Stability of surface states of weak $\mathbb{Z}_2$ topological insulators and superconductors

Takahiro Morimoto[1] and Akira Furusaki[1,2]

[1]*Condensed Matter Theory Laboratory, RIKEN, Wako, Saitama, 351-0198, Japan*
[2]*RIKEN Center for Emergent Matter Science (CEMS), Wako, Saitama, 351-0198, Japan*
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We study the stability against disorder of surface states of weak $\mathbb{Z}_2$ topological insulators (superconductors) which are stacks of strong $\mathbb{Z}_2$ topological insulators (superconductors), considering representative Dirac Hamiltonians in the Altland-Zirnbauer symmetry classes in various spatial dimensions. We show that, in the absence of disorder, surface Dirac fermions of weak $\mathbb{Z}_2$ topological insulators (superconductors) can be gapped out by a Dirac mass term which couples surface Dirac cones and leads to breaking of a translation symmetry (dimerization). The dimerization mass is a unique Dirac mass term in the surface Dirac Hamiltonian, and the two dimerized gapped phases which differ in the sign of the Dirac mass are distinguished by a $\mathbb{Z}_2$ index. In other words the dimerized surfaces can be regarded as a strong $\mathbb{Z}_2$ topological insulator (superconductor). We argue that the surface states are not localized by disorder when the ensemble average of the Dirac mass term vanishes.

I. INTRODUCTION

Three-dimensional topological insulators (TIs) [1–6] are classified into strong and weak TIs. A three-dimensional strong TI is characterized by an intrinsically three-dimensional topological index (strong $\mathbb{Z}_2$ index ν_0) and has an odd number of gapless Dirac cones on every surface. By contrast, a three-dimensional weak TI is adiabatically connected to stacked layers of two-dimensional TIs, characterized with three weak topological indices (ν_1, ν_2, ν_3) specifying the stacking direction, and has an even number (typically two) of Dirac cones on its side surfaces. Since an even number of Dirac cones can be gapped out without breaking time-reversal symmetry, it was initially considered that gapless surface states of weak TIs are fragile.

However, recent theoretical studies have revealed unexpected strength of weak TIs. It was first argued by Ringel *et al.* [7] that surface Dirac fermions of weak TIs are not localized by random potential which is weaker than a band gap and has zero mean. This was confirmed by a numerical study of effective Hamiltonian of two Dirac cones on the surface of a weak TI perturbed by various disorder potentials which preserve time-reversal symmetry [8]. The surface Dirac Hamiltonian used in this simulation has 4×4 matrix representation and has a single Dirac mass term which physically represents dimerization of stacked layers [3,7–10]. Mong *et al.* have also shown that a nonvanishing average of the Dirac mass induces a transition from a metallic phase to an insulating phase [8]. A more recent numerical study using a network model has shown that the metal-insulator transition in the presence of a finite dimerization belongs to the standard universality class of two-dimensional symplectic class of Anderson localization [11].

The remarkable stability against disorder of surface states of undimerized weak TIs is ascribed to the uniqueness of the dimerization mass term in the effective Hamiltonian for the surface states [8,10]. The point is that the sign of the unique Dirac mass term distinguishes topologically distinct phases, since the effective Hamiltonian has the same form as the Bernevig-Hughes-Zhang model [12] of two-dimensional quantum spin Hall insulators. This then leads to the following

semiclassical picture of surface transport. When random potential (including the Dirac mass) varies slowly in space, the two-dimensional surface of a weak TI is divided into positive-mass domains and negative-mass domains. Every domain boundary has helical gapless modes, which will percolate over the surface when positive- and negative-mass domains appear with the same probability, i.e., when the random potential has zero mean. As pointed out by Fu and Kane [10], this physics is similar to integer quantum Hall plateau transitions. It is well known that the two-dimensional Dirac Hamiltonian $H = k_x \sigma_x + k_y \sigma_y + m \sigma_z$ exhibits anomalous quantum Hall effect $\sigma_{xy} = -\text{sgn}(m)e^2/2h$, where σ_i are Pauli matrices and k_x and k_y are momenta. The critical point between the quantum Hall plateaus $\sigma_{xy} = \pm e^2/2h$ is realized by tuning ensemble average of the random mass m to zero [13]. Similarly, a clean surface of an undimerized weak $\mathbb{Z}_2$ TI is exactly at a quantum critical point separating two dimerized insulating phases which are distinguished by a $\mathbb{Z}_2$ index. A weak disorder then turns the quantum critical point into a metallic phase (because of antilocalization), as observed in numerical simulations [8].

The purpose of this paper is to show that the stability of surface states of weak TIs against disorder discussed above can be generalized to a much broader class of weak TIs and topological superconductors (TSCs) of any symmetry class which are characterized by weak $\mathbb{Z}_2$ indices. It is well known that, in every spatial dimension, two out of the ten Altland-Zirnbauer symmetry classes [14] of noninteracting fermion systems can have topologically nontrivial gapped phases of noninteracting fermions characterized by a strong $\mathbb{Z}_2$ index [15–17]. For example, symmetry class AII, a set of free-fermion Hamiltonians which are invariant under time-reversal operation T with $T^2 = -1$, has two- and three-dimensional TIs with a strong $\mathbb{Z}_2$ index [1,2]. In this paper we shall study $(d + 1)$-dimensional weak $\mathbb{Z}_2$ TIs (TSCs) which are stacks of d-dimensional strong $\mathbb{Z}_2$ TIs (TSCs). As a representative model for d-dimensional strong $\mathbb{Z}_2$ TIs (TSCs), we take a d-dimensional Dirac Hamiltonian satisfying symmetry conditions of a given symmetry class. We will show that a side surface of stacks of d-dimensional strong $\mathbb{Z}_2$ TIs (TSCs) has two Dirac cones which are again described by a d-dimensional Dirac Hamiltonian. It admits a unique Dirac

mass term which couples the two Dirac cones and opens a gap. To this end, we will employ Clifford algebras to treat a Dirac Hamiltonian and symmetry constraints on equal footing and make use of topological properties of classifying spaces which in our case are sets of all possible Dirac mass terms. The sign of the unique Dirac mass corresponds to a $\mathbb{Z}_2$ topological index of insulating phases. We will then argue that surface Dirac fermions cannot be localized by weak random potential if disorder average of the Dirac mass term vanishes.

The organization of this paper is as follows. In Sec. II, we briefly review the classification of TIs and TSCs using relevant Clifford algebras. In Sec. III, we describe a model of weak $(d + 1)$-dimensional TIs/TSCs which are stacks of strong $\mathbb{Z}_2$ TIs/TSCs for real symmetry classes, and derive an effective Dirac Hamiltonian for surface states with a unique Dirac mass term. In Sec. IV, we discuss a couple of examples of weak $\mathbb{Z}_2$ TIs and TSCs. We explicitly show that the mass term gapping out the surface states is of dimerization type and unique. In Sec. V, we conclude by summarizing the main results.

II. MINIMAL DIRAC MODEL AND CLIFFORD ALGEBRAS

In order to introduce theoretical formalism which we employ in the following sections, we give a brief review of Clifford algebras and their application to classification of TIs and TSCs. We consider a Dirac Hamiltonian

$$H = \gamma_0 m + \sum_{i=1}^{d} \gamma_i k_i, \tag{1}$$

where γ_i's $(i = 0, 1, \ldots, d)$ are gamma matrices anticommuting with each other,

$$\{\gamma_i, \gamma_j\} = 2\delta_{i,j}, \tag{2}$$

k_i is a momentum in the ith direction, and m is the Dirac mass that corresponds to a band gap [16]. We have set the velocity of Dirac fermions to unity. The Dirac Hamiltonian [Eq. (1)] is a minimal (irreducible) model, as we assume that no unitary operator (generator of continuous symmetry such as rotation) commutes with H. Such a Hamiltonian is classified as a member of one of the ten Altland-Zirnbauer (AZ) symmetry classes [14], according to the presence or absence of the three generic symmetries: time-reversal symmetry (TRS), particle-hole symmetry (PHS), and chiral symmetry. The Hamiltonian H has a TRS when it commutes with an antiunitary operator T for time-reversal transformation as

$$[T, H] = 0, \tag{3a}$$

which implies

$$\{T, \gamma_i\} = 0 \quad (\text{for } i \neq 0), \qquad [T, \gamma_0] = 0, \tag{3b}$$

for the Dirac Hamiltonian H, because complex conjugation operator $\mathcal{K}$ involved in T changes k_i to $-k_i$. Similarly, the Hamiltonian H has a PHS when it anticommutes with an antiunitary operator C,

$$\{C, H\} = 0, \tag{4a}$$

TABLE I. Real symmetry classes and their topological classification. The eight real symmetry classes are characterized by the presence or the absence of time-reversal symmetry (T) and particle-hole symmetry (C). Their presence is labeled by the sign of the squared operator, T^2 or C^2, and their absence is indicated by 0. For each class, the parameters (p,q) specifying the relevant real Clifford algebra, real classifying space R_{q-p}, and its zeroth homotopy group at $d = 0$ are listed.

class	T	C	Γ	(p,q)	R_{q-p}	$\pi_0(R_{q-p})\vert_{d=0}$
AI	+1	0	0	$(d+2,2)$	R_{0-d}	$\mathbb{Z}$
BDI	+1	+1	1	$(d+1,2)$	R_{1-d}	$\mathbb{Z}_2$
D	0	+1	0	$(d,2)$	R_{2-d}	$\mathbb{Z}_2$
DIII	−1	+1	1	$(d,3)$	R_{3-d}	0
AII	−1	0	0	$(d,4)$	R_{4-d}	$\mathbb{Z}$
CII	−1	−1	1	$(d+3,0)$	R_{5-d}	0
C	0	−1	0	$(d+2,0)$	R_{6-d}	0
CI	+1	−1	1	$(d+2,1)$	R_{7-d}	0

or

$$[C, \gamma_i] = 0 \quad (\text{for } i \neq 0), \quad \{C, \gamma_0\} = 0, \tag{4b}$$

where C serves as an operator for particle-hole transformation of Bogoliubov-de Gennes (BdG) Hamiltonian of a superconducting system. The Hamiltonian H has a chiral symmetry, if there exists a unitary operator Γ that anticommutes with H,

$$\{\Gamma, H\} = 0, \tag{5a}$$

or

$$\{\Gamma, \gamma_i\} = 0. \tag{5b}$$

We note that from two of the three relations (3)–(5) follows the third relation where the transformation operator is the product of those from the two relations. For example, if H has both TRS and PHS, then H has a chiral symmetry with $\Gamma = TC$. The antiunitary operators T and C square to plus or minus identity operator.

Among the ten AZ symmetry classes, two symmetry classes (A and AIII) which have neither TRS nor PHS are called complex classes, and the other eight symmetry classes are called real classes shown in Table I. For a more detailed introduction to the classification of single-particle Hamiltonians into the ten AZ classes, we refer the reader to Sec. 1.1 in Ref. [16].

It is known that, in each spatial dimension, five out of the ten AZ symmetry classes have topologically distinct gapped phases, which are characterized by either an integer ($\mathbb{Z}$) or a binary ($\mathbb{Z}_2$) topological index [15–17]. For example, gapped phases of minimal Dirac models can be topologically classified by examining how many distinct mass terms the Dirac Hamiltonians can have under given symmetry constraints [18]. When H can accommodate more than one mass terms, $m_1 \gamma_{0,1} + \cdots + m_n \gamma_{0,n}$, where $\gamma_{0,i}$'s anticommute with each other and with other γ_i's $(i = 1, \ldots, d)$, all the gapped ground states of H with different values of $\boldsymbol{m} = (m_1, \ldots, m_n) \neq 0$ are adiabatically connected without closing a gap. This means that the gapped phase of H is topologically trivial. On the other hand, when H has only a unique mass term ($m \gamma_0$),

the ground state of H with positive m (denoted by H_+), and the ground state of H with negative m (denoted by H_-), are topologically distinct gapped states separated by a critical point at $m = 0$; i.e., the two gapped phases with opposite signs of m are topologically distinct phases. Distinction between the two classifications, $\mathbb{Z}$ and $\mathbb{Z}_2$, becomes clear, when we consider a doubled system $H \otimes \sigma_0$, where σ_0 is a unit 2×2 matrix. For gapped phases with $\mathbb{Z}_2$ classification, we find an extra mass term in the doubled system, with which we can find a continuous deformation from $H_+ \otimes \sigma_0$ to $H_- \otimes \sigma_0$ or vice versa. For gapped phases with $\mathbb{Z}$ classification, on the other hand, we do not find an extra mass term in the doubled system; in this case topological indices of gapped ground states of $H_\pm$ can add up.

The classification of mass terms in minimal Dirac models described above can be systematically performed by considering an extension problem of Clifford algebra [17], as briefly summarized below. For more details see, e.g., Sec. III of Ref. [18]. In this paper we are concerned with real symmetry classes. For each real AZ class and each spatial dimension d, we can define a real Clifford algebra $Cl_{p,q}$ (as described later in this section) whose generators are symmetry operators (such as T, C, or Γ) and kinetic gamma matrices (γ_i, $i = 1, \dots, d$). We take a real representation of sufficiently large matrix dimension for Clifford algebras. We then examine the possibility of extending a given Clifford algebra (with a fixed representation) by adding a mass term γ_0 to the set of generators of the Clifford algebra. A set of possible representations of γ_0 form a manifold called a classifying space [17]. The classifying space for the extension $Cl_{p,q} \to Cl_{p,q+1}$ is given by R_{q-p}, whose explicit form can be found in literature [17,18]. The relation $R_{n+8} = R_n$ is known to hold (the Bott periodicity) [17,19]. The topological classification of the Dirac mass terms is then obtained from the connectivity of the classifying space, i.e., the zeroth homotopy group of the classifying space. The last columns of Table I show topological classification for the eight real symmetry classes at $d = 0$. The classification in d dimensions is obtained by using the Bott periodicity [17]. We note that insulators (superconductors) characterized by a nontrivial topological index discussed above are called strong TIs (TSCs), which should be distinguished from weak TIs (TSCs) discussed in the next section.

In the rest of this section we give a list of Clifford algebras and their extension problems which are used to obtain the above-mentioned classification of strong TIs and TSCs for the eight real symmetry classes and which will serve as a basis for the discussion in the following sections. To this end, we first introduce a real Clifford algebra $Cl_{p,q}$, which is a 2^{p+q}-dimensional real linear algebra generated by a set of generators $\{e_1, e_2, \dots, e_{p+q}\}$ satisfying the algebraic relations

$$\{e_i, e_j\} = 0 \quad \text{for } i \neq j \tag{6a}$$

and

$$e_i^2 = \begin{cases} -1, & 1 \leqslant i \leqslant p, \\ +1, & p+1 \leqslant i \leqslant p+q. \end{cases} \tag{6b}$$

We also introduce an operator J which plays a role of the imaginary unit "i" in real algebras and obeys the relations

$$J^2 = -1, \qquad \{T,J\} = \{C,J\} = [\gamma_i, J] = 0. \tag{7}$$

Symmetry classes C and D. These two classes have only a PHS: $C^2 = -1$ in class C and $C^2 = +1$ in class D. We define a Clifford algebra $Cl_{p,q}$ generated by the operators

$$\{C, CJ, J\gamma_1, \dots, J\gamma_d\}, \tag{8a}$$

where p and q are listed in Table I. For topological classification we consider extending $Cl_{p,q}$ to $Cl_{p,q+1}$ with the generators

$$\{\gamma_0, C, CJ, J\gamma_1, \dots, J\gamma_d\}. \tag{8b}$$

Symmetry classes BDI, CI, CII, and DIII. These four classes have both TRS and PHS. We have a Clifford algebra $Cl_{p,q}$ generated by

$$\{C, CJ, TCJ, J\gamma_1, \dots, J\gamma_d\}, \tag{9a}$$

which is to be extended to $Cl_{p,q+1}$ generated by

$$\{\gamma_0, C, CJ, TCJ, J\gamma_1, \dots, J\gamma_d\}, \tag{9b}$$

where (p,q) are listed for each class in Table I.

Symmetry classes AI and AII. These classes have a TRS only. We define a Clifford algebra $Cl_{p',q'}$ generated by

$$\{T, TJ, \gamma_1, \dots, \gamma_d\}, \tag{10a}$$

where p' and q' denote the numbers of generators squaring to -1 and $+1$, respectively;

$$(p',q') = \begin{cases} (0, d+2), & \text{AI}, \\ (2, d), & \text{AII}. \end{cases} \tag{10b}$$

We consider extending $Cl_{p',q'}$ to $Cl_{p'+1,q'}$, with the generators

$$\{J\gamma_0, T, TJ, \gamma_1, \dots, \gamma_d\}. \tag{10c}$$

Instead of directly studying the extension problem $Cl_{p',q'} \to Cl_{p'+1,q'}$, we make use of the isomorphism [17,18] $Cl_{p',q'} \otimes Cl_{0,2} \simeq Cl_{q',p'+2}$ by tensoring redundant degrees of freedom $Cl_{0,2} \simeq \mathbb{R}(2)$, to obtain the equivalent extension problem

$$Cl_{p,q} \to Cl_{p,q+1}, \qquad (p,q) = (q', p'+2), \tag{11}$$

with (p,q) listed in Table I. Here $\mathbb{R}(2)$ is an algebra of 2 by 2 matrices.

In the following sections we will study the stability of surface states of weak $\mathbb{Z}_2$ TIs and TSCs, using minimal Dirac models and Clifford algebras. We will make use of the one-to-one correspondence between the existence of a single mass (multiple masses) in a minimal Dirac Hamiltonian and nontrivial (trivial) topology of the corresponding classifying space.

III. GENERAL THEORY BASED ON CLIFFORD ALGEBRAS

In this section we study surface states of $(d+1)$-dimensional weak $\mathbb{Z}_2$ TIs and TSCs which are stacked layers of d-dimensional strong $\mathbb{Z}_2$ TIs and TSCs. We will show that the

TABLE II. Classification of mass terms and existence condition of an additional kinetic term in weak topological insulators and superconductors. They are determined by the value of $q - p$, where p and q are the numbers of generators squaring to -1 and $+1$ of the real Clifford algebra which is specified by the symmetry class and the spatial dimension as listed in Table I. The column with γ_0 shows classification of a mass term γ_0. The column with γ_{d+1} shows the existence condition of the kinetic term along the $(d+1)$th direction, where 0 indicates the existence of such a term, and both $\mathbb{Z}$ and $\mathbb{Z}_2$ mean the absence. The last column with $\tilde{\gamma}_0$ shows classification of the mass term $\tilde{\gamma}_0$, where $\mathbb{Z}$ or $\mathbb{Z}_2$ denotes uniqueness of the mass term gapping the surface states of a weak topological insulator or superconductor, while 0 indicates the existence of multiple mass terms.

$q - p$ (mod 8)	γ_0 $\pi_0(R_{q-p})$	γ_{d+1} $\pi_0(R_{p-q})$	$\tilde{\gamma}_0$ $\pi_0(R_{q-p})$
0	$\mathbb{Z}$	$\mathbb{Z}$	$\mathbb{Z}$
1	$\mathbb{Z}_2$	0	$\mathbb{Z}_2$
2	$\mathbb{Z}_2$	0	$\mathbb{Z}_2$
3	0	0	0
4	$\mathbb{Z}$	$\mathbb{Z}$	$\mathbb{Z}$
5	0	0	0
6	0	$\mathbb{Z}_2$	0
7	0	$\mathbb{Z}_2$	0

d-dimensional Dirac Hamiltonian for the surface states admits only a single mass term, which corresponds to dimerization of the stacked layers. The dimerized insulating states with a finite mass are labeled by a $\mathbb{Z}_2$ index (the sign of the mass). We will further argue that the surface states are not localized by disorder as long as disorder average of the dimerization mass term vanishes. We show these in several steps below.

Let us consider a d-dimensional strong $\mathbb{Z}_2$ TI or TSC described by the Hamiltonian H in Eq. (1). The gapped ground state of H has a nontrivial $\mathbb{Z}_2$ topological index in accordance with $\pi_0(R_{q-p}) = \mathbb{Z}_2$ for $q - p = 1,2$ (mod 8), where R_{q-p} is the classifying space associated with the extension problem

$$Cl_{p,q} \rightarrow Cl_{p,q+1} \qquad (12)$$

with (p,q) listed in Table I for each symmetry class; see also Table II. In the following discussions where we explain our theory based on Clifford algebras, we will use, as examples, the Clifford algebras defined in Eq. (9b) for time-reversal symmetric TSCs in class BDI, CI, CII, or DIII. The same theory can be directly applied to classes C and D which have a PHS only, since their relevant Clifford algebras (8b) are obtained by just dropping TCJ from Eq. (9b). It is also applicable to classes AI and AII with TRS only, since their equivalent extension problems (11) have the same mathematical structure.

We describe gapless surface states of d-dimensional strong $\mathbb{Z}_2$ TIs and TSCs as domain wall states of the massive Dirac Hamiltonian (1). Namely, we assume that the Dirac mass m is a function of x_d and changes its sign at $x_d = 0$ (a kink). This yields $(d-1)$-dimensional gapless surface Dirac fermions localized at $x_d = 0$. The wave function of the surface Dirac fermions can be written as $\Psi(x_1, \ldots, x_{d-1})\psi(x_d)$, where $\Psi(x_1, \ldots, x_{d-1})$ is an eigenfunction of the $(d-1)$-dimensional surface Dirac

Hamiltonian $H_{d-1} = -i \sum_{j=1}^{d-1} \gamma_j \partial_{x_j}$, and the localized wave function $\psi(x_d)$ is a solution to the equation $[-i\gamma_d \partial_{x_d} + m(x_d)\gamma_0]\psi(x_d) = 0$, i.e.,

$$\psi(x_d) = \exp\left[-i\int_0^{x_d} dx'_d\, m(x'_d)\gamma_d\gamma_0\right]|n\rangle, \qquad (13)$$

where $|n\rangle$ is chosen from eigenvectors of $-i\gamma_d\gamma_0$ (eigenvalue $+1$ or -1) such that $\psi(x_d)$ is normalizable. We note that $-i\gamma_d\gamma_0$ commutes with the gamma matrices γ_i ($i = 1, \ldots, d-1$) and symmetry operators in the Clifford algebra $Cl_{p,q+1}$. This is formally written as $Cl_{p,q+1} \simeq Cl_{p-1,q} \otimes Cl_{1,1} \simeq Cl_{p-1,q} \otimes \mathbb{R}(2)$. The $\mathbb{R}(2)$ degrees of freedom, which correspond to the localized wave function ψ, should be kept intact in the following procedures of building weak TIs (TSCs) by stacking "layers" of d-dimensional TIs (TSCs) in the $(d+1)$th direction. We set the "interlayer" spacing to unity for simplicity.

As we show later, there always exists a kinetic gamma matrix γ_{d+1} that satisfies the symmetry constraints [Eqs. (3) and (4)] and anticommutes with all the other gamma matrices, $\{\gamma_{d+1}, \gamma_i\} = 0$ ($i = 0, \ldots, d$). We can use the symmetry allowed operator γ_{d+1} for "interlayer" coupling between the $(d-1)$-dimensional Dirac surface states on neighboring "layers". The d-dimensional surface states of the $(d+1)$-dimensional weak TI (TSC) are then governed by the Schrödinger equation

$$-i\sum_{j=1}^{d-1} \gamma_j \frac{\partial \Psi_l}{\partial x_j} - \frac{i}{2}t\gamma_{d+1}(\Psi_{l+1} - \Psi_{l-1}) = E\Psi_l, \qquad (14)$$

where $\Psi_l(x_1, \ldots, x_{d-1})$ is the wave function of surface Dirac fermions in the lth layer, and t is an interlayer hopping matrix element. Note that the interlayer hopping term is compatible with TRS and PHS. In the momentum space the d-dimensional surface Hamiltonian reads

$$H_{d+1}^{(0)} = \sum_{i=1}^{d-1} \gamma_i k_i + t\gamma_{d+1}\sin k_{d+1}. \qquad (15)$$

After linearizing the dispersion near $k_{d+1} = 0$ and π, we have two surface Dirac cones centered at $(k_1, \ldots, k_{d-1}, k_{d+1}) = (0, \ldots, 0, 0)$ and $(0, \ldots, 0, \pi)$. While we have chosen a particular stacking structure in Eq. (14), this should suffice to discuss properties of weak TIs/TSCs that generally possess two surface Dirac cones.

We now prove the existence of γ_{d+1}. Let us look at the extension problem of $Cl_{p-1,q+1} \rightarrow Cl_{p,q+1}$, which is written in terms of generators as

$$\{\gamma_0, C, CJ, TCJ, J\gamma_1, \ldots, J\gamma_{d-1}\}$$
$$\rightarrow \{\gamma_0, C, CJ, TCJ, J\gamma_1, \ldots, J\gamma_{d-1}, J\gamma_d\}, \qquad (16)$$

whose classifying space is R_{p-q}. The topological classification for this extension of adding γ_d is trivial, $\pi_0(R_{p-q}) = 0$, for $q - p = 1,2$ as shown in Table II. This implies that, when we try to add one kinetic gamma matrix γ_d to a set of γ_i's ($i = 0, \ldots, d-1$), we can always find another kinetic gamma matrix, γ_{d+1}, that anticommutes with the other γ_i's and is compatible with symmetry constraints. In passing, we note that, when the d-dimensional TI or TSC is characterized by an integer topological index $\mathbb{Z}$ ($Cl_{p,q} \rightarrow Cl_{p,q+1}$ with

$q - p = 0,4$), the zeroth homotopy group of the classifying space R_{p-q} for the extension problem (16) is also $\mathbb{Z}$ (see Table II), implying that we cannot find γ_{d+1} to have surface Dirac cones; instead, we have a chiral metallic surface as in the case of the two-dimensional surface of layers of two-dimensional integer quantum Hall states [20]. The surface states can acquire finite dispersion along the k_{d+1} direction from interlayer hopping operators which do not anticommute with the $(d-1)$-dimensional Dirac Hamiltonian H_{d-1}.

We introduce a grading of 2 by 2 matrix τ_j to distinguish the two Dirac cones ($\tilde{\tau}_z = +1$ for $k_{d+1} = 0$ and $\tilde{\tau}_z = -1$ for $k_{d+1} = \pi$) on the d-dimensional surface and rewrite the surface Dirac Hamiltonian as

$$H_{d+1} = \sum_{i=1}^{d-1} \gamma_i \tau_0 k_i + t \gamma_{d+1} \tau_z k_{d+1}. \tag{17}$$

It is easy to see that there is only a single mass term $M\gamma_{d+1}\tau_y$ which can be added to H_{d+1}, as we show using Clifford algebras below. In fact, another candidate mass term $\gamma_{d+1}\tau_x$ is not allowed by TRS and PHS [Eqs. (3b) and (4b)] (here we have assumed $[\mathcal{K},\tau_x] = \{\mathcal{K},\tau_y\} = [\mathcal{K},\tau_z] = 0$ and $\{T,\gamma_{d+1}\} = [C,\gamma_{d+1}] = 0$). The mass term $\gamma_{d+1}\tau_y$ gaps out the two surface Dirac cones and is compatible with TRS and PHS. Physically, this mass term corresponds to dimerization of the "interlayer" hopping, as one can see from the fact that the translation in the x_{d+1} direction ($l \to l+1$) corresponds to an operation of τ_z, and this mass term breaks the translation symmetry as $\{\tau_z, \gamma_{d+1}\tau_y\} = 0$ [10].

The uniqueness of the dimerization mass term $\tilde{\gamma}_0 = \gamma_{d+1}\tau_y$ is understood by considering the extension problem $Cl_{p+1,q+1} \to Cl_{p+1,q+2}$, i.e.,

$$\{\gamma_0, C, CJ, TCJ, J\gamma_1, \ldots, J\gamma_d, J\gamma_{d+1}\tau_z\}$$
$$\to \{\tilde{\gamma}_0, \gamma_0, C, CJ, TCJ, J\gamma_1, \ldots, J\gamma_d, J\gamma_{d+1}\tau_z\}, \tag{18}$$

whose classifying space is again R_{q-p} with $\mathbb{Z}_2$ classification, $\pi_0(R_{q-p}) = \mathbb{Z}_2$ (Table II). Here we have included the original mass term γ_0 and all the kinetic gamma matrices γ_i ($i = 1, \ldots, d+1$) in the Clifford algebra $Cl_{p+1,q+1}$ to be extended, because we are seeking an extra mass term under the fixed representation of those gamma matrices and symmetry operators. Hence the dimerization term that we have found, $\tilde{\gamma}_0 = \gamma_{d+1}\tau_y$, is the unique mass term to gap out the surface Dirac cones of weak $\mathbb{Z}_2$ TIs and TSCs. The gapped d-dimensional surface is a (strong) $\mathbb{Z}_2$ TI or TSC.

Finally, let us discuss Anderson localization of the d-dimensional surface states of $(d+1)$-dimensional weak $\mathbb{Z}_2$ TIs and TSCs. We assume that disorder is weaker than the bulk band gap and changes slowly in space. The disorder potential gives rise to random signs of the dimerization mass M. The surface is then split into gapped regions (domains) of different $\mathbb{Z}_2$ indices, and there appear gapless helical states propagating along the domain boundaries. When we assume uniformity of the disorder-averaged surface and a vanishing mean of the dimerization mass term $M\tilde{\gamma}_0$, we expect that helical domain-wall states should percolate throughout the surface and never be localized. This mechanism is indeed at work for the metallic phase separating two insulating phases with distinct $\mathbb{Z}_2$ topological indices in the phase diagram of disordered two-dimensional insulators in class AII [21]. A similar physics

is known in the integer quantum Hall effect of Dirac fermions, where an unstable critical point between quantum Hall plateaus $\sigma_{xy} = \pm e^2/2h$ is realized under random magnetic fields and random mass, both with zero mean [13]. We thus conclude that, even in the presence of disorder, the surface states of weak $\mathbb{Z}_2$ TIs and TSCs are not localized and remain either metallic or critical, as long as the disorder average of the dimerization mass term vanishes. This conclusion is a natural generalization of the stability of surface states of three-dimensional weak $\mathbb{Z}_2$ topological insulators which was a subject of active research recently [7,8,10,11].

IV. EXAMPLES

In this section we consider three examples of weak $\mathbb{Z}_2$ topological insulators. We start with a three-dimensional weak TI of class AII, which is a stack of two-dimensional strong $\mathbb{Z}_2$ TIs [8,10]. Each TI layer is described as

$$H_{2D} = k_x \sigma_x \tau_x + k_y \tau_y + m(y)\tau_z, \tag{19}$$

where σ_i and τ_i are Pauli matrices ($i = x,y,z$). The Hamiltonian has a TRS with $T = i\sigma_y\mathcal{K}$. The mass $m(y)$ is assumed to have a kink, where a helical edge mode is formed as one of the eigenstates of $\tau_x = -i\tau_y\tau_z$. Here we take $\tau_x = +1$ without loss of generality.

We stack two-dimensional TI layers along the z direction to build a three-dimensional weak TI. The interlayer hopping term for the helical edge states is given by $t\sigma_y\tau_x$, which anticommutes with the gamma matrices in Eq. (19) and T. The effective Hamiltonian for the surface Dirac fermions of the three-dimensional weak TI then reads

$$H_{3D} = k_x \sigma_x + t \sin k_z \sigma_y, \tag{20}$$

where we have suppressed $\tau_x = +1$, since the τ sector is fixed in the helical edge states forming the surface Dirac cones. The original $\mathbb{Z}_2$ classification of two-dimensional TIs implies that there is no extra mass term in this two-dimensional representation with σ_i. However, since we have two valleys of Dirac cones at $k_z = 0$ and π, which we denote by $\rho_z = +1$ and -1 with another set of Pauli matrices ρ_i ($i = x,y,z$), we can find the dimerization mass term $\tilde{m}\sigma_y\rho_y$ which gaps out the surface Dirac cones. This yields the massive surface Dirac Hamiltonian

$$H_{3D} = k_x \sigma_x + t k_z \sigma_y \rho_z + \tilde{m}\sigma_y\rho_y. \tag{21}$$

One can easily verify that $\tilde{m}\sigma_y\tau_x\rho_y$ is the unique mass term that is invariant under $T = i\sigma_y\mathcal{K}$ and anticommutes with all the gamma matrices (τ_z, $\sigma_x\tau_x$, τ_y, $\sigma_y\tau_x\rho_z$). The uniqueness of the mass term means that the gapless surface states are neither gapped nor localized unless the translation symmetry in the layer direction is broken by dimerization. We note that the uniqueness of the mass term in the Dirac Hamiltonian in Eq. (21) was already pointed out in Refs. [8] and [10]. Mong *et al.* studied numerically the Anderson localization of this Hamiltonian with additional time-reversal invariant disorder and showed that the critical point $\tilde{m} = 0$ turns into a metallic phase separating two dimer insulating phases [8].

Next we discuss two examples of two-dimensional weak $\mathbb{Z}_2$ TSCs which are formed as a multileg ladder of

superconducting wires. The first of these is a weak two-dimensional TSC in class D. The BdG Hamiltonian for a one-dimensional spinless p-wave superconductor can be written as

$$H_{\rm 1D} = k_x \sigma_x + m(x)\sigma_z, \qquad (22)$$

where σ denotes particle-hole grading. The Hamiltonian has a PHS ($C = \sigma_x \mathcal{K}$). We introduce a kink in the mass $m(x)$ (which is nothing but the chemical potential of the electrons in the wire) to obtain a Majorana bound state localized at the kink, which is an eigenstate of $\sigma_y = -i\sigma_z\sigma_x$. We can set $\sigma_y = +1$ for the bound state for simplicity. We find that the same operator σ_y can be used as an interchain hopping operator which commutes with C and anticommutes with σ_x and σ_z. A Majorana bound state from each chain is coupled by the interchain hopping term and acquires a kinetic term $t\sigma_y \sin k_y$, where k_y is the momentum along the direction perpendicular to the chain direction x. The Majorana edge states thus formed have two Dirac points ($k_y = 0$ and π), which we denote by $\tau_z = +1$ and -1. We find that the Majorana edge states of the two-dimensional weak TSC are governed by the Hamiltonian

$$H_{\rm 2D} = tk_y \sigma_y \tau_z + \tilde{m}\sigma_y \tau_y, \qquad (23)$$

where $\tilde{m}\sigma_y\tau_y$ is the unique mass term which anticommutes with C and all the gamma matrices (σ_z, σ_x, $\sigma_y\tau_z$). In the presence of disorder the Majorana edge states remain critical (i.e., diverging localization length) as long as the disorder average of the dimerization mass term vanishes [22]. Incidentally, we note that, if we impose a chiral symmetry on this model (which is now in class BDI), the Majorana bound states form a stable flat band at zero energy as follows. In a TSC of class BDI which is described by the Hamiltonian (22) with a chiral symmetry $\Gamma = \sigma_y$, Majorana bound states are again an eigenstate of σ_y. However, the interchain hopping operator σ_y is not available anymore, if we impose the chiral symmetry $\Gamma = \sigma_y$. Hence the Majorana end states remain at zero energy as chiral zero modes and cannot be gapped, which is in agreement with the fact that one-dimensional BDI TSCs are characterized by an integer ($\mathbb{Z}$) topological index.

The last example we discuss in this section is a two-dimensional weak $\mathbb{Z}_2$ TSC in class DIII. We begin with a one-dimensional strong TSC with the Hamiltonian

$$H_{\rm 1D} = k_x \sigma_z \tau_z + m(x)\tau_x, \qquad (24)$$

where we have TRS $T = i\sigma_y \mathcal{K}$ and PHS $C = \sigma_y \tau_y \mathcal{K}$. This Hamiltonian was discussed in Ref. [23] as a model of Rashba wires in proximity to a $s_\pm$-wave superconductor, where we can regard the first term as a spin-orbit coupling and the second as a superconducting pair potential with σ and τ spanning spin and particle-hole degrees of freedom, respectively. At each end of a one-dimensional TSC, a Kramers pair of Majorana bound states appear, and they are an eigenstate of $\sigma_z\tau_y$. We may take the sector of $\sigma_z\tau_y = +1$ in the following discussion. When we stack one-dimensional chains of TSCs along the y direction, we can take $\sigma_x\tau_z \sin k_y$ as a kinetic term due to interchain

hopping. Denoting the two Dirac points at $k_y = 0$ and π by $\rho_z = +1$ and -1, we have the effective Hamiltonian for the Majorana edge states of the two-dimensional weak TSC,

$$H_{\rm 2D} = k_y \sigma_x \tau_z \rho_z + \tilde{m}\sigma_x \tau_z \rho_y, \qquad (25)$$

where $\tilde{m}\sigma_x\tau_z\rho_y$ is again the unique mass term which is compatible with TRS and PHS, and anticommutes with gamma matrices τ_x, $\sigma_z\tau_z$, and $\sigma_x\tau_z\rho_z$. The Majorana edge states should remain critical as long as the edge is uniform on average, i.e., when the dimerization term is absent after disorder average [22].

V. SUMMARY

We have discussed the surface stability of weak $\mathbb{Z}_2$ TIs (TSCs) which are stacked layers of strong $\mathbb{Z}_2$ TIs (TSCs), by examining the topological structure of the surface Dirac Hamiltonians, using Clifford algebras. We have shown the uniqueness of a Dirac mass term which causes scattering between the two surface Dirac cones and gaps them out by inducing dimerization of stacked layers. The dimerized insulating surface is a strong TI (TSC) with a $\mathbb{Z}_2$ index determined by the sign of the unique Dirac mass. Thus the point where the Dirac mass vanishes is a quantum critical point, which either remains to be critical or becomes metallic in the presence of disorder potential with a vanishing mean, i.e., without dimerization.

We note that our discussion based on Dirac Hamiltonians is valid only for small energy scale, where we can linearize the dispersion of gapless surface states. At larger energy scale one should include a quadratic momentum dependence and take into account renormalization of a Dirac mass [24]. Furthermore, when disorder strength is large and comparable with a bulk energy gap, the description with Dirac Hamiltonians is no longer appropriate. In that case, we have to consider original lattice Hamiltonians. Indeed numerical calculations on lattice models have shown that an insulating phase appears at strong disorder [25,26].

Finally, we point out that the physics we discussed here is also relevant for topological crystalline insulators which have gapless surface states protected by spatial symmetries (such as a mirror symmetry) [18,27–29]. An interesting question we may ask is the stability of the gapless surface states when the required spatial symmetry is retained only on average [30,31]. Using Clifford algebras, we can study stability of these gapless surface states against disorder which breaks spatial symmetries, which will be reported elsewhere [32]. This analysis can be applied to topological crystalline insulators with an average mirror symmetry, e.g., $Pb_{1-x}Sn_x Te$ materials where four Dirac cones appear on the (001) surface [27].

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