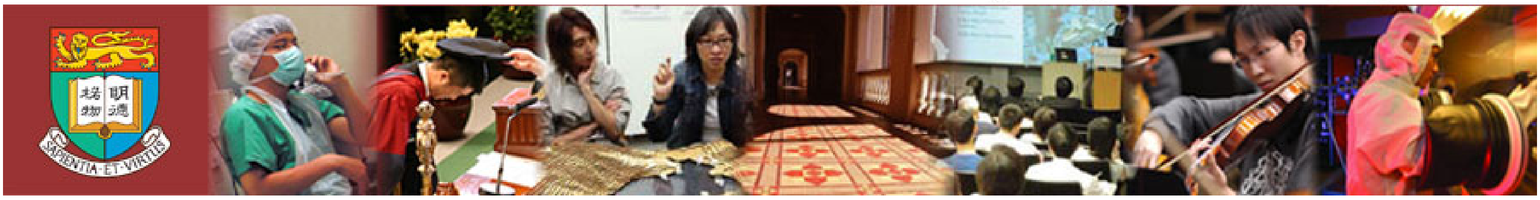

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Topological connection between the stability of Fermi surfaces and topological insulators and superconductors

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A topology-intrinsic connection between the stabilities of Fermi surfaces (FSs) and topological insulators/superconductors (TIs/TSCs) is revealed. First, through revealing the topological difference of the roles played by the time-reversal (or particle-hole) symmetry respectively on FSs and TIs/TSCs, a one-to-one relation between the topological types of FSs and TIs/TSCs is rigorously derived by two distinct methods with one relying on the direct evaluation of topological invariants and the other on K theory. Secondly, we propose and prove a general index theorem that relates the topological charge of FSs on the natural boundary of a TI/TSC to its bulk topological number. In the proof, FSs of all codimensions for all symmetry classes and topological types are systematically constructed by Dirac matrices. Moreover, implications of the general index theorem on the boundary quasiparticles are also addressed.

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I. INTRODUCTION

For the past several years, the research on topological insulators (TIs) and superconductors (TSCs) has greatly attracted both theoretical and experimental interests, which becomes a hot spot of contemporary physics [1,2]. As is known, a TI/TSC has a kind of nontrivial topology in its bulk band structure, preventing it from being deformed to an ordinary one without closing the energy spectrum gap in the bulk, and possesses robust gapless modes on its boundary against weak disorders and perturbations. Notably, all physical systems can be classified into ten classes by considering time-reversal (TRS), particle-hole (PHS), and chiral (CS) symmetries, which ubiquitously exist in physical systems and may be preserved in the presence of disorders from a viewpoint of random matrix theory [3–5]. Based on this, the restrictive effects of these symmetries on the bulk topology of a TI/TSC have been studied and a kind of complete classification for TIs/TSCs has been obtained using K theory to topologically classify the bulk configuration in momentum space directly [6,7] (or through checking whether eligible topological terms can exist on the surface of a TI/TSC responsible for robust gapless modes there [8–11]). According to a conventional wisdom, boundary gapless modes are originated from a fact that the boundary of a TI/TSC as a domain wall separates the system in different topological phases, with topological order-parameters being identified as the bulk topological numbers. As it is generally believed that there exists a faithful bulk-boundary correspondence [1,2,7–10,12], the above wisdom is practically useful, while it is likely to provide a qualitative insight on topology merely from the bulk to boundary, rather than a complete and quantitative description of this topological correspondence.

On the other hand, stimulated by Volovik's pioneering work on topological Fermi surfaces (FSs) without any antiunitary symmetry [13–15], a topological theory of FSs has recently been established for describing many-fermion systems with TRS or/and PHS, where a nontrivial topological charge of an FS with specific symmetries ensures its topological stability against symmetry-preserving weak disorders/perturbations and interactions [16,17]. Therefore, it is natural and insightful to look into directly the topological properties of boundary FSs of a TI/TSC and to reveal quantitatively their intrinsic connection to the bulk topology, particularly considering that the robustness of these gapless boundary modes may have the same topological origin as that of the bulk. This new sort of boundary-to-bulk insight on the topological essence of TIs/TSCs may further deepen our understanding of the bulk-boundary correspondence, supplementing the conventional one in a more efficient way because only information in the vicinity of FSs is actually needed to disclose the topological character.

This paper is organized as follows. In Sec. II, based on a well-established topological theory of FSs [16], we first derive a global-shift relation, Eq. (1), between the topological types of FSs and TIs/TSCs by means of two different methods: the direct evaluation of topological invariants and K theory. The former manifestly reveals that the shift is resulted from essentially different roles played by TRS(PHS) respectively on FSs and TIs/TSCs, while the latter is more formal by constructing mappings from FSs to TIs/TSCs. Actually, the classification of TIs/TSCs is repruduced by combining the classification of FSs and the global-shift relation. Intrigued by this relation, in Sec. III, we propose a general index theorem, Eq. (3), as a quantitive description for the topological boundary-bulk correspondence of TIs/TSCs, and prove it in the framework of Dirac-matrix construction. Moreover, we also address briefly the predictions and restrictions on the boundary low-energy effective theories of TIs/TSCs. Finally, a summary is presented in Sec. IV. Appendixes present technical details of relevant results in the main text and mathematical structures for constructing all types of FSs and TIs/TSCs. It is also noted that in Appendix C2, FSs of all codimensions for all symmetry classes and topological types in Table I are systematically constructed by Dirac matrices with their topological charges being explicitly computed.

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II. CLASSIFICATION RELATION BETWEEN FSS AND TIS/TSCS

Let us begin with a brief introduction to topological FSs. An FS is actually a region of fermionic gapless modes in the **k** space of energy spectrum. Some FSs are stable against disorders/perturbations, while some others are vulnerable and easy to be gapped [13]. It is found that the topological charge of an FS is responsible for its stability [13–16]. For a $(d_s - p)$-dimensional FS in a d_s-dimensional **k** space, we can choose a p-dimensional sphere S^p from $(\omega,\mathbf{k})$ space to enclose it from its transverse dimensions, where p is referred to as the codimension of the FS. Note that the spectrum is gapped on the whole S^p since the S^p is constructed in the transverse dimensions of an FS. For an FS without any discrete symmetry, its topological charge is given by the homotopy number of the inverse Green's function restricted on the S^p [13–15], i.e., $G^{-1}(\omega,\mathbf{k})|_{S^p} = [i\omega - \mathcal{H}(\mathbf{k})]|_{S^p}$. This idea has recently been generalized to FSs of the other classes for characterising the corresponding types of symmetry-dependent topological charges [16], as summarized in Table I (in a left-to-right manner), where the $\mathbf{Z}$, $2\mathbf{Z}$, $\mathbf{Z}_2^{(1)}$, and $\mathbf{Z}_2^{(2)}$ denote the integer topological charge, the even-integer topological charge, $\mathbf{Z}_2$-valued (integers of modular 2, i.e., 0 or 1) topological charge for the first descendant of a $\mathbf{Z}$ type, and $\mathbf{Z}_2$-valued topological charge for the second descendant of a $\mathbf{Z}$ type.

A. Derivation through topological invariants

We now derive the relation between the classification of FSs and that of TIs/TSCs, as indicated in Table I. First, It is crucial to observe that all six formulas for the topological charges of FSs can formally be used to calculate the topological numbers

TABLE I. Cartan classification of systems and topological classification of FSs [16] and TIs/TSCs. In the upper part of the table, T, C, and S denote TRS, PHS, and CS, respectively. 0 indicates the absence of the corresponding symmetry, ±1 indicates the sign of TRS or PHS, and 1 indicates the existence of CS. In the lower part, i is the index of symmetry classes, p is the codimension of an FS, and d is the spatial dimension of a TI/TSC. The elements $\mathbf{Z}$, $2\mathbf{Z}$, $\mathbf{Z}_2^{(1)}$, and $\mathbf{Z}_2^{(2)}$ in the above periodic (eightfold) table represent the corresponding topological types, respectively.

FS	AI	BDI	D	DIII	AII	CII	C	CI	TI/TSC
T	+1	+1	0	−1	−1	−1	0	+1	T
C	0	+1	+1	+1	0	−1	−1	−1	C
S	0	1	0	1	0	1	0	1	S
$p\backslash i$	1	2	3	4	5	6	7	8	i/d
1	0	0	$\mathbf{Z}$	$\mathbf{Z}_2^{(1)}$	$\mathbf{Z}_2^{(2)}$	0	$2\mathbf{Z}$	0	2
2	0	0	0	$\mathbf{Z}$	$\mathbf{Z}_2^{(1)}$	$\mathbf{Z}_2^{(2)}$	0	$2\mathbf{Z}$	3
3	$2\mathbf{Z}$	0	0	0	$\mathbf{Z}$	$\mathbf{Z}_2^{(1)}$	$\mathbf{Z}_2^{(2)}$	0	4
4	0	$2\mathbf{Z}$	0	0	0	$\mathbf{Z}$	$\mathbf{Z}_2^{(1)}$	$\mathbf{Z}_2^{(2)}$	5
5	$\mathbf{Z}_2^{(2)}$	0	$2\mathbf{Z}$	0	0	0	$\mathbf{Z}$	$\mathbf{Z}_2^{(1)}$	6
6	$\mathbf{Z}_2^{(1)}$	$\mathbf{Z}_2^{(2)}$	0	$2\mathbf{Z}$	0	0	0	$\mathbf{Z}$	7
7	$\mathbf{Z}$	$\mathbf{Z}_2^{(1)}$	$\mathbf{Z}_2^{(2)}$	0	$2\mathbf{Z}$	0	0	0	8
8	0	$\mathbf{Z}$	$\mathbf{Z}_2^{(1)}$	$\mathbf{Z}_2^{(2)}$	0	$2\mathbf{Z}$	0	0	9
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

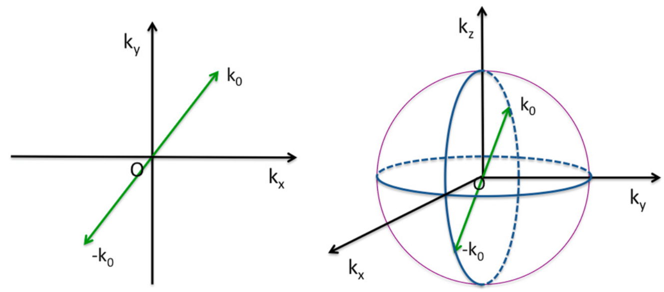

FIG. 1. (Color online) Symmetry identification. The left corresponds to a two-dimensional **k** space, and the right corresponds to an S^2 enclosing a Fermi point in a three-dimensional **k** space.

of TIs/TSCs, where we make the integration over the whole $(\omega,\mathbf{k})$ space in these formulas [2,19,20], instead of making it over S^p for an FS, as illustrated in Appendix A.

We emphasize here that the operation of TRS and PHS on the $(\omega,\mathbf{k})$ space of a TI/TSC is essentially different from that on an S^p for an FS, as shown in Fig. 1. If the symmetry operation is regarded as an identification, the resulting topological space of S^p for an FS is a p-dimensional projective space $RP(p)$ [21], while that of **k** space is not. This topological difference of symmetry operation leads to that the topological types of TIs/TSCs versus the dimension d have globally a one-dimension shift with respect to those of FSs versus the codimension p, i.e.,

$$K_{\mathrm{TI}}(d,i) = K_{\mathrm{FS}}(d-1,i), \tag{1}$$

where $K_{\mathrm{FS}}(p,i)$ and $K_{\mathrm{TI}}(d,i)$ denote, respectively, the topological types of FSs (with the codimension p) and TIs/TSCs (with the spatial dimension d) in the ith class. It is also noted that both the classifications of FSs and TIs/TSCs satisfy the elegant eightfold periodicity [6–10,16]:

$$K_{\Lambda}(p,i) = K_{\Lambda}(p+1,i+1), \tag{2}$$

where Λ is FS or TI, and both dimension and symmetry indexes are understood as modular eight.

Without loss of generality, we below consider class AII ($i = 5$) and highlight the key steps in the derivation of this relation. It is known that in the absence of any discrete symmetry, FSs with nontrivial topological charges can exist only when $p = 2n - 1$ with n being an integer [13,15], and TIs/TSCs can have nontrivial topological numbers only when $d = 2n$. After operations of the minus-sign TRS on S^p and $(\omega,\mathbf{k})$ space, with details in Appendix A, we obtain the following relations for FSs and TI/TSCs:

$$\nu_Z(2n+1,5) = (-1)^{n-1}\nu_Z(2n+1,5)$$
$$N_Z(2n,5) = (-1)^n N_Z(2n,5),$$

where $\nu_Z(p,i)$ and $N_Z(d,i)$ denote, respectively, the topological charge of an FS (with the codimension p) and the topological number of a TI/TSC (with the dimension d) in the ith class if they are of $\mathbf{Z}$ (or $2\mathbf{Z}$) type. It is found for class AII that nontrivial $\mathbf{Z}$ type (or $2\mathbf{Z}$ type) FSs can exist only when $p = 4m - 1$, while there are nontrivial $\mathbf{Z}$ type (or $2\mathbf{Z}$ type) TIs/TSCs only if $d = 4m$, where m is an integer. Since $\mathbf{Z}_2^{(1)}$ and $\mathbf{Z}_2^{(2)}$, as the first and second descendants of $\mathbf{Z}$, will follow $\mathbf{Z}$ successively when d is reduced, our remaining task is to fix the positions of $\mathbf{Z}$ and $2\mathbf{Z}$ for TIs/TSCs, which can be done for class AII as follows: noticing that FSs are of $\mathbf{Z}$ type when $p = 8(m-1)+3$, while TIs/TSCs, whose Hamiltonians can be constructed by Dirac matrices, possess unit topological number (i.e., $\mathbf{Z}$ type) for $d = 8(m-1)+4$ [19]. Thus we have $K_{\mathrm{TI}}(d,5) = K_{\mathrm{FS}}(d-1,5)$ by noting that the $2\mathbf{Z}$-type term should also exist for TIs/TSCs due to the same reason as that for FSs. Since similar derivations can be made for the other seven classes (not shown here), Eq. (1) is rigorously deduced and therefore the classification table of TIs/TSCs is established, as presented in Table I in a right-to-left manner.

An essentially same periodic table of TIs/TSCs was obtained before using K theory to topologically classify the bulk configurations in momentum space [6,7] or through checking whether eligible topological terms in the corresponding nonlinear sigma model can exist on the boundary of TIs/TSCs in the framework of random matrix theory [8–11]. Now from the above derivation, it is clear that all topological invariants for TIs/TSCs in Table I can be determined from the six formal formulas that we used to classify FSs. It is also noted that $\mathbf{Z}_2^{(1)}$ and $\mathbf{Z}_2^{(2)}$ are explicitly distinguishable types in our framework, which is different from that in previous studies and implies that they may correspond to different topologically protected behaviors, as will be seen in Sec. III B and in Ref. [22] about Majorana zero-modes at ends of one-dimensional superconductors.

B. Derivation through K theory

In the framework of K theory, the topological type of an FS or a TI/TSC with a given symmetry class and dimension corresponds to a K group [6,7]. Now we proceed to a more formal proof of Eq. (1) by constructing isomorphisms between K groups of FSs and those of TIs/TSCs. We will construct mappings from the Green's functions of FSs with codimension $p = 1$ in ith class to Hamiltonians of one-dimensional TIs/TSCs in class $(i-1)$th class. Since these mappings are invertible in a homotopic sense, the desired isomorphisms are established. For FSs with codimension $p = 1$, in $(\omega,\mathbf{k})$ space, we choose a S^1 to enclose the FS, where the Green's function is parametrized as

$$G_{(i)}^{-1}(\phi) = ia\cos\phi - \mathcal{H}_{\mathrm{FS}}^{(i)}(a\sin\phi),$$

where a is the radius of the chosen S^1 and $\phi \in [-\pi,\pi)$ (we simply set $a = 1$ hereafter). The operations of TRS and PHS on $\mathcal{H}_{\mathrm{FS}}^{(s)}$ are

$$T\mathcal{H}_{\mathrm{FS}}^{(i)}(\sin\phi)T^\dagger = \mathcal{H}_{\mathrm{FS}}^{(i)T}(\sin(-\phi))$$
$$C\mathcal{H}_{\mathrm{FS}}^{(i)}(\sin\phi)C^\dagger = -\mathcal{H}_{\mathrm{FS}}^{(i)T}(\sin(-\phi))\,.$$

In a viewpoint of K theory, the classification of FSs with codimension $p = 1$ is to compute the corresponding K group for each class.

We first construct a mapping for FSs without chiral symmetry, i.e., $i = 2n$, which reads

$$G_{(2n)}^{-1}(\phi) \longrightarrow \mathcal{H}_{\mathrm{TI}}^{(2n-1)}(\phi) = \mathcal{H}_{\mathrm{FS}}^{(2n)}(\sin\phi)\otimes\tau_z + \cos\phi\otimes\tau_\alpha,$$

where $\alpha = x$ (or y) depending on whether the $2n$-th class has TRS (or PHS). Here the $\mathcal{H}_{\mathrm{TI}}^{(2n-1)}$ corresponds a TI/TSC in the $(2n-1)$th class. This is justified by regarding ϕ as a momentum coordinate and the two facts: (i) the original TRS(PHS) is preserved by the mapping; and (ii) the new Hamiltonian has an additional PHS(TRS) $T\otimes\tau_y$ $(C\otimes\tau_x)$.

For FSs with chiral symmetry, i.e., $i = 2n+1$, we consider another mapping:

$$G_{(2n+1)}^{-1}(\phi) \longrightarrow \mathcal{H}_{\mathrm{TI}}^{(2n)}(\phi) = \mathcal{H}_{\mathrm{FS}}^{(2n+1)}(\sin\phi) + \mathcal{K}\cos\phi,$$

where $\mathcal{K}$ represents the chiral symmetry. The first term preserves the original TRS and PHS, but the second one breaks one of them depending on $\eta = \eta_T\eta_C$ with $\eta_T(\eta_C)$ being the sign of the TRS(PHS) in Table I, since $\mathcal{K}\sim C^\dagger T$ and $(C^\dagger T)^T = \eta T C^\dagger$. It is verified case by case that $\mathcal{H}_{\mathrm{TI}}^{(2n)}(\phi)$ is a one-dimensional TI/TSC in the $2n$-th class.

As a result, the desired mappings from FSs with codimension $p = 1$ in ith class to one-dimensional TIs/TSCs in $(i-1)$th class have been established, which leads to K-group homomorphisms:

$$K_{\mathrm{FS}}(s,1) \longrightarrow K_{\mathrm{TI}}(s-1,1).$$

Noting that the invertibility of these mappings in a homotopic sense can be proven by Mose theory [7], we thus have

$$K_{\mathrm{FS}}(s,1) = K_{\mathrm{TI}}(s-1,1).$$

Combining it with the eightfold periodicity, Eq. (2), the above equation just leads to the global dimension-shift relation, Eq. (1).

III. GENERAL INDEX THEOREM

It has been known from many examples that the boundary gapless modes of a given TI/TSC with one (or more) above symmetry are robust against disorders/perturbations that do not break the corresponding symmetry. This implies that the FSs corresponding to these gapless modes are actually protected by their nontrivial topological charge with the same symmetry class according to a theory of topologically stable FSs [16], while such robustness can also be attributed to a nontrivial topological number of bulk. Therefore we attempt to find a quantitative relation between the topological number N of a bulk TI/TSC and the topological charge ν of its boundary FSs. Let us consider a d-dimensional semi-infinite TI/TSC of a symmetry class i with a boundary being at $x = 0$ on its left-side. Under the natural boundary condition of the TI/TSC, i.e., no dramatic anisotropy is induced and the symmetries in the ith class are preserved when the system approaches to its boundary, FSs on the boundary will always be some Fermi points in a topological sense. This conclusion is obviously valid for $d = 1,2$. In addition, its validity can also be extended to TIs/TSCs for $d > 2$ [23]. As a result, the boundary codimension $p = d-1$. Then by appropriately choosing an S^{d-1} in the $(\omega,\mathbf{k})$ space of the boundary to enclose all the FSs, we are able to compute the total topological charge $\nu(d-1,i)$ of all FSs. Therefore, from Eq. (1), which enables the same type of nontrivial topological charge of boundary FSs and bulk number to protect the FSs, we may expect a general index theorem as a quantitive topological description of the boundary-bulk correspondence of a TI/TSC:

$$\nu(d-1,i) = N(d,i). \tag{3}$$

Clearly, the above equation reflects essentially that the same topological origin protects the stability of the boundary FSs and the gapped feature of bulk spectrum against disorders/perturbations. We note that Eq. (3) accounts for the earlier statements for classification of TIs/TSCs based on the random-matrix theory by assuming certain boundary topological terms in a nonlinear σ model [8–10], and reveals that the bulk topology can also be quantified by the topological charge of boundary FSs. More remarkably, comparing with some existing results in the literature [24–27], where merely some specific index theorems with various forms for several concrete models or a few symmetry types are addressed or argued, we here have rigorously established a complete topological theory of the bulk-boundary correspondence for all TGSs in a unified simple equation, which seems highly nontrivial and has a significant impact. Moreover, our general index theorem (3) reveals also the topological stabilities of boundary modes against disorders/perturbations in the framework of an established topological theory for FSs.

To see Eq. (3) more clearly, we first present two typical examples, with the proof to be given later. Firstly, we note that detailed calculations of the topological charges in the examples below can be found in Appendix B. Consider a three-dimensional TI described by the Dirac-lattice model [19], i.e., $\mathcal{H}_D = \sum_{i=1}^{3} \sin k_i \Gamma^{i+2} + (3 + \sum_{i=1}^{3} \cos k_i)\Gamma^1$ with $\Gamma_i (i = 1,\ldots,5)$ being 4×4 Hermitian Dirac matrices [28] and $T = \Gamma^1\Gamma^3$. This model has TRS with a minus sign and thus may have a nontrivial $\mathbf{Z}_2^{(1)}$ type, as seen from Table I ($d = 3$). On the other hand, its boundary effective model reads $\mathcal{H} = k_z\sigma_2 - k_y\sigma_3$ with σ_i being Pauli matrices [27], which preserves the same TRS and has a Fermi point with codimension $p = 2$. One can find that $\nu(2,5) = 1 = N(3,5)$, verifying Eq. (3). Similarly, another two-dimensional model, which describes the quantum spin Hall effect, is given by $\mathcal{H}_{\text{spin}} = \sum_{i=1}^{2} \sin k_i \Gamma^{i+3} + (3 + \sum_{i=1}^{2} \cos k_i)\Gamma^1$. It has also TRS with a minus sign and therefore belongs to class AII with a $\mathbf{Z}_2^{(2)}$-type topological number. Its boundary effective Hamiltonian is $\mathcal{H} = \sigma_z k_z$, which has a Fermi point ($p = 1$) with the same $\mathbf{Z}_2^{(2)}$-type topological charge. We can also find that $\nu(1,5) = 1 = N(2,5)$.

A. A proof of the general index theorem

At this stage, we turn to brief readers the proof of the general index theorem expressed by Eq. (3), with full details being presented in Appendix C. First, it is seen from the topological nature of a TI/TSC that the total topological charge of FSs on its boundary and the topological number of its bulk are both invariant under a continuous symmetry-preserving deformation of its Hamiltonian without closing the bulk spectrum gap. Secondly, it is noted that Hamiltonian of each type of FS (point) for a given codimension p and class i with a unit charge (or double-unit charge for $2\mathbf{Z}$ type) can be expressed by Dirac matrices in a unified form:

$$\mathcal{H}_{\text{FS}}(\mathbf{k}) = \sum_{a=1}^{p} k_a \Gamma^{a+b}_{(2n+1)}, \tag{4}$$

where $\Gamma^a_{(2n+1)}$ are $2^n \times 2^n$ Dirac matrices, and b is an integer that is specified by the corresponding topological type of the FS. Here, we pinpoint that in Appendix C2, FSs of all codimensions in all topological types and symmetry classes are first systematically constructed by Dirac matrices with their topological charges being explicitly computed.

Thirdly, a modified Dirac-type model for each type of bulk TI/TSC with unit topological number(or double-unit for $2\mathbf{Z}$ type) can also be constructed in a unified form:

$$\mathcal{H}_{\text{TI}}(\mathbf{k}) = \sum_{a=1}^{d} k_a \Gamma^{a+b-1}_{(2n+1)} + (m - \epsilon k^2)\Gamma^{\alpha}_{(2n+1)}, \tag{5}$$

where ϵ is a constant, $\Gamma^\alpha = i\Gamma^1\Gamma^2\Gamma^3$ for $2\mathbf{Z}$ cases and $\Gamma^\alpha = \Gamma^1$ otherwise. Note that ϵ term is necessary for a prescription of the singularity of $\mathcal{H}_{\text{TI}}$ when k approaches to infinity [13]. Note that the construction of TIs/TSCs using Dirac matrices has been systematically studied in literatures [8,29,30]. This model has a unified expression of the topological number for all types of TIs/TSCs:

$$N(d,i) = (1 \text{ or } 1/2)\,[\mathbf{sgn}(m) + \mathbf{sgn}(\epsilon)]\,, \tag{6}$$

where the coefficient is 1 for $2\mathbf{Z}$ cases, and 1/2 otherwise. Next, we proceed to consider an arbitrarily given TI/TSC in a certain type with the topological number $N(d,i)$, which can be deformed continuously to a model that is N multiple [or for $2\mathbf{Z}$ cases, $(N/2)$ multiple] of the model (5), preserving the corresponding symmetries and without closing the bulk spectrum gap. After this deformation, both the bulk topological number and the total topological charge of boundary FSs are preserved, as indicated above [31], and therefore it is sufficient to consider the unit model (5) for proof of Eq. (3). The advantage of this deformation lies in that the boundary low-energy effective theory of the model (5) can be systematically derived by using a standard perturbation theory of quantum mechanics under the open boundary condition, see Appendix C. After some tedious derivations detailed in Appendix C, the boundary effective theory of the model (5) turns out to be

$$\mathcal{H}_{\text{eff}} = \frac{1}{2}\,[\mathbf{sgn}(m) + \mathbf{sgn}(\epsilon)] \sum_{a=2}^{d} k_a \Gamma^{a+b-3}_{(2n-1)}, \tag{7}$$

for the boundary at $x = 0$. Note that the symmetries of the system are now represented in the boundary effective theory (7). By matching the symmetry representation of the theory (7) to that of our constructed model (4), we find that not only the topological charge of Fermi point in the boundary effective theory (7) is equal to the topological number of the model (5), but also the topological type of the FS is the same as that of the bulk model (5), namely, the general index theorem is validated.

B. Topological implications on boundary effective theories

Before concluding this paper, we address briefly implications of Eq. (3) on the form of a boundary effective theory with a given bulk topological number. Based on the Atiyah-Bott-Singer (ABS) construction in K theory and a fact that an FS of multiple charge can be perturbed to a more stable state consisting of a number of unit FSs [15,32,33], we assert that a typical low-energy effective theory of boundary for a **Z** type TI/TSC is a collection of $\sum_{i=1}^{2n+1} k_i\Gamma^i_{(2n+1)}$ for nonchiral cases or $\sum_{i=1}^{2n} k_i\Gamma^i_{(2n+1)}$ for chiral cases, with the total topological charge being equal to the bulk topological number. On the other hand, for $\mathbf{Z}_2^{(1,2)}$ type TIs/TSCs, the constraint from ABS construction is not as strong as that of the above cases, while the constraint on $\mathbf{Z}_2^{(1)}$ type is stronger than that on $\mathbf{Z}_2^{(2)}$ type, since the latter needs one more extra parameter. Nevertheless, a boundary effective theory can still be constructed by Dirac matrices, whose expression is not uniquely determined. For instance, $\mathcal{H} = k_z\sigma_3 + \alpha k_z^{(2n+1)} + \beta k_z^{(2m+1)}$ and $\mathcal{H} = k_z^3\sigma_3 + \alpha k_z^{(2n+1)} + \beta k_z^{(2m+1)}$ are both eligible as the boundary effective theory of a quantum spin hall system.

IV. SUMMARY

In summary, the topology-intrinsic connection between the stabilities of FSs and TIs/TSCs has been revealed. The relation between the classification of FSs and that of TIs/TSCs has been revealed both through using topological invariants to clarify the topologically different roles played by TRS and PHS on FSs and TIs/TSCs, respectively, and through establishing isomorphisms between K groups of FSs and those of TIs/TSCs. Furthermore, we have proposed and proven a general index theorem, providing a quantitive description of the bulk-boundary correspondence of TIs/TCSs. In the proof, all kinds of FSs are constructed systematically by Dirac matrices with their topological charges being explicitly calculated. It is anticipated that the present work will also provide a deeper insight and open a wider door for exploring exotic boundary gapless modes of TIs/TSCs such as Majorana fermions [22].

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APPENDIX A: DERIVATION OF EQ. (1) THROUGH TOPOLOGICAL INVARIANTS

In the derivation, the first key point is that for a $\mathcal{H}(\mathbf{k})$ with either TRS or PHS, the symmetries can be preserved on the S^p if it is chosen to be centrosymmetric with respect to the origin of $(\omega,\mathbf{k})$ space. Secondly, It is crucial to observe that all six formulas for the topological charges of FSs can formally be used to calculate the topological numbers of TIs/TSCs, where we make the integration over the whole $(\omega,\mathbf{k})$ space, instead of making it over S^p for an FS.

The topological difference of symmetry identification plays an essential role in the derivation of the topological classification table of TIs/TSCs. In practical calculations for FSs, we use the following spherical coordinates for the chosen S^{p-1},

$$\begin{aligned}
k_1 &= \cos s_1\\
k_2 &= \sin s_1 \cos s_2\\
k_3 &= \sin s_1 \sin s_2 \cos s_3\\
&\vdots\\
k_{p-1} &= \sin s_1 \sin s_2 \cdots \sin s_{p-2} \cos s_{p-1}\\
k_p &= \sin s_1 \sin s_2 \cdots \sin s_{p-2} \sin s_{p-1}
\end{aligned} \tag{A1}$$

with $s_i \in [0,\pi]$ for $i = 1,2,\ldots,p-2$ and $s_{p-1} \in [0,2\pi)$. Without loss of generality, we have assumed that the FS is a Fermi point with codimension p in a $(p+1)$-dimensional $(\omega,\mathbf{k})$ space. In the following, we focus on the class AII as an illustration, which has only TRS with $\eta_T = -1$, while other seven classes can be treated in the same way and results are the same. The TRS on the chosen S^{p-1} with the spherical coordinates can be represented as

$$T^\dagger \mathcal{H}(s) T = \mathcal{H}^T(\pi - s_1, \ldots, \pi - s_{p-2}, \pi + s_{p-1}).$$

Note that the transformation of s_{p-1} is different from those of the others. Correspondingly, Green's function $G(\omega,\mathbf{k}) = [i\omega - \mathcal{H}(\mathbf{k})]^{-1}$ is transformed as

$$T^\dagger G(\omega,s) T = G^T(\omega,\pi - s_1,\ldots,\pi - s_{p-2},\pi + s_{p-1}). \tag{A2}$$

While the Green's function for a TI in the class AII satisfies

$$T^\dagger G(\omega,\mathbf{k}) T = G^T(\omega,-\mathbf{k}). \tag{A3}$$

It is seen that that all **k**s of the TI/TSC reverse the signs under the TRS transformation, which is in contrast to the situation of the chosen S^{p-1} enclosing an FS where the last coordinate s_{p-1} does not reverse its sign. We first illustrate how TRS makes the **Z**-type topological charge of an FS with codimension $p = 4m+1$ vanishing. The formula for the **Z**-type topological charge with codimension $p = 2n+1$ is given by

$$\begin{aligned}
&\nu(2n+1,5)\\
&= C_{2n+1}\int_{S^p} d\omega d^{2n}s\, \epsilon^{\mu_1\mu_2\cdots\mu_{2n+1}}\\
&\quad\times \mathbf{tr}(G\partial_{\mu_1}G^{-1}G\partial_{\mu_2}G^{-1}\cdots G\partial_{\mu_{2n+1}}G^{-1}(\omega,s)),
\end{aligned} \tag{A4}$$

where $C_{2n+1} = -n!/(2n+1)!(2\pi i)^{n+1}$. Implementing the TRS transformation, i.e., Eq. (A2), and the coordinate substitution $s_i' = \pi - s_i$ with $i = 1,2,\ldots,2n-1$ and $s_{2n}' = \pi + s_{2n}$, we have

$$\begin{aligned}
&\nu(2n+1,5)\\
&= -C_{2n+1}\int_{S^p} d\omega d^{2n}s'\, \epsilon^{\mu_1'\mu_2'\cdots\mu_{2n+1}'}\\
&\quad\times \mathbf{tr}(G^T\partial_{\mu_1'}G^{T-1}\cdots G^T\partial_{\mu_{2n+1}'}G^{T-1}(\omega,s'))\\
&= C_{2n+1}\int_{S^p} d\omega d^{2n}s\, \epsilon^{\mu_1\mu_2\cdots\mu_{2n+1}}\\
&\quad\times \mathbf{tr}(G\partial_{\mu_{2n+1}}G^{-1}G\partial_{\mu_{2n}}G^{-1}\cdots G\partial_{\mu_1}G^{-1}(\omega,s)).
\end{aligned} \tag{A5}$$

Making a permutation that reverses the order of all the indices of ϵ, we obtain

$$\nu(2n+1,5) = (-1)^{n-1}\nu(2n+1,5), \tag{A6}$$

where the extra $(-1)^n$ comes from the permutation. Now it is clear that when $n = 2m$ with m being an integer, i.e.,

$p = 4m + 1$, the **Z**-type topological charge of an FS is vanished for the class AII. For the corresponding case of TIs, the procedure is almost the same. First, the integral form of topological number is the same as Eq. (A4), but the integration is made over the whole $(\omega,\mathbf{k})$ space:

$$\begin{aligned} N(2n,5) &= C_{2n+1}\int d\omega d^{2n}k\, \epsilon^{\mu_1\mu_2\cdots\mu_{2n+1}} \\ &\quad\times \mathbf{tr}(G\partial_{\mu_1}G^{-1}G\partial_{\mu_2}G^{-1}\cdots G\partial_{\mu_{2n+1}}G^{-1}(\omega,\mathbf{k})). \end{aligned}\tag{A7}$$

In a similar way to the case of FS, we make the variable substitution $\mathbf{k}' = -\mathbf{k}$, matrix transposition, and then a permutation to reverse all the indices of ϵ. The only difference is that when substituting the variables, we could not obtain an extra minus sign as that in the second equality of Eq. (A5), since the number of partial derivatives of k_i is even. Thus we have

$$N(2n,5) = (-1)^n\, N(2n,5),\tag{A8}$$

which implies the topological number of a TI with $d = 4m + 2$ in the class AII is always trivial, but that with $d = 4m$ can be nontrivial.

Comparing Eq. (A3) with Eq. (A6), we see clearly a one-dimension shift from $K_{\mathrm{FS}}(p,5)$ to $K_{\mathrm{TI}}(d,5)$. From the established classification table of FSs in class AII, we know that a sole but minor remaining uncertainty is whether the topological types of TIs for $d = 8m + 4$ are **Z** or 2**Z**, which can surely be fixed by examining an appropriately chosen case. Since the Dirac model of $d = 4$ can have a unit topological charge belonging to **Z** type, the topological charges for $d = 8m + 4$ is of **Z** type, and thus $K_{\mathrm{FS}}(d-1,5) = K_{\mathrm{TI}}(d,5)$. The same results are obtained for the other seven classes due to the same reason. Thus we show rigorously that $K_{\mathrm{FS}}(d-1,i) = K_{\mathrm{TI}}(d,i)$, which reflects the topological difference between the **k** space and the chosen S^{p-1} to enclose an FS when the symmetry class is concerned.

APPENDIX B: TOPOLOGICAL CHARGE OF FERMI POINTS ON THE BOUNDARY OF TOPOLOGICAL INSULATORS

1. Topological charge of the Fermi point on the boundary of three-dimensional topological insulator

The boundary effective theory for a three-dimensional topological insulator reads

$$\mathcal{H}(\mathbf{k}) = k_y\sigma_1 - k_x\sigma_2 + \alpha(k_x + k_y)\sigma_3,$$

where the term $\alpha(k_x + k_y)\sigma_3$ merely indicates that the Hamiltonian in the class AII allows such term, which will turn out to be irrelevant for the topological charge of the Fermi point. This Hamiltonian has a TRS with sign $-$, i.e., see Ref. [16],

$$\mathcal{H}(\mathbf{k}) = \sigma_2\mathcal{H}^T(-\mathbf{k})\sigma_2^{-1},\quad \sigma_2^T = -\sigma_2.$$

It belongs to the class AII. The Fermi surface is the point $\mathbf{k} = 0$ with the codimension 2. According to Ref. [16], we can calculate its $\mathbf{Z}_2^{(1)}$-topological charge from Eq. (6) there. In order to do this, we choose an S^2 in the $(\omega,\mathbf{k})$ space enclosing the Fermi point, and make the following continuous extension of the Green's function restricted on the S^2:

$$\begin{aligned} G^{-1} &= i\omega - \Delta\sigma_3\sin\theta \\ &\quad - [k\sin\phi\sigma_1 - k\cos\phi\sigma_2 + k(\cos\phi + \sin\phi)\sigma_3]\cos\theta, \end{aligned}$$

where $\phi \in [0,2\pi]$ parametrizes the circle in the **k**-space enclosing the Fermi surface, $\theta \in [0,\pi/2]$ is the parameter for extension, and Δ is a positive constant. Substituting this Green's function into Eq. (6) in Ref. [16], we obtain

$$\begin{aligned} \nu(2,5) &= \frac{1}{12\pi^2}\int d\omega d\phi d\theta\, \epsilon^{\mu\nu\lambda} \\ &\quad\times \mathbf{tr}(G\partial_\mu G^{-1}G\partial_\nu G^{-1}G\partial_\lambda G^{-1}) \\ &= \frac{1}{2\pi}\int_0^{2\pi} d\phi\int_0^{\frac{\pi}{2}} d\theta\ \frac{1}{|g|^3}\mathbf{g}\cdot(\partial_\theta\mathbf{g}\times\partial_\phi\mathbf{g}), \end{aligned}$$

with

$$\begin{aligned} \mathbf{g} = (&k\sin\phi\cos\theta, \\ &-k\cos\phi\cos\theta, k(\cos\phi + \sin\phi) + \Delta\sin\theta). \end{aligned}$$

For simplicity, setting $\alpha = k = \Delta = 1$, we obtain

$$\nu(2,5) = \frac{1}{2\pi}\int_0^{2\pi} d\phi\int_0^{\frac{\pi}{2}} d\theta\ \frac{n(\theta,\phi)}{m(\theta,\phi)} = 1,$$

where

$$n(\theta,\phi) = \cos\theta$$

and

$$\begin{aligned} m(\theta,\phi) = \{&\sin^2\theta + \sin(2\theta)(\cos\phi + \sin\phi) \\ &+ \cos^2\theta[2 + \sin(2\phi)]\}^{\frac{3}{2}}. \end{aligned}$$

It is then found that a nontrivial $\mathbf{Z}_2^{(1)}$ topological charge $\nu(2,5) = 1$, which is equal to $N(3,5)$ obtained before.

2. Topological charge of the Fermi point on the boundary of quantum spin Hall systems

For the boundary of a quantum spin Hall system, the effective boundary theory can be written as

$$\mathcal{H}(k_x) = k_x\sigma_1 + \alpha k_x\sigma_2 + \beta k_x\sigma_3,\tag{B1}$$

where the last two terms preserving TRS will turn out to be irrelevant for the topological charge. When we choose a circle in the (ω,k_x) plane, the Green's function restricted on this circle is given by

$$G^{-1}(\psi) = ia\sin\psi - \mathcal{H}(a\cos\psi)$$

with $\psi \in [0,2\pi)$. Noting that TRS for the Green's function is $TG(\omega,k)T^\dagger = G^T(\omega,-k)$, this TRS is accordingly represented as $\sigma_2 G(\psi)\sigma_2 = G(\pi - \psi)$ on the circle. Then following Ref. [16], we extend the Green's function restricted on the circle with two additional parameters, i.e.,

$$\begin{aligned} G^{-1}(\psi,\theta,\phi) = ia\sin\psi - [(&\mathcal{H}(a\cos\psi)\cos\theta + \sin\theta\sigma_2)\cos\phi \\ &+ \sin\phi\sigma_3] \end{aligned}$$

with $\theta \in [0,\pi]$ and $\phi \in [0,\pi]$. It is straightforward to verify that TRS is preserved for this extension:

$$\sigma_2 G\,(\psi,\theta,\phi)\,\sigma_2 = G^T\,(\pi - \psi, -\theta, -\phi)\,.$$

The $\mathbf{Z_2}^{(2)}$-type topological charge is calculated as

$$\nu(1,5) = \frac{1}{24\pi^2}\int d\psi d\theta d\phi \epsilon^{\mu\nu\lambda} \times \mathbf{tr}(G\partial_\mu G^{-1} G\partial_\nu G^{-1} G\partial_\lambda G^{-1}), = 1,$$

which equals to $N(2,5)$ calculated before.

APPENDIX C: DIRAC MATRIX CONSTRUCTION OF FSS AND TIS/TSCS AND THE PROOF OF GENERAL INDEX THEOREM

1. Preliminaries of Dirac matrices

The purpose of this section is to introduce the preliminaries about Dirac matrices needed for our construction of topologically protected FSs and TI/TSCs. As for a pedagogical introduction to Dirac matrices, it is seen in Ref. [34]. Although most results may be basis-independent, we still introduce explicitly our convention of Dirac matrices below.

$$\begin{aligned}\Gamma^a_{(2n+1)} &= \Gamma^a_{(2n-1)} \otimes \sigma_1, \quad a = 1,2,3,\ldots,2n-1,\\ \Gamma^{2n}_{(2n+1)} &= \mathbf{1}_{2^{n-1}} \otimes \sigma_2,\\ \Gamma^{2n+1}_{(2n+1)} &= \mathbf{1}_{2^{n-1}} \otimes \sigma_3,\end{aligned} \tag{C1}$$

where σ_i are Pauli matrices and $\mathbf{1}_{2^{n-1}}$is the $2^{n-1}\times 2^{n-1}$unit matrix. We input the initial condition: $\Gamma^1_{(3)} = \sigma_1, \Gamma^2_{(3)} = \sigma_2$ and $\Gamma^3_{(3)} = \sigma_3$, to obtain Dirac matrices in all dimensions. Notably, Γ matrices with odd superscript are purely real, while ones with even superscript are purely imaginary. All Dirac matrices are hermitian, and satisfy the Clifford algebra:

$$\left\{\Gamma^a_{(2n+1)}, \Gamma^b_{(2n+1)}\right\} = 2\delta^{ab}\mathbf{1}_{2^n\times 2^n}. \tag{C2}$$

We will construct Hamiltonians by Dirac matrices and discuss their TRS and PHS. For this purpose, we introduce the following operators:

$$\begin{aligned}B^1_{(2n+1)} &:= \Gamma^3_{(2n+1)}\Gamma^5_{(2n+1)}\cdots\Gamma^{2n+1}_{(2n+1)},\\ B^2_{(2n+1)} &:= \Gamma^2_{(2n+1)}\Gamma^4_{(2n+1)}\cdots\Gamma^{2n}_{(2n+1)},\\ \tilde{B}^1_{(2n+1)} &:= B^1_{(2n+1)}\Gamma^{2n+1}_{(2n+1)},\\ \tilde{B}^2_{(2n+1)} &:= B^2_{(2n+1)}\Gamma^{2n+1}_{(2n+1)}.\end{aligned} \tag{C3}$$

It is direct to verify the following commutation relations below:

$$\begin{aligned}&B^1_{(2n+1)}\Gamma^a_{(2n+1)}\left(B^1_{(2n+1)}\right)^{-1}\\ &\quad= \begin{cases}(-1)^{n+1}\left(\Gamma^a_{(2n+1)}\right)^T, & a = 2,\ldots,2n+1\\ (-1)^n\left(\Gamma^1_{(2n+1)}\right)^T\end{cases},\\ &B^2_{(2n+1)}\Gamma^a_{(2n+1)}\left(B^2_{(2n+1)}\right)^{-1}\\ &\quad= (-1)^n\left(\Gamma^a_{(2n+1)}\right)^T, \quad a = 1,2,\ldots,2n+1.\end{aligned} \tag{C4}$$

The transposition matrices of B^1, B^2, $\tilde{B}^1$, and $\tilde{B}^2$ satisfy, respectively,

$$\begin{aligned}B^1_{(2n+1)} &= (-1)^{n(n-1)/2}\left(B^1_{(2n+1)}\right)^T,\\ B^2_{(2n+1)} &= (-1)^{n(n+1)/2}\left(B^2_{(2n+1)}\right)^T,\\ \tilde{B}^1_{(2n+1)} &= -(-1)^{n(n+1)/2}\left(\tilde{B}^1_{(2n+1)}\right)^T,\\ \tilde{B}^2_{(2n+1)} &= (-1)^{n(n-1)/2}\left(\tilde{B}^2_{(2n+1)}\right)^T.\end{aligned} \tag{C5}$$

2. Construction of all topological types of Fermi surfaces

a. Fermi surfaces in nonchiral classes AI, AII, D, and C

$\mathbf{Z}$ *and* $\mathbf{Z}_2^{(1,2)}$. The simplest way to construct a Hamiltonian with Dirac matrices is to make Weyl-type Hamiltonian, namely,

$$\mathcal{H}^W_{(2n+1)}(\mathbf{k}) = \sum_{a=1}^{2n+1} k_a\Gamma^a_{(2n+1)}. \tag{C6}$$

This Hamiltonian has either TRS or PHS depending on its spatial dimension $2n+1$. To be explicit, the Hamiltonian satisfies

$$B^2_{(2n+1)}\mathcal{H}^W_{(2n+1)}(\mathbf{k})\left(B^2_{(2n+1)}\right)^{-1} = (-1)^{n+1}\left(\mathcal{H}^W_{(2n+1)}\right)^T(-\mathbf{k}), \tag{C7}$$

which can be seen from Eq. (C5). B^2 represents a TRS with $n = 2m+1$ or a PHS with $n = 2m$, where m is an integer or zero, and the corresponding symmetry sign is given by Eq. (C5). This Hamiltonian has a Fermi point at the origin of $\mathbf{k}$ space, whose codimension is $p = 2n+1$. The Fermi point is in classes AI, AII, D, and C, respectively, for $p = 8m+7$, $8m+3$, $8m+1$, and $8m+5$, which precisely coincides with that of $\mathbf{Z}$-type topological charge for the same class in the classification table of Fermi surfaces (Table I in the main text).

Our next task is to show that this Fermi point has a unit $\mathbf{Z}$-type topological charge. It can be enclosed by a cylinder $A := (-\infty,\infty)\times S^{2n}$ in $(\omega,\mathbf{k})$ space with S^{2n} centered at the origin of $\mathbf{k}$ space and ω being in $(-\infty,\infty)$. We parametrize the Green's function on this cylinder A as

$$G^{-1}|_A(\omega,\mathbf{k}) = i\omega - k_a(s)\Gamma^a_{(2n+1)},$$

where $k_a(s)$ are the same as those defined in Eq. (A1) with $p = 2n+1$. For the Green's function, the cylinder A is essentially a topological $(2n+1)$-dimensional sphere S^{2n+1} since G^{-1} tends to a constant matrix when ω approaches to $\pm\infty$. To compute its topological charge, we make the following integral on the cylinder with Eq. (C2):

$$\begin{aligned}\nu &= C_{2n+1}\int_A (G\mathbf{d}G)^{2n+1}\\ &= (2n+1)C_{2n+1}\int_{-\infty}^{\infty} d\omega\int_{S^{2n}} d^{2n}s\ \epsilon^{\mu_1\mu_2\cdots\mu_{2n}}\\ &\quad\times \mathbf{tr}(G\partial_\omega G^{-1} G\partial_{\mu_1}G^{-1}\cdots G\partial_{\mu_{2n}}G^{-1})\\ &= \frac{1}{2^{n-1}\Omega_{2n+1}}\int_{S^{2n}} d^{2n}s\ \frac{1}{|\mathbf{n}|^{2n+1}}\epsilon^{\mu_1\mu_2\cdots\mu_{2n+1}}\epsilon^{\nu_1\nu_2\cdots\nu_{2n}}\\ &\quad\times n_{\mu_1}\partial_{\nu_1}n_{\mu_2}\partial_{\nu_2}n_{\mu_3}\cdots\partial_{\nu_{2n}}n_{\mu_{2n+1}}\\ &= 1\end{aligned} \tag{C8}$$

with Ω_{2n+1} being the total solid angle of $(2n+1)$-dimensional space. Now it is clear that all Fermi points of unit topological charge with either a TRS or PHS can be constructed by the Dirac matrices in the form of Eq. (C6). Note that we can construct an N-charged Fermi point for each case simply by multiplying the unit Hamiltonian N times for $\mathbf{Z}$ types, or the double-unit models (to be constructed latter) $N/2$ times for $2\mathbf{Z}$ types. This also holds for $\mathbf{Z}$-type and $2\mathbf{Z}$-type TIs/TSCs with multiple topological numbers, which will not be repeated any more.

We now turn to construct FSs protected by $\mathbf{Z}_2^{(1,2)}$ type topological charge. According to our general classification table, each $\mathbf{Z}$ type topological charge is followed by $\mathbf{Z}_2^{(1)}$ and $\mathbf{Z}_2^{(2)}$ with decreasing codimensions, which motivates us to construct corresponding models by lowering spatial dimensions, i.e., the number of ks from the Weyl-type model (C6). For $\mathbf{Z}_2^{(1)}$ cases, we consider the following model:

$$\mathcal{H}_W^{(1)} = \sum_{a=1}^{2n} k_a \Gamma^{a+1} + \lambda \sum_{a=1}^{2n} k_a \Gamma^1, \tag{C9}$$

where the last term with a coefficient λ is added to merely indicate that the considered model, while keeping TRS or PHS with the topological character unchanged, may not need to have an additional CS. We may set $\lambda = 0$ without changing the topological property of the Fermi point at $k = 0$. For brevity, we have dropped the awkward subscript $(2n+1)$ in the above expression and will do it hereafter if it can be recovered from the context. To calculate the $\mathbf{Z}_2^{(1)}$ type topological charge of the Fermi point, we first choose an S^{2n-1} in $\mathbf{k}$ space, which is parametrized by the spherical coordinates s_i with $i = 1,2,\ldots,2n-1$, and restrict the Hamiltonian on it, i.e., $\mathcal{H}_W^{(2)}|_{S^{2n-1}} = \mathcal{H}_W^{(2)}(s)$. According to the formulation of $\mathbf{Z}_2^{(1)}$ type topological charge, we make a one-parameter extension of $\mathcal{H}_W^{(2)}(s)$, which may be chosen as

$$\mathcal{H}(s,\alpha) = \mathcal{H}(s)\cos\alpha + \sin\alpha\Gamma^1,$$

with $\alpha \in [-\pi/2,\pi/2]$. It is straightforward to check that this extension satisfies all the requirements [16]. Using the extended Green's function $G^{-1}(\omega,s,\alpha) = i\omega - \mathcal{H}(s,\alpha)$, we compute the topological charge as

$$\nu = C_{2n+1} \int_{\tilde{A}} \mathbf{tr}(G\mathbf{d}G^{-1}(\omega,s,\alpha))^{2n+1},$$

where $\tilde{A} = A \times S^1$ with A being the original domain $(-\infty,\infty) \times S^{2n-1}$ in $(\omega,\mathbf{k})$ space. After replacing the variable α with $\alpha' = \alpha + \pi/2$, we are able to treat α as the $2n$-th spherical coordinate of S^{2n} made by S^{2n-1} and the extended dimension. Thus referring to our calculation of $\mathbf{Z}$ type topological charge, we find that $\nu = 1 \mod 2$, which means that the Fermi point at $k = 0$ for model (C9) is nontrivial.

With the experience of constructing nontrivial $\mathbf{Z}_2^{(1)}$ type topological charge, we now give the following model as a candidate for $\mathbf{Z}_2^{(2)}$:

$$\mathcal{H}_W^{(2)} = \sum_{a=1}^{2n-1} k_a \Gamma^{a+2} + \lambda_1 \sum_{a=1}^{2n-1} k_a \Gamma^1 + \lambda_2 \sum_{a=1}^{2n-1} k_a^3 \Gamma^2, \tag{C10}$$

where analogous to the previous case, terms with $\lambda_{1,2}$ are added to mean that the model does not require additional symmetries, and again they may be set as zero without changing the topological property of the Fermi point. To see the topological property of the Fermi point, we choose an S^{2n-2}, which is parametrized with a spherical coordinates s_i with $i = 1,2,\ldots,2n-2$, in $\mathbf{k}$ space to enclose it. The Hamiltonian restricted on the S^{2n-2} is denoted by $\mathcal{H}_W^{(2)}(s)$, and then according to the formulation of $\mathbf{Z}_2^{(2)}$ type topological number, we make two-parameter extension of $\mathcal{H}_W^{(2)}(s)$, which may be written as

$$\mathcal{H}_W^{(2)}(s,\alpha,\beta) = \left(\mathcal{H}_W^{(2)}(s)\cos\alpha + \sin\alpha\Gamma^1\right)\cos\beta + \sin\beta\Gamma^2,$$

where $\alpha,\beta \in [-\pi/2,\pi/2]$. The above extension satisfies all the requirements for computing the topological charge of the Fermi point [16]. Using the extended Green's function $G^{-1}(\omega,s,\alpha,\beta) = i\omega - \mathcal{H}_W^{(2)}(s,\alpha,\beta)$, we have the topological charge as

$$\nu = C_{2n+1} \int_{\tilde{\tilde{A}}} \mathbf{tr}(G\mathbf{d}G^{-1}(\omega,s,\alpha,\beta)),$$

where $\tilde{\tilde{A}} = A \times T^2$ with $A = [-\infty,\infty] \times S^{2n-2}$ and T^2 being the domain of α and β. Through the variable transformation: $\alpha' = \alpha + \pi/2$ and $\beta' = \beta + \pi/2$, we can combine T^2 and S^{2n-2} as S^{2n}. Thus the Fermi point has nontrivial topological charge $\nu = 1 \mod 2$.

$2\mathbf{Z}$ *type.* To construct $2\mathbf{Z}$ type Fermi surface in our classification table, we introduce the following operator:

$$\mathcal{B}^1 = \Gamma^2\Gamma^5\Gamma^7\cdots\Gamma^{2n+1},$$

which is a modified version of B^1 with Γ^3 being replaced by Γ^2. $\mathcal{B}^1$ satisfies

$$\mathcal{B}^1 = -(-1)^{n(n-1)/2}(\mathcal{B}^1)^T \tag{C11}$$

and

$$\begin{cases} \mathcal{B}^1\Gamma^a\left(\mathcal{B}^1\right)^{-1} = (-1)^{n+1}\left(\Gamma^a\right)^T, & 4 \leqslant a \leqslant 2n+1 \\ \mathcal{B}^1\tilde{\Gamma}\left(\mathcal{B}^1\right)^{-1} = (-1)^{n+1}\tilde{\Gamma}^T \end{cases} \tag{C12}$$

with $\tilde{\Gamma} = i\Gamma^1\Gamma^2\Gamma^3$. We construct the model as

$$\mathcal{H}_W^2(\mathbf{k}) = \sum_{a=2}^{2n-1} k_a \Gamma_{(2n+1)}^{a+2} + \tilde{\Gamma}_{(2n+1)} k_1. \tag{C13}$$

As $\mathcal{H}_W^2$ can be diagonalized into two equivalent $2^{n-1} \times 2^{n-1}$ blocks since $[\mathcal{H}_W^2, i\Gamma^1\Gamma^2] = 0$, up to a unitary transformation it can rewritten as

$$\mathcal{H}_W^2(\mathbf{k}) \sim \begin{pmatrix} \sum_{a=1}^{2n-1} k_a \Gamma_{(2n-1)}^a & \\ & \sum_{a=1}^{2n-1} k_a \Gamma_{(2n-1)}^a \end{pmatrix}.$$

Since each block has unit $\mathbf{Z}$ type topological charge, the Fermi point of $\mathcal{H}(\mathbf{k})$ has topological charge 2. We then analyze its TRS and PHS by using Eq. (C12), which leads to

$$\mathcal{B}^1\mathcal{H}_W^2(\mathbf{k})(\mathcal{B}^1)^{-1} = (-1)^n \mathcal{H}_W^{2T}(-\mathbf{k}).$$

Thus based on the relation Eq. (C11) and the above relation, we summarize that the Fermi point is in class AI, AII, D, and C, respectively, for the codimension $p = 8m+3, 8m+7, 8m+5$, and $8m+1$.

b. Fermi surfaces in chiral classes CI, CII, DIII, and BDI

$\mathbf{Z}$ *type and* $\mathbf{Z}_2^{(1,2)}$ *type.* To handle the remaining four symmetry classes with chiral symmetry (CS), we construct the Dirac-type Hamiltonian as

$$\mathcal{H}_D(\mathbf{k}) = \sum_{a=1}^{2n} k_a \Gamma^a. \tag{C14}$$

In other words, we sum over all Γs except the last one, which leads to CS, i.e.,

$$\{\mathcal{H}_D, \Gamma^{2n+1}\} = 0.$$

As is known that this Hamiltonian has a TRS(PHS) represented by B^2 just like that of $\mathcal{H}^W$, using $\Gamma^{2n+1}_{(2n+1)}$ we are able to newly construct a PHS(TRS), which is represented by $\tilde{B}^2 = B^2\Gamma^{2n+1}$ as in Eq. (C3). It is verified that

$$\begin{aligned}\tilde{B}^2\mathcal{H}_D(\mathbf{k})(\tilde{B}^2)^{-1} &= -B^2\mathcal{H}_D(\mathbf{k})(B^2)^{-1}\\ &= (-1)^n(\mathcal{H}_D(-\mathbf{k}))^T.\end{aligned}$$

Compared with Eq. (C7), if B^2 refers to a TRS, then $\tilde{B}^2$ refers to a PHS, and vice versa. The sign of $\tilde{B}^2$ as a TRS/PHS can be seen from Eq. (C5). As the codimension of the Fermi point for the Hamiltonian of Eq. (C14) is $2n$, the Fermi point is in class CI, DIII, BDI, and CII respectively when $p = 8m + 6$, $8m + 2$, $8m$, and $8m + 4$, which is in agreement with the appearance of $\mathbf{Z}$-type topological charge for the four classes with CS in the classification table. Parallel to the case without CS, we will show that the Fermi point of Eq. (C14) has unit charge. Before doing it, it is noted that $\mathcal{H}_D$ can be expressed as

$$\mathcal{H}_D = \begin{pmatrix} 0 & u \\ u^\dagger & 0 \end{pmatrix}, \tag{C15}$$

where $u = -ik_{2n}\mathbf{1}_{2^{n-1}\times 2^{n-1}} + \sum_{a=1}^{2n-1} k_a \Gamma^a_{(2n-1)}$ with our convention of Dirac matrices in Eq. (C1). To calculate the topological charge, we choose an S^{2n-1} in the $\mathbf{k}$ space to enclose the Fermi point, which is parametrized by s_i with i being from 1 to $2n - 1$. Thus we have

$$\nu = \frac{C_{2n-1}}{2}\int_{S^{2n-1}} \mathbf{tr}[\Gamma^{2n+1}((\mathcal{H}_D)^{-1}\mathbf{d}\mathcal{H}_D)^{2n-1}].$$

Without loss of generality, we choose the S^{2n-1} to be unit, which implies $u^\dagger u = 1$ and leads to

$$\nu = C_{2n-1}\int_{S^{2n-1}} \mathbf{tr}(u\mathbf{d}u^\dagger)^{2n-1}.$$

As $u^\dagger$ can be regarded as an inversion of Green's function in $(2n - 1)$ spatial dimensions with k_{2n} as ω, referring to the case of Eq. (C8), it is seen that $\nu = 1$.

Analogous to the cases without CS, we can construct $\mathbf{Z}_2^{(1,2)}$ type topological Fermi surfaces by lowering spatial dimension from the model (C14). The process is entirely analogous to that of nonchiral cases, so we simply write down the corresponding models below:

$$\begin{cases}\mathcal{H}_D^{(1)} = \sum_{a=1}^{2n-1} k_a\Gamma^{a+1} & for \quad \mathbf{Z}_2^{(1)} \\ \mathcal{H}_D^{(2)} = \sum_{a=1}^{2n-2} k_a\Gamma^{a+2} & for \quad \mathbf{Z}_2^{(2)}\end{cases}. \tag{C16}$$

Note that although the above two models have additional symmetries, e.g., Γ^1 anticommutes with $\mathcal{H}_D^{(1)}$, these symmetries are not required, which means that we can add some terms to break them without changing the corresponding topological properties, such as the λ terms in models (C9) and (C10).

$2\mathbf{Z}$ *type*. According to the corresponding model of classes AI, AII, C, and D, we can define

$$\tilde{\mathcal{B}}^1 := \mathcal{B}^1\Gamma^{2n+1},$$

which satisfies the relation

$$\tilde{\mathcal{B}}^1 = (-1)^{n(n+1)/2}(\tilde{\mathcal{B}}^1)^T. \tag{C17}$$

Accordingly, we introduce the following model:

$$\mathcal{H}_D^2(\mathbf{k}) = \sum_{a=2}^{2n-2} k_a\Gamma^{a+2} + k_1\tilde{\Gamma}, \tag{C18}$$

whose Fermi point has a topological charge 2 from the same reasoning for model (C13). It has a CS (represented by Γ^{2n+1}), and, moreover, when $\mathcal{B}^1$ represents a TRS(PHS), $\tilde{\mathcal{B}}^1$ denotes a PHS(TRS). Considering the relation (C17) and the results of nonchiral cases, it is found that the Fermi point is in classes DIII, CI, CII, and BDI, respectively, when $p = 8m + 6$, $8m + 2$, $8m$, and $8m + 4$, which is in consistence with our classification table of Fermi surfaces. To conclude this section, all types of Fermi surfaces in the classification table have been constructed by Dirac matrices.

3. Construction of all topological types of TIs/TSCs

a. TIs/TSCs in nonchiral classes AI, AII, D, and C

$\mathbf{Z}$ *type and* $\mathbf{Z}_2^{(1,2)}$ *type*. We first wish to indicate that a part of results to be presented for the relationship of Dirac matrices with TIs/TSCs were addressed in Ref. [8]. As the bulk energy spectrum of a TI/TSC is fully gaped, we need one of Γs with a coefficient as a mass term, which is chosen to be Γ^1. Thus a typical Hamiltonian reads

$$\mathcal{H}(\mathbf{k}) = \sum_{a=2}^{2n+1} k_{a-1}\Gamma^a + (m - \epsilon k^2)\Gamma^1. \tag{C19}$$

Note that the term of $\epsilon k^2\Gamma^1$, in which a constant ϵ can be regarded to be infinitesimally small, is included as a prescription for the singularity of this kind of continuum model at the infinity in the $\mathbf{k}$ space [35]. It will turn out that the topological number of this Hamiltonian is either ± 1 or 0.

Let us look into the TRS/PHS of Hamiltonian in Eq. (C19), which is now represented by B^1. Using Eq. (C4), we obtain the relation

$$B^1\mathcal{H}(\mathbf{k})(B^1)^{-1} = (-1)^n\mathcal{H}^T(-\mathbf{k}). \tag{C20}$$

Thus when $n = 2m$, i.e., the spatial dimension $d = 4m$, B^1 represents a TRS, while it corresponds to a PHS when $n = 2m + 1$ or $d = 4m + 2$. Equation (C5) can tell us the sign of the TRS/PHS, so that we can encapsulate that Hamiltonian of Eq. (C19) is in classes AI, AII, D, and C, respectively, for $d = 8m$, $8m + 4$, $8m + 2$, and $8m + 6$, which is in agreement with the distribution of $\mathbf{Z}$-type topological numbers in the classification of TIs/TSCs. The remaining task for these classes is to verify that Hamiltonian of Eq. (C19) has indeed unit topological number. Substituting Eq. (C19) into the corresponding formula for the integer topological number, i.e.,

$$N = C_{d+1}\int_{\mathcal{M}} \mathbf{tr}(G\mathbf{d}G^{-1}(\omega,\mathbf{k}))^{d+1},$$

where $\mathcal{M}$ is the whole $(\omega,\mathbf{k})$ space, we can obtain

$$N = \frac{1}{2}\,[\mathbf{sgn}(m) + \mathbf{sgn}(\epsilon)]\,, \tag{C21}$$

which indicates unit topological number when both m and ϵ have the same sign. Thus it is clear that the model of Eq. (C19) can be regarded as a representative for each $\mathbf{Z}$ type of the classes AI, AII, D, and C.

Since the procedures to construct the $\mathbf{Z}_2^{(1,2)}$-type TIs/TSCs are similar to those for constructing $\mathbf{Z}_2^{(1,2)}$-type Fermi surfaces, to avoid redundant derivations, we here write down the results directly with some necessary remarks. The corresponding models for cases of $\mathbf{Z}_2^{(1)}$ and $\mathbf{Z}_2^{(1)}$ are, respectively,

$$\mathcal{H}^{(1)} = \sum_{a=1}^{2n-1} k_a\Gamma^{a+2} + (m-\epsilon k^2)\Gamma^1 \quad \text{for} \quad \mathbf{Z}_2^{(1)}$$

$$\mathcal{H}^{(2)} = \sum_{a=1}^{2n-2} k_a\Gamma^{a+3} + (m-\epsilon k^2)\Gamma^1 \quad \text{for} \quad \mathbf{Z}_2^{(2)}.$$

To see that nontrivial topological property of $\mathcal{H}^{(1,2)}$, we need to make continuous extension with new parameters, which can be chosen as the omitted momenta, compared with model (C19). Concretely, for $\mathcal{H}^{(1)}$ the extension can be made by adding the term $\alpha\Gamma^2 - \epsilon\alpha^2\Gamma^1$ with $\alpha \in (-\infty,\infty)$. When $\alpha = 0$, we obtain the original $\mathcal{H}^{(1)}$, and by changing α from 0 to $\pm\infty$, $\mathcal{H}^{(1)}$ is deformed smoothly without closing its gap to a trivial model $\sim \alpha\Gamma^2 - \epsilon\alpha^2\Gamma^1$. Since the extended model is equivalent to the model (C19) whose $\mathbf{Z}$-type topological number is given by Eq. (C21), it is concluded that the $\mathbf{Z}_2^{(1)}$-type topological number of $\mathcal{H}^{(1)}$ is also given by Eq. (C21). The same reasoning is applicable to $\mathcal{H}^{(2)}$ when we make two-parameter extension, thus $\mathcal{H}^{(2)}$ has a nontrivial $\mathbf{Z}_2^{(2)}$-type topological number when m and ϵ have the same sign. We note again that only the symmetries in the corresponding symmetry class are required, while other terms preserving topological properties may be added to break unwanted additional symmetries.

2$\mathbf{Z}$ *type*. Similar to the case of 2$\mathbf{Z}$-type Fermi surface, we introduce a model:

$$\mathcal{H}^2(\mathbf{k}) = \sum_{a=1}^{2n-2} k_a\Gamma^{a+3} + (m-\epsilon k^2)\tilde{\Gamma}$$

with topological number $\mathbf{sgn}(m) + \mathbf{sgn}(\epsilon)$, which can be seen from our previous discussion of 2$\mathbf{Z}$ type Fermi surfaces. Noting that

$$B^2\tilde{\Gamma}(B^2)^{-1} = (-1)^{n+1}\,\tilde{\Gamma}$$

and relation (C4), we have

$$B^2\mathcal{H}^2(\mathbf{k})(B^2)^{-1} = (-1)^{n+1}\,\mathcal{H}^{2T}(-\mathbf{k}). \tag{C22}$$

Combining Eq. (C5) with Eq. (C22), it can be found that the classes of model belong, respectively, to AI, AII, D, and C for $d = 8m+4$, $8m$, $8m+6$, and $8m+2$, consistent with our classification of TIs/TSCs.

b. TIs/TSCs in chiral classes CI, CII, BDI, and DIII

$\mathbf{Z}$ *type and* $\mathbf{Z}_2^{(1,2)}$ *type*. For the other classes with CS, the term Γ^{2n+1} is excluded for the presence of CS, and the corresponding model may be written as

$$\mathcal{H}_{\text{CS}}(\mathbf{k}) = \sum_{a=2}^{2n} k_{a-1}\Gamma^a + (m-\epsilon k^2)\Gamma^1. \tag{C23}$$

Here, the additional TRS/PHS is represented by $\tilde{B}^1 = B^1\Gamma^{2n+1}$ referring to Eq. (C3), and we can check that

$$\begin{aligned}\tilde{B}^1\mathcal{H}_{\text{CS}}(\mathbf{k})(\tilde{B}^1)^{-1} &= -B^1\mathcal{H}_{\text{CS}}(\mathbf{k})(B^1)^{-1}\\ &= (-1)^{n+1}\mathcal{H}_{\text{CS}}^T(-\mathbf{k}).\end{aligned}$$

Compared with Eq. (C20), it is seen that if B^1 denotes a TRS(PHS), then $\tilde{B}^1$ corresponds to a PHS(TRS). The sign of $\tilde{B}^1$ is given by Eq. (C5), and thus it can be seen that the classes of model (C23) belong, respectively, to CI, DIII, BDI, and CII for $d = 8m+7$, $8m+3$, $8m+1$, and $8m+5$. To check the $\mathbf{Z}$-type topological number, we use the corresponding formula

$$N = \frac{C_{2n-1}}{2}\int_M \mathbf{tr}\big[\Gamma^{2n+1}\big(\mathcal{H}_{\text{CS}}^{-1}\mathbf{d}\mathcal{H}_{\text{CS}}\big)^{2n-1}\big],$$

where M denotes the whole $\mathbf{k}$ space. If we recover the Γ matrices with their subscript to be $\Gamma^a_{(2n+1)}$, we recall Eq. (C15) of $\mathcal{H}_{\text{CS}}$ with

$$u = -ik_{2n-1}\mathbf{1}_{2^{n-2}} + \sum_{a=2}^{2n-1} k_{a-1}\Gamma^a_{(2n-1)} + (m-\epsilon k^2)\Gamma^1_{(2n-1)}.$$

Similar to the calculation of topological charge for Fermi point, we have

$$N = C_{2n-1}\int_M \mathbf{tr}(u\mathbf{d}u^\dagger)^{2n-1}.$$

Thus the topological number is given by

$$N = \frac{1}{2}\,[\mathbf{sgn}(m) + \mathbf{sgn}(\epsilon)]\,,$$

which implies $N = 1$ when both m and ϵ are positive. Note that the correct definition of k^2 should be $k^2 = \sum_{a=1}^{2n-2} k_a^2$ in order to obtain the above expression, since adding k_{2n-1}^2 in the summation will always make the topological number vanish.

$\mathbf{Z}_2^{(1,2)}$-type TIs/TSCs in these classes can be obtained directly by the method used in the previous section, thus we here present the result:

$$\mathcal{H}_{\text{CS}}^{(1)} = \sum_{a=1}^{2n-2} k_a\Gamma^{a+2} + (m-\epsilon k^2)\Gamma^1 \quad \text{for} \quad \mathbf{Z}_2^{(1)}$$

$$\mathcal{H}_{\text{CS}}^{(2)} = \sum_{a=1}^{2n-3} k_a\Gamma^{a+3} + (m-\epsilon k^2)\Gamma^1 \quad \text{for} \quad \mathbf{Z}_2^{(2)}.$$

The two models have nontrivial $\mathbf{Z}_2^{(1,2)}$ type topological numbers when m and ϵ have the same sign.

2$\mathbf{Z}$ *type*. From our experience, a desired mode in this case can be written as

$$\mathcal{H}_{\text{CS}}^2(\mathbf{k}) = \sum_{a=1}^{2n-3} k_a\Gamma^{a+3} + (m-\epsilon k^2)\tilde{\Gamma},$$

which has topological number $\mathbf{sgn}(m) + \mathbf{sgn}(\epsilon)$. If B^2 corresponds to a TRS(PHS), $\tilde{B}^2$ represents a PHS(TRS). Then the classes of the above model belong, respectively, to DIII, CI, BDI, and CII when $d = 8m+7, 8m+3, 8m+5$, and $8m+1$, in agreement with our classification table of TIs/TSCs. To conclude this section, all types of TIs/TSCs in our classification table have been constructed by using Dirac matrices.

4. Boundary modes of Dirac models and the general index theorem

Up to now, all types of TIs/TSCs have been constructed by Dirac matrices, and all of our constructed models may be written in the unified form:

$$\mathcal{H}_G(\mathbf{k}) = \sum_{a=1}^{d} k_a \Gamma^{a+b-1} + (m - \epsilon k^2)\Gamma^{\alpha}, \tag{C24}$$

where d is the bulk dimension, b is the starting superscript of $\Gamma_{(2n+1)}$ matrices, and $\Gamma^{\alpha} = \Gamma^1$ except in the cases of $2\mathbf{Z}$-type where $\Gamma^{\alpha} = \tilde{\Gamma}$. The advantage of this kind of construction in the form of Eq. (C24) lies in that its boundary low-energy effective theory can be formulated systematically through the perturbation theory of quantum mechanics. The method used here is a generalization of that in Ref. [36]. We consider that a boundary at $x = 0$ is on the left of a d-dimensional model of Eq. (C19) and translation invariance is still preserved along the other $d-1$ directions. To implement the perturbation method, we will first identify the gapless subspace of the model residing on the boundary, i.e., concentrated near $x = 0$, and then compute the transition elements in this subspace by regarding the remaining translation invariant terms as perturbations.

A physical boundary state $\varphi(\mathbf{x})$ has zero energy and should vanish at $x = 0$ and $x \to +\infty$. If such a state exists, it satisfies the following equation:

$$\left[-i\Gamma^b \partial_x + \left(m + \epsilon\partial_x^2\right)\Gamma^1\right]\varphi(x) = 0,$$

where momenta along the other directions are set to be zero since only the ground state is relevant at present. Also note that we have set $\Gamma^{\alpha} = \Gamma^1$ for explicitness, since there is no difference essential for the cases of $\tilde{\Gamma}$. The above equation can be rewritten as

$$\left[\partial_x + \left(m + \epsilon\partial_x^2\right) i\Gamma^b\Gamma^1\right]\varphi(x) = 0.$$

Assuming that $\varphi(x) = \chi_\eta f(x)$, where $\eta = \pm$ and $\chi_\pm$ is the eigenvector of $i\Gamma^b\Gamma^1$ with $\pm$ being the corresponding eigenvalue. Then

$$\partial_x f(x) + \eta\left(m + \epsilon\partial_x^2\right) f(x) = 0,$$

with the boundary conditions:

$$f(0) = 0 \quad \text{and} \quad f(x)|_{x\to\infty} = 0.$$

Seeking solutions with the form $f \sim e^{-\lambda x}$, we have

$$\lambda^2 - \frac{\eta}{\epsilon}\lambda + \frac{m}{\epsilon} = 0.$$

To satisfy the boundary condition, we need the two roots $\lambda_{1,2}$ are both positive, which requires $\eta = \mathbf{sgn}(\epsilon)$ and $m\epsilon > 0$. Thus the condition of the existence of the boundary states is

$$\mathbf{sgn}(m) = \mathbf{sgn}(\epsilon), \tag{C25}$$

which is in consistence with the bulk topological number, e.g., expressed in Eq. (C21). It turns out that there exist 2^{n-1} degenerate solutions with degeneracy originated from the internal space:

$$\varphi_i(x) = \chi^i_{\mathbf{sgn}(\epsilon)}(e^{-\lambda_1 x} - e^{-\lambda_2 x}),$$

where i labels the 2^{n-1} degenerate eigenvectors of $i\Gamma^b\Gamma^1$ with eigenvalue $\mathbf{sgn}(\epsilon)$.

To obtain the low-energy effective Hamiltonian on the boundary, we consider the remaining terms along the other directions of Eq. (C19),

$$\Delta\mathcal{H} = \sum_{a=2}^{d} k_a\Gamma^{a+b-1} - \epsilon\sum_{a=2}^{d} k_a^2\Gamma^1,$$

as perturbations. Since we are only interested in the low-energy behavior of the boundary, it is sufficient to implement the perturbation theory of quantum mechanics in this subspace with zero energy to obtain the low-energy effective Hamiltonian $\mathcal{H}_{\text{eff}}$, that is,

$$\mathcal{H}_{\text{eff}}^{ij} = \langle\chi^i|\Delta\mathcal{H}|\chi^j\rangle.$$

We first show that the quadratic terms vanish as follows. Note that

$$\begin{aligned}\langle\chi^i|\Gamma^1|\chi^j\rangle &= \langle\chi^i|\Gamma^2\Gamma^2\Gamma^1|\chi^j\rangle\\ &= -i\langle\chi^i|\Gamma^2(i\Gamma^2\Gamma^1)|\chi^j\rangle\\ &= -i\,\mathbf{sgn}(\epsilon)\langle\chi^i|\Gamma^2|\chi^j\rangle\end{aligned}$$

and

$$\begin{aligned}\langle\chi^i|\Gamma^1|\chi^j\rangle &= \langle\chi^i|\Gamma^1\Gamma^2\Gamma^2|\chi^j\rangle\\ &= -i\langle\chi^i|i\Gamma^1\Gamma^2\Gamma^2|\chi^j\rangle\\ &= i\langle\chi^i|(i\Gamma^2\Gamma^1)\Gamma^2|\chi^j\rangle\\ &= i\,\mathbf{sgn}(\epsilon)\langle\chi^i|\Gamma^2|\chi^j\rangle.\end{aligned}$$

As a result, $\langle\chi^i|\Gamma^1|\chi^j\rangle = -\langle\chi^i|\Gamma^1|\chi^j\rangle$, and thus the quadratic terms have no contribution to $\mathcal{H}_{\text{eff}}$. For the linear terms of $\Delta\mathcal{H}$, noting that

$$[i\Gamma^b\Gamma^1, \Gamma^a] = 0, \quad \text{for} \quad a \neq 1 \text{ or } b,$$

all Γ^as with $a \neq 1$ *or* b can be diagonalized into $2^{n-1} \times 2^{n-1}$ blocks as

$$\Gamma^a = \begin{pmatrix}\Gamma^a_+ & \\ & \Gamma^a_-\end{pmatrix},$$

where each block satisfies

$$\left\{\Gamma^a_\eta, \Gamma^b_\eta\right\} = 2\delta^{ab}\mathbf{1}_{2^{n-1}\times 2^{n-1}}, \quad a,b \neq 1 \text{ or } b.$$

Thus either $\{\Gamma^a_+\}$ or $\{\Gamma^a_-\}$ forms a $2^{n-1} \times 2^{n-1}$ representation of the Clifford algebra. Thus up to a unitary transformation, we can express the effective theory as

$$\mathcal{H}_{\text{eff}} = \frac{1}{2}[\mathbf{sgn}(m) + \mathbf{sgn}(\epsilon)]\sum_{a=2}^{d} k_a\Gamma^{a+b-3}_{(2n-1)}, \tag{C26}$$

subject to the condition of Eq. (C25). Note that for $2\mathbf{Z}$ cases, the first Γ matrix in the above expression should be $\tilde{\Gamma}$.

It is crucial to observe that the low-energy effective theory (C26), which is obtained on the boundary of the unified model (C24) of TIs/TSCs, takes also a unified form for all types of FSs, i.e., models (C6), (C9), (C10), (C13), (C14), (C16), and (C18). Since our final aim is to prove the general index theorem, namely, to show that the same topological information is encoded in both bulk and boundary, our remaining task is to look into the topological charge of the Fermi point with the obtained effective theory. To be explicit, we shall complete two tasks: the first one is to identify the symmetry operators of a boundary effective theory according to those of its bulk Hamiltonian; the second one is to check whether the topological charge of the Fermi point on the boundary matches the bulk topological number on both magnitude and topological type. The first one can be done by comparing the symmetries and their signs, and thereby it turns out that, for a given symmetry case, the corresponding symmetry operators are just those we defined previously in the constructions of that kind of FS with unit topological charge. This can be clearly seen from the fact that our constructions of Fermi surfaces and TIs/TSCs matches to our classification table of both FSs and TIs/TSCs, where the symmetry situation of an FS of codimension $d-1$ is the same as that of a d-dimensional TIs/TSCs. For the second task, again from our classification table of FSs and TIs/TSCs, we see that the topological charge of the Fermi point has the same type as that of the corresponding bulk topological number, and furthermore their numerical equality is obvious. Thus we finally have the following general index theorem:

$$\nu(i,d-1) = N(i,d),$$

where i is the index of the symmetry classes, $d-1$ is the codimension of the Fermi point on the boundary, and d is the spatial dimension, for a concerned TI/TSC.

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