -B^* \\ B & A^* \end{pmatrix} \tag{4.84}$$

with $N \times N$ matrices A and B. Repeating the same argument in the class AII, the matrix V defined in this way is an element of the symplectic group $Sp(N)$. Furthermore, Eq. (4.82) is invariant under the transformation

$$V \to V \begin{pmatrix} U & 0 \\ 0 & U^* \end{pmatrix}, \qquad U \in U(N). \tag{4.85}$$

Therefore, the classifying space of U_B is given by

$$R_6 = \frac{Sp(N)}{U(N)}. \tag{4.86}$$

10. Class CI

The class CI has the three symmetries, $\mathcal{T}_+$, $\mathcal{C}_-$, and $\mathcal{T}_+\mathcal{C}_-$. The additional conditions for U_B are

$$T_+ U_B T_+^{-1} = U_B, \qquad T_+ = \mathcal{K}, \tag{4.87}$$

$$C_- U_B C_-^{-1} = -U_B, \qquad C_- = (1_N \otimes i\sigma_2)\mathcal{K}, \tag{4.88}$$

$$\Gamma_- U_B \Gamma_-^{-1} = -U_B, \qquad \Gamma_- = 1_N \otimes \sigma_2. \tag{4.89}$$

Since the CS is present, the Witten index in the class CI is

$$\Delta_W = 0. \tag{4.90}$$

When we take the basis

$$\tilde{\Gamma}_- = \tilde{V}^\dagger \Gamma_- \tilde{V} = \sigma_3 \otimes 1_N, \tag{4.91}$$

$$\tilde{T}_+ = \tilde{V}^\dagger T_+ \tilde{V} = (\sigma_1 \otimes 1_N)\mathcal{K} = \begin{pmatrix} 0 & 1_N \cdot \mathcal{K} \\ 1_N \cdot \mathcal{K} & 0 \end{pmatrix} \tag{4.92}$$

with the unitary matrix $\tilde{V}$

$$\tilde{V} = W_{N\leftrightarrow 2} \frac{1}{\sqrt{2}} \begin{pmatrix} 1_N & 1_N \\ i1_N & -i1_N \end{pmatrix}, \tag{4.93}$$

the matrix $\tilde{U}_B = \tilde{V}^\dagger U_B \tilde{V}$ is given by

$$\tilde{U}_B = \begin{pmatrix} 0 & u_B \\ u_B^\dagger & 0 \end{pmatrix} u_B^\dagger u_B = 1_N, \qquad u_B^\top = u_B. \tag{4.94}$$

Since u_B is a unitary matrix, it can be diagonalized, using the unitary matrix v, as

$$u_B = v^\dagger u_d v, \qquad u_d = \begin{pmatrix} e^{i\alpha_1} & & 0 \\ & \ddots & \\ 0 & & e^{i\alpha_N} \end{pmatrix},$$
$$v \in U(N), \qquad \alpha_i \in \mathbb{R} \quad (i = 1, \dots, N). \tag{4.95}$$

From the relation $u_B^\top = u_B$, we obtain

$$(vv^\top) u_d = u_d (vv^\top), \tag{4.96}$$

or equivalently

$$(vv^\top)_{ij} (u_d)_{jj} = (u_d)_{ii} (vv^\top)_{ij}, \tag{4.97}$$

where i, j denote the indices of the matrix elements and are not summed up. If $(vv^\top)_{ij} \neq 0$, the above relation implies that $(u_d)_{ii} = (u_d)_{jj}$. Then, by dividing both sides of the above equation by $u_d^{1/2}$, we can also obtain the following relation:

$$(vv^\top)_{ij} \sqrt{(u_d)_{jj}} = \sqrt{(u_d)_{ii}} (vv^\top)_{ij}. \tag{4.98}$$

This relation is also trivially satisfied in the case of $(vv^\top)_{ij} = 0$. Using this relation, u_B can be rewritten as

$$u_B = w^\top w, \qquad w \equiv v^\top u_d^{1/2} v^*, \tag{4.99}$$

where w satisfies

$$ww^\dagger = 1_N. \tag{4.100}$$

This means the parameter space of u_B is specified by the unitary matrix w. However, Eq. (4.99) is invariant under the replacement

$$w \to gw, \qquad g \in O(N). \tag{4.101}$$

Therefore, the classifying space of U_B is given by

$$R_7 = \frac{U(N)}{O(N)}. \tag{4.102}$$

B. $\mathbb{Z}_2$ index

Finally, let us discuss the $\mathbb{Z}_2$ index, which is the number of Dirac zero modes in module 2.

The topological property of this index results from the degeneracy of massive mode functions due to the symmetry $\mathcal{C}_+$. As we have seen in Sec. III E 2, by the $\mathcal{C}_+$, the mode functions are transformed as follows:

$$f_n^{(i)}(y) \xrightarrow{\mathcal{C}_+} f_n^{\mathcal{C}_+(i)}(y) = Q_y P_y g_n^{(i)*}(y), \tag{4.103}$$

$$g_n^{(i)}(y) \xrightarrow{\mathcal{C}_+} g_n^{\mathcal{C}_+(i)}(y) = Q_y P_y f_n^{(i)*}(y). \tag{4.104}$$

Using Eqs. (2.10) and (2.11), we can show that the $f_n^{(i)}(y)$ and $f_n^{\mathcal{C}_+(i)}(y)$ with the same index i are orthogonal with each other for $n \neq 0$. Furthermore, if we have a massive mode $f_n^{(j)}(y) (i \neq j)$ which is orthogonal with $f_n^{(i)}(y)$ and $f_n^{\mathcal{C}_+(i)}(y)$, $f_n^{\mathcal{C}_+(j)}(y)$ is also orthogonal with them. This is also the same for $g_n^{(i)}(y)$. Therefore the degeneracy of the massive mode functions $f_n^{(i)}(y)$ and $g_n^{(i)}(y) (n \neq 0)$ with the symmetry $\mathcal{C}_+$ is always multiple of two respectively, and their mass eigenvalues move together by deformations of the parameters. On the other hand, zero mode functions $f_0^{(i)}(y)$ and $g_0^{(i)}(y)$ are not necessarily degenerate respectively (although the number of independent zero mode $f_0^{(i)}(y)$ and that of $g_0^{(i)}(y)$ are equal to each other by $\mathcal{C}_+$). Then, the number of massless Dirac fields $N_D (\equiv (N_{f_0} + N_{g_0})/2) \bmod 2$ is invariant by continuous deformations of the parameters in the boundary conditions as described in Fig. 8, and this index can be topologically nontrivial if the symmetry $\mathcal{C}_+$ is present.

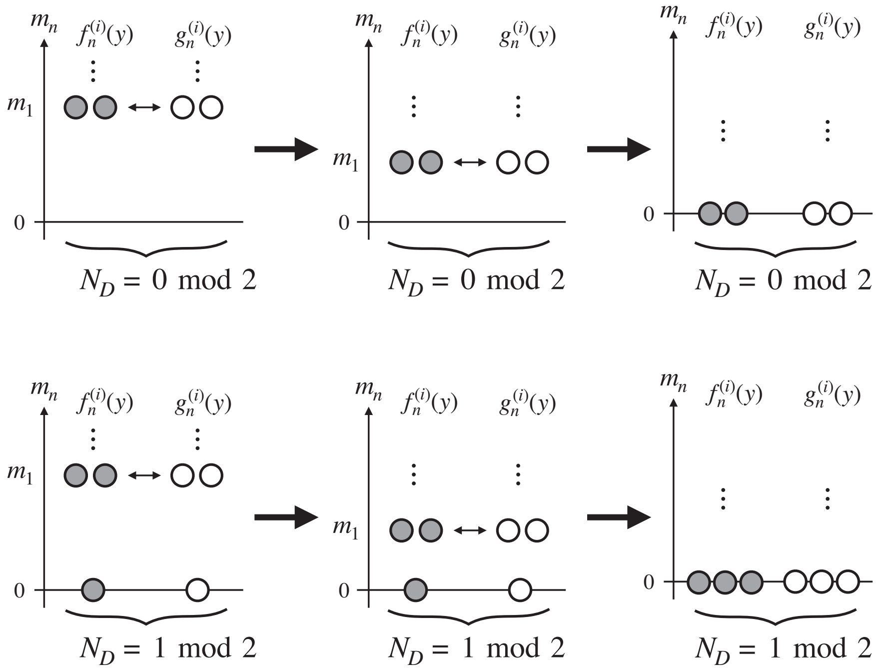

FIG. 8. The figures represent the change in the number of zero modes under continuous deformations of parameters with the symmetry $\mathcal{C}_+$. Comparing the top three figures with the bottom three figures, we can see that the number of massless Dirac fields N_D mod 2 is invariant.

In the following subsection, we confirm that the $\mathbb{Z}_2$ index becomes topologically nontrivial and take the $\mathbb{Z}_2$ values in the class D and BDI depending on the discontinuity of their classifying spaces, while it is topologically trivial in the other classes.

1. Class D

First, let us consider the case of the class D. Since this class has the $\mathcal{C}_+$ symmetry, there is a possibility that the $\mathbb{Z}_2$ index becomes topologically nontrivial. In this class, from the discussion in Sec. IV A 5, the matrix U_B can be written as follows:

$$U_\mathrm{B} = \tilde{V}R(-\sigma_2 \otimes 1_N)R^\top \tilde{V}^\dagger, \qquad R \in O(2N), \tag{4.105}$$

where

$$\tilde{V} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1_N & 1_{N/2} \otimes i\sigma_1 \\ -1_{N/2} \otimes i\sigma_2 & 1_{N/2} \otimes i\sigma_3 \end{pmatrix}. \tag{4.106}$$

The classifying space of this class is given by the disconnected space $O(2N)/U(N)$ from the matrix R and divided into two connected regions by $\det R = +1$ and $\det R = -1$. This determinant is related to the number of Dirac zero modes N_D. The result is

$$\det R = (-1)^{N_D}. \tag{4.107}$$

Therefore, $N_D = 0$ mod 2 for the parameter space with $\det R = +1$ and $N_D = 1$ mod 2 for the parameter space with $\det R = -1$. This is the topological invariant as discussed in the beginning of this subsection, and we can find that this index corresponds to the topological number $\mathbb{Z}_2$ of the 0th homotopy group of the classifying space.

To confirm this result, it is enough to see a simple example since this index is invariant by continuous deformations of parameters. Then, as an example, we take R as

$$R = \begin{pmatrix} 1_m \otimes \sigma_3 & & & \\ & 1_{N-2m} & & \\ & & 1_{2m} & \\ & & & 1_{N-2m} \end{pmatrix}$$
$$(m = 0, \ldots, N/2) \tag{4.108}$$

with $\det R = (-1)^m$. For this R, U_B is given by

$$U_\mathrm{B} = \left(\begin{array}{cc|cc} 0_{2m} & & 1_{2m} & \\ & 1_{N/2-m} \otimes \sigma_1 & & 0_{N-2m} \\ \hline 1_{2m} & & 0_{2m} & \\ & 0_{N-2m} & & 1_{N/2-m} \otimes \sigma_1 \end{array}\right). \tag{4.109}$$

Then the boundary condition (2.16) and (2.17) for the zero modes are written as

$$\left(\begin{array}{cc|cc} 1_{2m} & & -1_{2m} & \\ & 1_{N/2-m}\otimes(1_2-\sigma_1) & & 0_{N-2m} \\ \hline -1_{2m} & & 1_{2m} & \\ & 0_{N-2m} & & 1_{N/2-m}\otimes(1_2-\sigma_1) \end{array}\right)\begin{pmatrix} F_1^{(i)}e^{-M(L_0+\varepsilon)} \\ F_1^{(i)}e^{-M(L_1-\varepsilon)} \\ \vdots \\ F_N^{(i)}e^{-M(L_{N-1}+\varepsilon)} \\ F_N^{(i)}e^{-M(L_N-\varepsilon)} \end{pmatrix} = 0, \tag{4.110}$$

$$\left(\begin{array}{cc|cc} 1_{2m} & & 1_{2m} & \\ & 1_{N/2-m}\otimes(1_2+\sigma_1) & & 0_{N-2m} \\ \hline 1_{2m} & & 1_{2m} & \\ & 0_{N-2m} & & 1_{N/2-m}\otimes(1_2+\sigma_1) \end{array}\right)\begin{pmatrix} G_1^{(j)}e^{M(L_0+\varepsilon)} \\ -G_1^{(j)}e^{M(L_1-\varepsilon)} \\ \vdots \\ G_N^{(j)}e^{M(L_{N-1}+\varepsilon)} \\ -G_N^{(j)}e^{M(L_N-\varepsilon)} \end{pmatrix} = 0, \tag{4.111}$$

where the $F_a^{(i)}$ and $G_a^{(j)}$ $(a = 1, \ldots, N)$ are the coefficients in Eqs. (2.27) and (2.28). Here we assume that the bulk mass $M \neq 0$. Then the coefficients are given by

$$F_1^{(i)} = F_{N/2+1}^{(i)} e^{M(L_0-L_{N/2})}, \ldots, \qquad F_m^{(i)} = F_{N/2+m}^{(i)} e^{M(L_{m-1}-L_{N/2+m-1})}, \tag{4.112}$$

$$G_1^{(j)} = -G_{N/2+1}^{(j)} e^{-M(L_0-L_{N/2})}, \ldots, \qquad G_m^{(j)} = -G_{N/2+m}^{(j)} e^{-M(L_{m-1}-L_{N/2+m-1})}, \tag{4.113}$$

and the others vanish for the case of $M \neq 0$. Therefore, the independent coefficients are $F_1^{(i)}, \ldots, F_m^{(i)}$ and $G_1^{(i)}, \ldots, G_m^{(i)}$, and the number of independent zero mode functions is m for $f_0^{(i)}(i = 1, \ldots, m)$ and $g_0^{(j)}(j = 1, \ldots, m)$, respectively. Thus $N_D = m$ for the case of $M \neq 0$ and we can find that the relation (4.107) is satisfied. We also mention that we obtain $N_D = N - m$ Dirac zero modes for $M = 0$ unlike the case of $M \neq 0$. But the result (4.107) does not change since N is even in this class.

2. Class BDI

Next, we consider the class BDI. This class has the $\mathcal{T}_+$ symmetry in addition to $\mathcal{C}_+$. From the discussion in Sec. IV A 4, U_B can be written as follows:

$$U_\mathrm{B} = \tilde{V}\begin{pmatrix} 0 & u_\mathrm{B} \\ u_\mathrm{B}^\top & 0 \end{pmatrix}\tilde{V}^\top, \qquad u_\mathrm{B} \in O(N), \tag{4.114}$$

where

$$\tilde{V} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1_N & 1_{N/2}\otimes\sigma_1 \\ -1_{N/2}\otimes i\sigma_2 & 1_{N/2}\otimes\sigma_3 \end{pmatrix}. \tag{4.115}$$

We mention that if we restrict the matrix R in (4.105) as

$$R = \begin{pmatrix} u_\mathrm{B} & 0 \\ 0 & 1_N \end{pmatrix}, \tag{4.116}$$

Eq. (4.114) can be obtained.

The classifying space in this class is $O(N)$ specified by the matrix u_B and divided into two spaces by $\det u_\mathrm{B} = +1$ and $\det u_\mathrm{B} = -1$ disconnected with each other. By considering the same example in the class D, we obtain the following relation between this determinant and the number of Dirac zero modes N_D:

$$\det u_\mathrm{B} = (-1)^{N_D}. \tag{4.117}$$

Therefore, we see that the $\mathbb{Z}_2$ index in this class corresponds to the topological number $\mathbb{Z}_2$ of the 0th homotopy group of this classifying space.

3. The other classes

In the class DIII, the $\mathcal{T}_-$ symmetry is present in addition to $\mathcal{C}_+$. Under the $\mathcal{T}_-$ transformation, the mode functions are transformed as

$$f_n^{(i)}(y) \xrightarrow{\mathcal{T}_-} f_n^{\mathcal{T}_-(i)}(y) = Q_y f_n^{(i)*}(y), \tag{4.118}$$

$$g_n^{(i)}(y) \xrightarrow{\mathcal{T}_-} g_n^{\mathcal{T}_-(i)}(y) = Q_y g_n^{(i)*}(y). \tag{4.119}$$

Then we can show that the $f_n^{(i)}(y)(g_n^{(i)}(y))$ and $f_n^{\mathcal{T}_-(i)}(y)(g_n^{\mathcal{T}_-(i)}(y))$ with the same index i are orthogonal to each other for all n. Therefore this $\mathcal{T}_-$ symmetry leads to the twofold degeneracy of not only the massive modes but also zero modes like the Kramers degeneracy. Then the number of zero mode N_D mod 2 is always trivial in this class. Instead of the $\mathbb{Z}_2$ index, one may consider a fourfold degeneracy of massive mode functions by the combination of $\mathcal{T}_-$ and $\mathcal{C}_+$ and N_D mod 4 to become topologically nontrivial, but this is not the case since the fourfold degeneracy of massive modes does not generally hold. Actually, when we consider the boundary condition

$$U_\mathrm{B} = \left(\begin{array}{ccc|ccc} u_1 & & & & & \\ & \ddots & & & 0 & \\ & & u_{N/2} & & & \\ \hline & & & u_1 & & \\ & 0 & & & \ddots & \\ & & & & & u_{N/2} \end{array}\right), \tag{4.120}$$

$$u_a = \begin{pmatrix} \cos\theta_a & \sin\theta_a \\ \sin\theta_a & -\cos\theta_a \end{pmatrix}, \qquad \theta_a \in [0, 2\pi)$$
$$(a = 1, \ldots, N/2), \tag{4.121}$$

two Dirac zero modes appear for each θ_a which satisfies $\tan(\theta_a/2) = e^{-M(L_a - L_{a-1})}$. Then we find that the Dirac zero modes vanish by continuous deformations of the parameters $\theta_a (a = 1, \ldots, N/2)$, and thus it is topologically trivial.

We can also show that the $\mathbb{Z}_2$ index is trivial in the other classes since they have no symmetries which leads to the degeneracy only for massive modes.

V. SUMMARY AND DISCUSSION

In this paper, we studied 5D fermions of which extra dimension is on quantum graphs. We showed that the boundary conditions of the quantum graphs are classified into ten symmetry classes according to the presence or absence of time-reversal, charge conjugation, and extra-spatial symmetries of 5D fermions. The obtained symmetry classes are identical to the AZ symmetry classes of SPT phases of gapped free-fermion systems. A Hermitian matrix U_B specifying the boundary conditions corresponds to a 0d Hamiltonian of gapped free fermion systems. Furthermore, the constraints for U_B originating from symmetries of 5D fermions are the same as those for the 0d Hamiltonian with AZ symmetries. Based on these results, we introduced topological numbers for the boundary conditions in the same manner as those of 0d topological insulators and superconductors. Importantly, the topological numbers of the boundary conditions coincide with the number of KK 4D chiral or Dirac fermions localized at the vertex of quantum graphs, which would be a generalization of the bulk-boundary correspondence for gapped free-fermion systems.

Our classification implies that class A with no symmetries or class AI with the time-reversal symmetry is preferable for realizing the fermion flavor structure in the standard model. The nontrivial topological number $\mathbb{Z}$ in these classes may provide three generations of 4D chiral fermions.[9] To fully reproduce the standard model in our quantum graph approach, we must investigate gauge fields on quantum graphs. (Higgs bosons can be obtained by five-dimensional gauge fields.) Although Refs. [25–29] take into account gauge fields, they consider the only simple boundary conditions such as the Dirichlet and Neumann conditions. In general graphs, more involved boundary conditions are possible for gauge fields. The boundary conditions for gauge fields are related to those of fermions by 5D gauge symmetry since the 5D fermions after the gauge transformation should satisfy the same boundary condition, which restricts an allowed gauge parameter space. This restriction affects the 4D spectra of the gauge fields and can induce gauge symmetry breaking. We should also take care of the gauge anomalies due to the 4D chiral fermions, but our quantum graph approach is based on a 5D theory, so it should be anomaly free. The anomalies of 4D chiral fermions at the vertex of quantum graphs are canceled with the contributions of massive modes at the edges of quantum graphs by the anomaly inflow mechanism [41–43].

The key point in the classification of the boundary conditions for the 5D fermions is the existence of chiral spinors in four dimensions. The Hermiticity of the boundary matrix U_B originates from the independence of the left and right-handed chiral fields under the 4D Lorentz invariance. We expect that the same discussion works for general odd D-dimensional cases since chiral spinors exist in $D-1$ dimensions. In contrast, for even D-dimensions, we cannot apply the same discussions. In fact, the matrix for the boundary conditions is not generally Hermitian in even dimensions (See, e.g. [19]). We leave the extension of our results to other spacetime dimensions as a future problem. In particular, the investigations for lower dimensions would be important from the viewpoint of condensed matter physics.

We are also interested in the correspondence to SPT phases in other dimensions. So far, we have discussed the

[9] For example, Refs. [25–29] discuss the realization of the mass hierarchies and CP-violating phase by using the 1D extra space consisting of three line segments with the Dirichlet boundary conditions for fermions. This corresponds to the case with $|\Delta_W| = 3$, and thus three generations of 4D chiral fermions appear.

relation between the boundary conditions for quantum graphs and $1+0$d SPT phases for gapped free fermion systems, assuming that the 4D spacetime and the extra dimension are factorized, and the boundary conditions on the extra space do not have a 4D momentum dependence. However, if we consider the boundary conditions depending on the 4D momentum (or equivalently the 4D derivative), the boundary condition matrix would be regarded as a higher dimensional Hamiltonian, and thus we may obtain the correspondence to SPT phases in other dimensions.

Another future direction is the effect of interactions. So far, we have considered free fermions on quantum graphs. However, by considering interactions and also quantum corrections, the boundary conditions would be changed, and breakdowns of the topological phases may occur, which affects low-energy physics. For the topological matter side, it has been known that SPT phases of gapped free-fermion systems may break down by interactions preserving symmetries (see, e.g. [44–51]). For example, the $\mathbb{Z}$ classification of class BDI for 1D topological superconductor reduces to the $\mathbb{Z}_8$ classification if quartic interactions are present. We are interested in whether a similar breakdown occurs in the topological classification of boundary conditions. It is also known that interacting SPT phases in bulk can be characterized by perturbative and/or nonperturbative anomalies on boundary [42,52–55]. This is described by an anomaly inflow. Thus, it could be interesting to consider the boundary conditions from the viewpoint of anomalies. We hope to revisit these issues in the near future.

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