Homotopy theory of strong and weak topological insulators

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We use homotopy theory to extend the notion of strong and weak topological insulators to the nonstable regime (low numbers of occupied/empty energy bands). We show that for strong topological insulators in d spatial dimensions to be "truly d-dimensional," i.e., not realizable by stacking lower-dimensional insulators, a more restrictive definition of "strong" is required outside the stable regime. However, this does not exclude weak topological insulators from being "truly d-dimensional," which we demonstrate by an example. Additionally, we prove some useful technical results, including the homotopy theoretic derivation of the factorization of invariants over the torus into invariants over spheres in the stable regime, as well as the rigorous justification of the parameter space replacements $T^d \to S^d$ and $T^{d_k} \times S^{d_x} \to S^{d_k+d_x}$ used widely in the current literature.

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I. INTRODUCTION

In recent years, there has been considerable interest in topological phases of band insulators, fueled by their theoretical prediction [1–3] and subsequent experimental realization [4–6] in two- and three-dimensional time-reversal invariant systems. On the theoretical side the obvious question arose: under what circumstances (dimensions, symmetries, etc.) do topological phases occur? For the case of free fermions, a partial answer was given in the seminal paper [7] using K-theory, the result of which is displayed in Table I (the "Periodic Table of topological insulators and superconductors"). It is only a partial answer, since it has the limitation of assuming that the number of occupied as well as empty energy bands is large enough for K-theory to apply. In this *stable regime*, it can be shown using K-theory [7,8] that invariants defined for a torus T^d as momentum space factorize into a product of $\binom{d}{l}$ independent invariants over S^l, where l runs from 0 to d and Table I shows the answer for each l (we give an alternative, homotopy theoretic derivation of this result in Appendix A). This factorization of invariants in the stable regime leads to a natural definition of *strong* topological insulators as those insulators that have a nontrivial invariant in the factor with domain S^d, while the remaining insulators are dubbed *weak* topological insulators [9]. This distinction, which we refer to as the *stable* definition, becomes problematic beyond the stable regime. In this paper, we propose an alternative definition of strong/weak topological insulators outside the stable regime, which defines a topological insulator to be strong if and only if it has a nontrivial invariant over S^d *and all other invariants are trivial*, while all remaining insulators are called weak. The additional restriction is necessary in order to guarantee strong topological insulators to be "truly d-dimensional," meaning that they cannot be realized by stacking lower-dimensional insulators into d dimensions. We demonstrate the necessity of this definition by inspecting a two-dimensional setting in which all topological phases with nontrivial weak invariants have a representative that is obtained by stacking a one-dimensional insulator, irrespective of the value of the strong invariant.

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After formalizing the notion of stacking insulators, we further demonstrate through an example in the stable regime that there may be weak topological insulators that cannot be realized through stacking. In other words, there may be also be "truly d-dimensional" weak topological insulators.

In order for the nonstable definition to be well-defined, we prove that distinct phases over a sphere as momentum space always remain distinct over the torus with the same dimension. By a straightforward generalization, we show that they also always remain distinct over any product of sphere and torus with the same (total) dimension, which provides a rigorous justification for the replacement $S^{d_x} \times T^{d_k} \to S^{d_x+d_k}$ in Ref. [10], where invariants for topological insulators in d_k dimensions with a defect of codimension $d_x + 1$ are calculated.

In this paper, we use the natural notion of homotopy (also known as adiabatic or continuous deformation) as an equivalence relation between insulator ground states. This generalizes two definitions of topological insulators in the current literature: the first one is based on K-theory and the generalization is the extension to the nonstable regime. The second definition, as adopted in Ref. [11], defines an insulator to have nontrivial topology if there is no adiabatic deformation to the atomic limit, where fermions are localized at lattice points. While this second definition already uses the notion of homotopy (=adiabatic deformation), it only distinguishes nontrivial from trivial and is generalized here by the additional distinction between different nontrivial insulators.

II. SETTING AND STATEMENT OF RESULTS

If the symmetry group contains only translations and internal symmetries (those that commute with all translations), any translation invariant free fermion ground state of an insulator can be reduced to a collection of ground states each belonging to one of ten symmetry classes, which we divide into two "complex" and eight "real" ones [12]. A ground state in one of the two complex symmetry classes (upper two rows in Table I) is described by a continuous map

$$\psi : T^d \to C_s, \tag{1}$$

where T^d is the Brillouin zone torus and C_s is either a Grassmannian $\mathrm{Gr}_m(\mathbb{C}^n)$ [13] for even s (class A) describing an n-band model with m filled bands, or a unitary group U_n for odd s describing a $2n$-band model with n filled bands in

TABLE I. This table (the "Periodic Table of topological insulators and superconductors" [7]) lists the sets $[S^d,C_s]^*_{\mathbb{Z}_2}$ for dimensions $0 \leqslant d \leqslant 3$ for the eight real and two complex symmetry classes indexed by s mod 8. In the complex case, the involution on S^d and C_s is trivial, while in the real case, it is nontrivial with fixed point sets S^0 and R_s, respectively.

symmetry		target	fixed point set	$[S^d,C_s]^*_{\mathbb{Z}_2}$			
s	label	C_s	R_s	$d=0$	1	2	3
even	A	$\cup_{m=0}^{n}\mathrm{Gr}_m(\mathbb{C}^n)$	$\cup_{m=0}^{n}\mathrm{Gr}_m(\mathbb{C}^n)$	$\mathbb{Z}_{n+1}$	0	$\mathbb{Z}$	0
odd	AIII	U_n	U_n	0	$\mathbb{Z}$	0	$\mathbb{Z}$
0	D	$\cup_{m=0}^{2n}\mathrm{Gr}_m(\mathbb{C}^{2n})$	O_{2n}/U_n	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
1	DIII	U_{2n}	U_{2n}/Sp_{2n}	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
2	AII	$\cup_{m=0}^{n}\mathrm{Gr}_{2m}(\mathbb{C}^{2n})$	$\cup_{m=0}^{n}\mathrm{Gr}_m(\mathbb{H}^n)$	$\mathbb{Z}_{n+1}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
3	CII	U_{2n}	Sp_{2n}	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$
4	C	$\cup_{m=0}^{2n}\mathrm{Gr}_m(\mathbb{C}^{2n})$	Sp_{2n}/U_n	0	0	$\mathbb{Z}$	0
5	CI	U_n	U_n/O_n	0	0	0	$\mathbb{Z}$
6	AI	$\cup_{m=0}^{n}\mathrm{Gr}_m(\mathbb{C}^n)$	$\cup_{m=0}^{n}\mathrm{Gr}_m(\mathbb{R}^n)$	$\mathbb{Z}_{n+1}$	0	0	0
7	BDI	U_n	O_n	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0

the chiral class AIII. A ground state in one of the eight real classes (eight lower rows in Table I) satisfies the additional requirement

$$\tau_s\left(\psi(k)\right) = \psi(-k), \tag{2}$$

where $\tau_s : C_s \to C_s$ is an involution. This restricts the image of ψ at momenta with $k=-k$ to a subspace $R_s \subset C_s$ (see Table I). An equivalent formulation of condition (2) is to say that ψ is $\mathbb{Z}_2$-*equivariant* with respect to the $\mathbb{Z}_2$-actions generated by $k \mapsto -k$ on T^d and τ_s on C_s. A detailed description of all C_s, R_s, and τ_s can be found in Ref. [12].

A topological phase in this setting is an equivalence class of ground-state maps ψ, denoted $[\psi]$. In this paper, we use the equivalence relation of being homotopic, i.e., two ground states ψ_0 and ψ_1 represent the same class $[\psi_0]=[\psi_1]$ if and only if there is a continuous interpolation ψ_t $(0 \leqslant t \leqslant 1)$ respecting the additional equivariance condition (2) in the real cases. The set of all topological phases in d dimensions will be denoted $[T^d,C_s]$ (homotopy classes of maps $T^d \to C_s$) for the complex classes and $[T^d,C_s]_{\mathbb{Z}_2}$ (homotopy classes of $\mathbb{Z}_2$-equivariant maps $T^d \to C_s$) for the real ones. We will mainly use the latter since it includes the former as the special case with trivial $\mathbb{Z}_2$-actions on T^d and C_s.

As outlined in the Introduction, this definition of a topological phase refines two definitions given in the current literature. One of them views an insulator ground state as a vector bundle of occupied eigenstates (of a Hamiltonian) over the Brillouin zone and defines equivalence classes through the notion of isomorphism of vector bundles [14,15]. These bundles may be constructed using pullback under ψ (the *classifying map*) of the tautological bundle over the Grassmannian [16]. If there is no isomorphism between the vector bundles associated to two ground state maps ψ_0 and ψ_1, then there is no homotopy between them, i.e., $[\psi_0] \neq [\psi_1]$. However, the converse is only true for a large number of empty bands (large $n-m$). The equivalence relation of isomorphism of vector bundles is relaxed further when going to K-theory, where the equivalence relation called *stable equivalence* only requires isomorphism of vector bundles up to direct sums with arbitrary trivial bundles [7,17]. Here, two vector bundles that represent different stable equivalence classes in K-theory are in particular not isomorphic, but the converse is only true for large bundle dimensions (large number m of occupied bands). Therefore the notion of homotopy classes refines that of isomorphism classes of vector bundles, which in turn refines that of stable equivalence in K-theory. Note that the intermediate step of considering isomorphism classes of vector bundles is limited to classes A, AII, and AI, where there are two parameters m and n (see Table I).

The other definition of topological phases [11] uses the atomic limit as a reference ground state, which corresponds to a constant map ψ. It defines an insulator ground state to have nontrivial topology if there exists no adiabatic deformation to the atomic limit. This translates to no homotopy existing to the constant map. Using homotopy as an equivalence relation also refines this definition since it additionally distinguishes between different nontrivial states.

We note here that the notion of homotopy is natural in that it is the direct mathematical formalization of the physical concept of "adiabatically connecting": two ground states can be adiabatically connected *if and only if* there is a homotopy between them. This implies that two insulators in different topological phases cannot be adiabatically connected without a quantum phase transition (closing of the energy gap). While, therefore, the situation is clear for translation invariant, infinitely extended systems, the challenging task remains of establishing the bulk-boundary correspondence, which states that the boundary of a topological insulator is gapless. The bulk-boundary correspondence has been addressed primarily in the stable regime [18–21], but numerical results indicate that it also holds in the nonstable regime [22,23].

We emphasize that the additional, nonstable topological phases introduced by the refining equivalence relation of homotopy rely on a fixed number of (occupied and empty) energy bands. A fixed number of bands is natural in the effective description of superconductors (included here as insulators of quasi-particles), but for normal insulators one may object that adding trivial bands should not change the physics. Indeed, the nonstable invariants are not well defined if further bands are added, but we conjecture that if additional trivial bands are well separated in energy, the physical implications (metallic surface states) of a nontrivial nonstable invariant will remain the same. Similarly, there is no obvious protection against arbitrary amounts of disorder (as already noted in Refs. [22,23]), but the effect of small amounts of disorder remains to be investigated. This problem is shared by so-called topological crystalline insulators [24] (topological insulators with spatial symmetries), which rely on translational invariance. Some optimism can be gained by recent experiments confirming the presence of gapless surface states for these types of materials [25].

Based on the refined definition of equivalence, we propose to define strong topological insulators in the nonstable regime as nontrivial classes in the subset

$$[S^d,Y]_{\mathbb{Z}_2} \subset [T^d,Y]_{\mathbb{Z}_2}, \tag{3}$$

while weak topological insulators are defined as the complement. We will refer to this as the nonstable definition. In Appendix B, we prove that the above inclusion is indeed well-defined for all spaces Y including the physically relevant (products of) classifying spaces. Using similar arguments, we show that there is also an inclusion

$$[S^{d_x+d_k},Y]_{\mathbb{Z}_2} \subset [S^{d_x} \times T^{d_k},Y]_{\mathbb{Z}_2}, \tag{4}$$

a useful technical result for determining topological phases in the presence of (single) defects with codimension $d_x + 1$, which is used (without proof for the nonstable regime) in Ref. [10].

The result (3) and the corresponding nonstable definition is to be contrasted with the well established stable definition (see [9]) of strong/weak. In terms of homotopy theory, the latter is based on the decomposition of $[T^d,C_s]_{\mathbb{Z}_2}$ into a product containing $\binom{d}{l}$ factors of each set $[S^l,C_s]^*_{\mathbb{Z}_2}$ with $l = 0,\ldots,d$:

$$[T^d,C_s]_{\mathbb{Z}_2} \simeq \prod_{l=0}^{d} \left([S^l,C_s]^*_{\mathbb{Z}_2}\right)^{\binom{d}{l}}, \tag{5}$$

where $[X,Y]^*_{\mathbb{Z}_2}$ denotes the set of homotopy classes of equivariant maps $X \to Y$ mapping a base point x_0 in the fixed point set $X^{\mathbb{Z}_2}$ to a base point $y_0 \in Y^{\mathbb{Z}_2}$ with all homotopies respecting this property. This formula holds for all symmetry classes s with a slight modification for classes A, AI, and AII, where we replace C_s by its connected components $(C_s)_0$ containing the base point (i.e., we fix a number of occupied bands) and omit the factor with $l = 0$ on the right-hand side. The decomposition above can be obtained via K-theory [7,8], but we give an independent homotopy theoretic proof in Appendix A.

As an example, consider three-dimensional insulators in class AII [9]. In that case,

$$[T^3,(C_2)_0]_{\mathbb{Z}_2} \simeq \mathbb{Z}_2 \times (\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2), \tag{6}$$

since $[S^3,C_2]^*_{\mathbb{Z}_2} = [S^2,C_2]^*_{\mathbb{Z}_2} = \mathbb{Z}_2$ and $[S^1,C_2]^*_{\mathbb{Z}_2} = 0$ (we use "0" here to denote the set with only one element). According to the stable definition, the strong topological insulators are given by the subset of $[T^d,C_s]_{\mathbb{Z}_2}$ which is nontrivial in the factor $[S^d,C_s]^*_{\mathbb{Z}_2}$ [9]. Here, this gives a set of eight strong topological insulators. In the language of Ref. [9], there is a strong invariant ν_0 and three weak invariants ν_i, $i = 1,2,3$, all taking values 0 or 1 so that every phase is described by the tuple $(\nu_0;\nu_1,\nu_2,\nu_3)$. A strong insulator is any element of the form $(1;\nu_1,\nu_2,\nu_3)$, giving eight possibilities, while the weak topological insulators are the complementary set of eight phases with invariants $(0;\nu_1,\nu_2,\nu_3)$.

To motivate the definition of strong/weak outside the stable regime, consider now the example given by the Hopf topological insulators. These are three-dimensional insulators with one occupied and one empty band in class A. The topological phases for this setting have been computed in Ref. [26] and investigated from a physics perspective in Refs. [22,23]:

$$\begin{aligned}[T^3,\mathrm{Gr}_1(\mathbb{C}^2)] = \{&(n_0;n_1,n_2,n_3) \mid n_1,n_2,n_3 \in \mathbb{Z};\\ &n_0 \in \mathbb{Z} \text{ for } n_1 = n_2 = n_3 = 0 \text{ and}\\ &n_0 \in \mathbb{Z}_{2\cdot\gcd(n_1,n_2,n_3)} \text{ otherwise}\}. \end{aligned}\tag{7}$$

The invariant n_0 is known as the Hopf invariant and the three invariants n_1,n_2,n_3 are the Chern numbers obtained by restricting a representative $\psi : T^3 \to \mathrm{Gr}_1(\mathbb{C}^2)$ to the three independent subtori $T^2 \subset T^3$ (by setting one of the three coordinates to zero). This example shows that the factorization in Eq. (5) may not hold outside the stable regime. In fact, the range of distinct values for the Hopf invariant n_0 is finite unless the Chern numbers satisfy $n_1 = n_2 = n_3 = 0$, in which case $n_0 \in \mathbb{Z} = [S^3,\mathrm{Gr}_1(\mathbb{C}^2)] \subset [T^3,\mathrm{Gr}_1(\mathbb{C}^2)]$. The extended definition that we propose for the nonstable regime only considers the nontrivial elements in this subset to be strong topological insulators. In other words, only phases with invariants $(n_0;0,0,0)$ and $n_0 \neq 0$ are strong, while the rest is weak. In the next section, we will give a further example that demonstrates that only this definition has the property that all strong topological insulators in d dimensions are "truly d-dimensional" (we use this phrase synonymously for the property of not being realizable by stacking lower-dimensional systems).

III. STACKED INSULATORS

Before we introduce the example that motivates the extended definition of strong/weak, we formally describe stacking of insulators into higher dimensions.

Let the translation-invariant Hamiltonian $\hat{H}$ of an n-band model act on the Hilbert space $l^2(\mathbb{Z}^d) \otimes \mathbb{C}^n$ of a d-dimensional lattice. In a basis $\{|x,\alpha\rangle\}$, with $x \in \mathbb{Z}^d$ and $\alpha = 1,\ldots,n$,

$$\hat{H}\,|x,\alpha\rangle := \sum_{x',\beta} h_{\alpha\beta}(x')|x + x',\beta\rangle, \tag{8}$$

where $h_{\alpha\beta}(x') = \overline{h_{\beta\alpha}(-x')}$ in order to ensure hermiticity.

In the following, we will fix the given basis and work only with the matrix $h(x')$. After a Fourier transform, the Bloch Hamiltonian is given by

$$H(k) = \sum_{x\in\mathbb{Z}^d} h(x)e^{i\langle k,x\rangle}, \tag{9}$$

for $k \in T^d$.

We now view $\mathbb{Z}^d$ as being embedded into some bigger lattice $\mathbb{Z}^D$ with $D > d$. In Eq. (8), a canonical embedding is given by letting $x,x' \in \mathbb{Z}^D$ and setting $h_{\alpha\beta}(x') = 0$ whenever $x'_i \neq 0$ for $i = d+1,\ldots,D$. Physically, this means no hopping into the new $D - d$ directions or, equivalently, stacking of the d-dimensional system into these directions.

To generalize the stacking direction, we introduce an invertible, integer D-by-D matrix $A \in \mathrm{GL}_D(\mathbb{Z})$ and define the stacked Hamiltonian to be given by the replacement $h_{\alpha\beta}(x') \mapsto h_{\alpha\beta}(A^{-1}x')$, corresponding to changing the hopping from the x' direction to the Ax' direction.

Defining the projection $P : T^D \to T^d$ by $P(k_1,\ldots,k_D) := (k_1,\ldots,k_d)$, the Bloch Hamiltonian of the stacked system can be expressed by the lower-dimensional Bloch Hamiltonian:

$$\begin{aligned} H_{\text{stack}}(k) &= \sum_{x\in\mathbb{Z}^D} h(A^{-1}x)e^{i\langle k,x\rangle} = \sum_{x\in\mathbb{Z}^D} h(x)e^{i\langle k,Ax\rangle}\\ &= \sum_{x\in\mathbb{Z}^D} h(x)e^{i\langle A^Tk,x\rangle} = \sum_{x\in\mathbb{Z}^d} h(x)e^{i\langle PA^Tk,x\rangle}\\ &= H(PA^Tk). \end{aligned}\tag{10}$$

The change in k-dependence descends to the level of ground-state maps. Therefore given a ground state $\psi : T^d \to C_s$, stacking it in D dimensions according to the matrix A yields a map

$$\psi_{\text{stack}}(k) = \psi(PA^T k). \tag{11}$$

A. Necessity of the new definition

We are now in a position to analyze another example, which will illustrate three points. (1) In general, only nontrivial elements in $[S^d,Y]_{\mathbb{Z}_2} \subset [T^d,Y]_{\mathbb{Z}_2}$ cannot be realized by stacking lower-dimensional systems. (2) Strong invariants can "break down" in the nonstable regime. (3) Fixing base points can make a difference in the nonstable regime.

The model we consider is a two-dimensional system with three bands, one of which is occupied. We assume that the combination $\mathcal{T} \circ \mathcal{I} = \mathcal{I} \circ \mathcal{T}$ of time-reversal $\mathcal{T}$ (with $\mathcal{T}^2 = 1$) and inversion $\mathcal{I}$ (with $\mathcal{I}^2 = 1$) is a symmetry, but individually, both $\mathcal{T}$ and $\mathcal{I}$ symmetries are broken. Since this symmetry does not commute with translations, the setting belongs to the realm of topological crystalline insulators. However, since the symmetry fixes all momenta, the image of any ground-state map lies within the fixed point set $\mathrm{Gr}_1(\mathbb{R}^3) \subset \mathrm{Gr}_1(\mathbb{C}^3)$, so we can consider nonequivariant ground-state maps

$$\psi : T^2 \to \mathrm{Gr}_1(\mathbb{R}^3), \tag{12}$$

which is the setting of the complex symmetry class A with a real instead of complex Grassmannian. The homotopy classification of such maps has been studied in the context of nematics in Refs. [27–29], where the torus plays the role of a measuring surface around closed defect lines. The result, here interpreted as the set of topological phases, is the following (see Appendix C for a derivation):

$$\begin{aligned}[T^2,\mathrm{Gr}_1(\mathbb{R}^3)] = \{(n_0;n_1,n_2) \mid\ & n_1,n_2 \in \mathbb{Z}_2;\\ & n_0 \in \mathbb{N}_0 \text{ for } n_1 = n_2 = 0 \text{ and}\\ & n_0 \in \mathbb{Z}_2 \text{ otherwise}\}.\end{aligned} \tag{13}$$

The strong invariant $n_0 \in \mathbb{N}_0 = [S^2,\mathrm{Gr}_1(\mathbb{R}^3)]$ originates from the mapping degree of maps $S^2 \to S^2$ composed with the projection $S^2 \to S^2/\mathbb{Z}_2 = \mathrm{Gr}_1(\mathbb{R}^3)$. In the language of physics, n_0 represents the skyrmion charge [see Fig. 1(a)]. Note that preserving base points gives $[S^2,\mathrm{Gr}_1(\mathbb{R}^3)]^* = \mathbb{Z}$, on which the fundamental group $[S^1,\mathrm{Gr}_1(\mathbb{R}^3)]^*$ acts via multiplication by -1. Hence, after identification to obtain the unbased classes (see Appendix B), $\mathbb{Z}$ changes to $\mathbb{N}_0$ (skyrmions of charge n_0 are homotopic to ones with charge $-n_0$).

Again, the strong invariants $\mathbb{N}_0$ "break down" to $\mathbb{Z}_2$ in the presence of nontrivial lower-dimensional invariants $n_1,n_2 \in \mathbb{Z}_2 = [S^1,\mathrm{Gr}_1(\mathbb{R}^3)]$, which are nontrivial if they involve a π rotation of lines along the loop, a configuration known as a Moebius strip [see Fig. 1(b) for an example that is canonically embedded into two dimensions].

In this model, *all* classes except those of the form $(n_0;0,0)$ with $n_0 \neq 0$, which correspond to nontrivial elements in $[S^2,\mathrm{Gr}_1(\mathbb{R}^3)] \subset [T^2,\mathrm{Gr}_1(\mathbb{R}^3)]$, have representatives that are stacked versions of one-dimensional systems [27–29] (see Appendix C for details). This gives a total of *seven* stackable classes (four with $n_0 = 0$ and three with $n_0 = 1$), which is remarkable since, naively, the $\mathbb{Z}_2$ classification in one

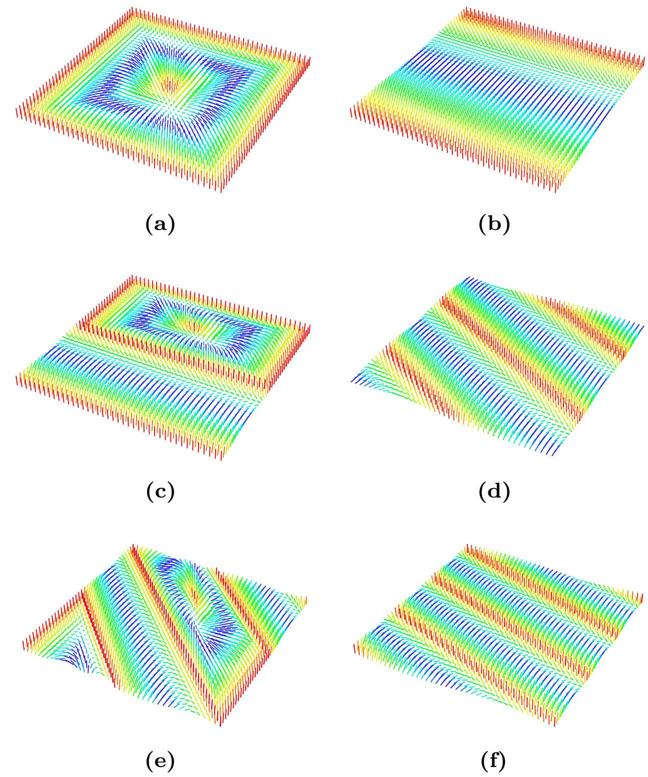

FIG. 1. (Color online) Maps $T^2 \to \mathrm{Gr}_1(\mathbb{R}^3)$ visualized by placing the image of a point (a line in $\mathbb{R}^3$) on the point itself. T^2 is modeled here as a square with periodic boundary conditions. Colors represent the angle to the axis out of the plane. Using the notation $(n_0;n_1,n_2)$, (a) corresponds to $(1;0,0)$, (b) to $(0;1,0)$, (c) and (d) to $(1;1,0)$, and (e) and (f) to $(1;1,1)$. Remarkably, all except (a) are homotopic to stacked one-dimensional insulators.

dimension would suggest only *four* classes ($\mathbb{Z}_2$ in both linearly independent directions and $n_0 = 0$). Hence, in general, only the proposed nonstable definition of strong/weak can guarantee that no stackable strong topological insulators can occur.

Figure 1 illustrates some representatives. While a single skyrmion representing $(1;0,0)$ cannot be realized by stacking, having a skyrmion combined with nontrivial projections allows for this possibility.

B. Weak but not stackable

The following is an example of a weak topological insulator in the stable regime, which cannot be realized through stacking; in two dimensions, consider a $4n$-band model with $2n$ occupied and $2n$ empty bands in class AIII, which has a target space $C_1 = U_{2n}$. Let there be a U_1-symmetry, for example, conservation of the spin S_z-component, which commutes with the chiral operator (which in turn anticommutes with the Hamiltonian). This effectively splits the target U_{2n} into a product $U_n \times U_n$ or, in other words, the ground state can be described as a collection of two class AIII ground states (one for spin up and one for spin down). Thus the ground state is a map

$$\psi : T^2 \to U_n \times U_n \tag{14}$$

and the topological phases (homotopy classes) are given by

$$[T^2,U_n \times U_n] = [T^2,U_n] \times [T^2,U_n] = (\mathbb{Z} \times \mathbb{Z}) \times (\mathbb{Z} \times \mathbb{Z}). \quad (15)$$

Since $[S^2,U_n] = 0$ (only weak topological insulators are possible here) and U_n is connected, the factors $\mathbb{Z}$ originate from $[S^1,U_n] = \mathbb{Z}$. Writing $\psi(k_1,k_2) = (\psi_1(k_1,k_2),\psi_2(k_1,k_2)) \in U_n \times U_n$, the invariants (15) are given by the winding numbers of $\det(\psi_i(k_1,0))$ and $\det(\psi_i(0,k_2))$ for $i = 1,2$.

One-dimensional versions of this model are classified by $[S^1,U_n \times U_n] = \mathbb{Z} \times \mathbb{Z}$, with invariants given by the winding numbers of $\det(\psi_i(k))$ with $i = 1,2$ and $k \in S^1$. Stacking a representative of the class (n,m) according to some matrix $A \in \mathrm{GL}_2(\mathbb{Z})$ yields an element in the class

$$(A_{11}n,A_{11}m) \times (A_{21}n,A_{21}m) \in (\mathbb{Z} \times \mathbb{Z}) \times (\mathbb{Z} \times \mathbb{Z}). \quad (16)$$

Clearly, not all classes can be of this form, the simplest counterexample being $(1,0) \times (0,1)$. The mathematical reason is the fact that $\mathbb{Z} \times \mathbb{Z}$ is not generated by a single element. The physical reason is that the nontrivial winding for spin up happens along a linearly independent direction from that of the nontrivial winding for spin down and therefore there is no corresponding one-dimensional system.

IV. CONCLUSION

We have proposed to use the natural concept of homotopy theory to extend the results from K-theory (and the intermediate step of considering isomorphism classes of vector bundles) beyond the stable regime, which includes *all* insulators independent of the number of occupied/empty bands. We showed that the definition of strong topological insulators has to be more restrictive in the nonstable regime in order to avoid the possibility of a realization by stacking lower-dimensional systems. Furthermore, we demonstrated that there are d-dimensional topological insulators in the stable regime that are "truly d-dimensional" despite being weak, meaning they cannot be realized by stacking lower-dimensional systems.

Along the way, we derived some useful technical results: we showed how the factorization of topological invariants in the stable regime can be understood from the perspective of homotopy theory and proved that in general (in the stable and nonstable regime), it is legitimate to replace a domain consisting of products of spheres by a single sphere of the same total dimension, even in the presence of $\mathbb{Z}_2$-equivariance.

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APPENDIX A: PROOF OF (5)

The crucial feature of the stable regime is a result called *Bott periodicity* [30,31]: denoting by ΩY the space of all based loops in Y, it states that there are maps

$$B_s^{\mathbb{C}} : C_s \to \Omega C_{s-1}, \quad (A1)$$

$$B_s^{\mathbb{R}} : R_s \to \Omega R_{s-1}, \quad (A2)$$

inducing isomorphisms

$$B_{s*}^{\mathbb{C}} : [S^d,C_s]^* \xrightarrow{\sim} [S^d,\Omega C_{s-1}]^* = [S^{d+1},C_{s-1}]^*, \quad (A3)$$

$$B_{s*}^{\mathbb{R}} : [S^d,R_s]^* \xrightarrow{\sim} [S^d,\Omega R_{s-1}]^* = [S^{d+1},R_{s-1}]^*, \quad (A4)$$

for all $1 \leqslant d \leqslant d_{\max}$, where $d_{\max}$ depends on the symmetry class and increases monotonously with m and n. In the stable limit $m,n \to \infty$, we have $d_{\max} \to \infty$ and $B_s^{\mathbb{C}}$ as well as $B_s^{\mathbb{R}}$ become what is called weak homotopy equivalences. The case $d = 0$ may only be included for $B_{s*}^{\mathbb{C}}$ if s is odd and for $B_{s*}^{\mathbb{R}}$ if $s \neq 2,6$. The reason is that the spaces C_s (s even), R_2 and R_6 have $n + 1$ connected components (see Table I), whereas the corresponding right-hand sides of Eqs. (A3) and (A4) are isomorphic to $\mathbb{Z}$. The set $[S^d,Y]^*$ can be equipped with a group structure for $d \geqslant 1$, which is given by concatenation of loops for $d = 1$ and a similar construction using only one coordinate for $d > 1$ [32]. These groups are known as the homotopy groups $\pi_d(Y)$ and the group structure will be important in the following.

Bott periodicity sets apart the stable from the nonstable regime and therefore, not surprisingly, will be central to our proof. This distinction is to be expected from the nonstable examples in the main text, for which (5) does not hold.

The torus T^d is a $\mathbb{Z}_2$-CW complex [33–35] (a space with $\mathbb{Z}_2$-action built by inductively attaching disks of increasing dimensions along their boundary spheres) and as such the relations between homotopy groups give a lot of information about the relations between the sets of topological phases in the different classes. This statement is formalized by the equivariant Whitehead theorem [33–35], which states that the fact that $B_s^{\mathbb{C}}$ is equivariant and restricts to $B_s^{\mathbb{R}}$ (see [36]), both of which induce bijections on homotopy groups for $d \leqslant d_{\max}$ and odd s, implies that $B_s^{\mathbb{C}}$ also induces a bijection

$$B_{s*}^{\mathbb{C}} : [T^d,C_s]_{\mathbb{Z}_2} \xrightarrow{\sim} [T^d,\Omega C_{s-1}]_{\mathbb{Z}_2}, \quad (A5)$$

for $d < d_{\max}$ and odd s.

The last ingredient needed in order to further evaluate the right-hand side of (A5) is the equivariant free loop fibration, which requires the introduction of some notation: if $g \in \mathbb{Z}_2$ is the nontrivial element, then for a space Y with $\mathbb{Z}_2$-action, we denote by $Y^{\mathbb{Z}_2}$ the subset that is fixed under g. An important space is the space of free (i.e., unbased) loops in a space Y, denoted by LY, which is equipped with the $\mathbb{Z}_2$-action $f \mapsto g \circ f \circ g^{-1}$ for $f : S^1 \to Y$ (with the action $g \cdot \phi = -\phi$ on the angle coordinate of S^1). The space of equivariant free loops is then given by $(LY)^{\mathbb{Z}_2}$. The equivariant free loop fibration is a map $p : (LY)^{\mathbb{Z}_2} \to Y^{\mathbb{Z}_2}$ assigning to a free equivariant loop $S^1 \to Y$ its value at a fixed point $s_0 \in (S^1)^{\mathbb{Z}_2} = S^0$. The fiber at a point $y_0 \in Y^{\mathbb{Z}_2}$ is $(\Omega Y)^{\mathbb{Z}_2}$ (based equivariant loops at y_0). Importantly, this fibration has a section $q : Y^{\mathbb{Z}_2} \to (LY)^{\mathbb{Z}_2}$ given by assigning to $y_0 \in Y^{\mathbb{Z}_2}$ the constant loop at y_0, which yields $p \circ q = \mathrm{Id}_{Y^{\mathbb{Z}_2}}$.

All fibrations provide a long exact sequence of homotopy groups. In the case of the equivariant free loop fibration, the existence of the section q implies that this sequence splits into short exact sequences:

$$0 \to \pi_k((\Omega Y)^{\mathbb{Z}_2}) \xrightarrow{i_*} \pi_k((LY)^{\mathbb{Z}_2}) \underset{q_*}{\overset{p_*}{\rightleftarrows}} \pi_k(Y^{\mathbb{Z}_2}) \to 0 \quad \text{(A6)}$$

for all $k \geqslant 0$, where i_* is induced by the inclusion i of the fiber $(\Omega Y)^{\mathbb{Z}_2}$ into $(LY)^{\mathbb{Z}_2}$. As stated previously, π_k has a group structure for $k \geqslant 1$ and in that case, all maps in Eq. (A6) are homomorphisms. In this situation, every element of $\pi_k((LY)^{\mathbb{Z}_2})$ can be written uniquely as a sum $i_*[a] + s_*[b]$ for $[a] \in \pi_k((\Omega Y)^{\mathbb{Z}_2})$ and $[b] \in \pi_k(Y^{\mathbb{Z}_2})$. In other words,

$$\pi_k((LY)^{\mathbb{Z}_2}) \overset{\text{as sets}}{\simeq} \pi_k((\Omega Y)^{\mathbb{Z}_2}) \times \pi_k(Y^{\mathbb{Z}_2}). \quad \text{(A7)}$$

The fact that this decomposition only works for $k \geqslant 1$ is crucial: the left-hand side of (A5), which we want to evaluate in the end, is the same as $\pi_0((L^d C_s)^{\mathbb{Z}_2})$. Here, $(L^d C_s)^{\mathbb{Z}_2}$ is the d-fold iterated equivariant free loop space of C_s, which is the space of equivariant maps from T^d to C_s and π_0 is the set of its connected components. In other words, it is the set of d-dimensional topological phases in symmetry class s. Equations (7) and (13) show that the decomposition cannot work in general at the level of π_0, and consequently, we really need to go to the loop space ΩC_{s-1} in order to arrive at the case $k = 1$ and complete the proof:

$$\begin{aligned}[T^d, C_s]_{\mathbb{Z}_2} &\simeq [T^d, \Omega C_{s-1}]_{\mathbb{Z}_2} \\ &\simeq \pi_1((L^d C_{s-1})^{\mathbb{Z}_2}) \\ &\simeq \pi_1((L^{d-1}\Omega C_{s-1})^{\mathbb{Z}_2}) \times \pi_1((L^{d-1} C_{s-1})^{\mathbb{Z}_2}) \\ &\vdots \\ &\simeq \prod_{l=0}^{d} [\pi_1((\Omega^l C_{s-1})^{\mathbb{Z}_2})]^{\binom{d}{l}} \\ &\simeq \prod_{l=0}^{d} [(\pi_0((\Omega^l C_s)^{\mathbb{Z}_2})]^{\binom{d}{l}} \\ &\simeq \prod_{l=0}^{d} \left([S^l, C_s]^*_{\mathbb{Z}_2}\right)^{\binom{d}{l}}. \end{aligned} \quad \text{(A8)}$$

In the second to last equality, the equivariant Whitehead theorem was used again (this time in its base-point preserving version) in order to arrive at a result for the target space C_s. This completes the proof for both the real and the complex classes (the latter are included by choosing trivial $\mathbb{Z}_2$-actions) with odd s.

For even s, the requirements for the equivariant Whitehead theorem are not met since the complex Bott maps $B^{\mathbb{C}}_{s*}$ in Eq. (A3) are not a bijection for $d = 0$. This shortcoming is remedied by replacing C_s by its connected component $(C_s)_0$ containing the base point as well as ΩC_{s-1} by its connected component $(\Omega C_{s-1})_0$ containing the constant loop at the base point of C_{s-1}. The equivariant Whitehead theorem then gives a bijection

$$[T^d, (C_s)_0]_{\mathbb{Z}_2} \simeq [T^d, (\Omega C_{s-1})_0]_{\mathbb{Z}_2}. \quad \text{(A9)}$$

The right-hand side of this equation is a subset of $[T^d, \Omega C_{s-1}]_{\mathbb{Z}_2}$. It can be identified in the decomposition in Eq. (A8) as the subset with the factor $\pi_1(C^{\mathbb{Z}_2}_{s-1}) = \pi_1(R_{s-1})$ replaced by $\ker((i_{s-1})_*) \subset \pi_1(R_{s-1})$, where

$$(i_{s-1})_* : \pi_1(R_{s-1}) \to \pi_1(C_{s-1}) \quad \text{(A10)}$$

is the induced map of the inclusion $i_{s-1} : R_{s-1} \hookrightarrow C_{s-1}$.

For the real classes with $s \neq 2,6$, $\ker((i_{s-1})_*) = \pi_1(R_{s-1})$ and $[T^d, C_s]_{\mathbb{Z}_2} = [T^d, (C_s)_0]_{\mathbb{Z}_2}$, where the latter follows from the observation that for $s \neq 2,6$, $R_s \subset (C_s)_0$ and therefore the image of equivariant maps from T^d is always contained in $(C_s)_0$. Thus the result in these cases is equivalent to the result for odd s. In the symmetry classes A, AII ($s = 2$) and AI ($s = 6$), the set $\ker((i_{s-1})_*)$ contains only one element and $[T^d, C_s]_{\mathbb{Z}_2} \neq [T^d, (C_s)_0]_{\mathbb{Z}_2}$, so the result needs to be modified as stated below Eq. (5).

APPENDIX B: PROOF OF (3) AND (4)

In this section, we give a proof of the following theorem [Eqs. (3) and (4)].

Theorem 1. There are inclusions

$$\begin{aligned}[S^d, Y]_{\mathbb{Z}_2} &\subset [T^d, Y]_{\mathbb{Z}_2} \\ [S^{d_x+d_k}, Y]_{\mathbb{Z}_2} &\subset [S^{d_x} \times T^{d_k}, Y]_{\mathbb{Z}_2}.\end{aligned}$$

The first line allows defining *strong* topological insulators as nontrivial elements of the left-hand side, while the second line shows that in the presence of defects with codimension $d_x + 1$, one may replace the product of sphere and torus by a single sphere of equal total dimension, at the cost of potentially missing nontrivial classes.

As a model for maps from both torus and sphere, we will use the d-dimensional cube $[-\pi,\pi]^d$ as the domain, with coordinates $-\pi \leqslant x_i \leqslant \pi$, $i = 1,\ldots,d$. Maps from the torus are realized by requiring them to be periodic in all directions (same values on opposing sides of the cube), while maps from the sphere are required to map the entire boundary of the cube to a single point. The action of $\mathbb{Z}_2$ on the cube is given coordinatewise as either $x_i \mapsto -x_i$ (nontrivial or momentumlike) or $x_i \mapsto +x_i$ (trivial or positionlike), which gives a total of 2^d possible actions.

A crucial ingredient in the proof is the $\mathbb{Z}_2$-equivariant version of the relation between homotopy classes of maps with fixed basepoints, denoted $[S^d, Y]^*_{\mathbb{Z}_2}$, and those without fixed basepoints, denoted $[S^d, Y]_{\mathbb{Z}_2}$. If the fixed point set $Y^{\mathbb{Z}_2}$ is connected, then any representative of an unbased class can be homotoped to a based map (we assume that the basepoint $y_0 \in Y^{\mathbb{Z}_2}$). However, two based maps that represent different elements in $[S^d, Y]^*_{\mathbb{Z}_2}$ may represent the same element in $[S^d, Y]_{\mathbb{Z}_2}$, meaning there can be an unbased homotopy even though no based one exists. This unbased homotopy takes the image of the basepoint $s_0 \in (S^d)^{\mathbb{Z}_2}$ to a loop in $Y^{\mathbb{Z}_2}$ and identifying all based maps up to these loops gives a bijection [37,38]:

$$[S^d, Y]_{\mathbb{Z}_2} \simeq [S^d, Y]^*_{\mathbb{Z}_2} / [S^1, Y^{\mathbb{Z}_2}]^*. \quad \text{(B1)}$$

If $Y^{\mathbb{Z}_2}$ is disconnected, we denote by $Y^{\mathbb{Z}_2}_0$ the component containing the base point and introduce the notation $[(X,x_0),(Y,Z)]_{\mathbb{Z}_2}$ for equivariant homotopy classes of maps $X \to Y$, which map $x_0 \in X$ to $Z \subset Y$. For example, given base points $s_0 \in S^d$ and $y_0 \in Y^{\mathbb{Z}_2} \subset Y$, we have $[S^d, Y]^*_{\mathbb{Z}_2} = [(S^d, s_0),(Y,\{y_0\})]_{\mathbb{Z}_2}$. Then Eq. (B1) holds in the

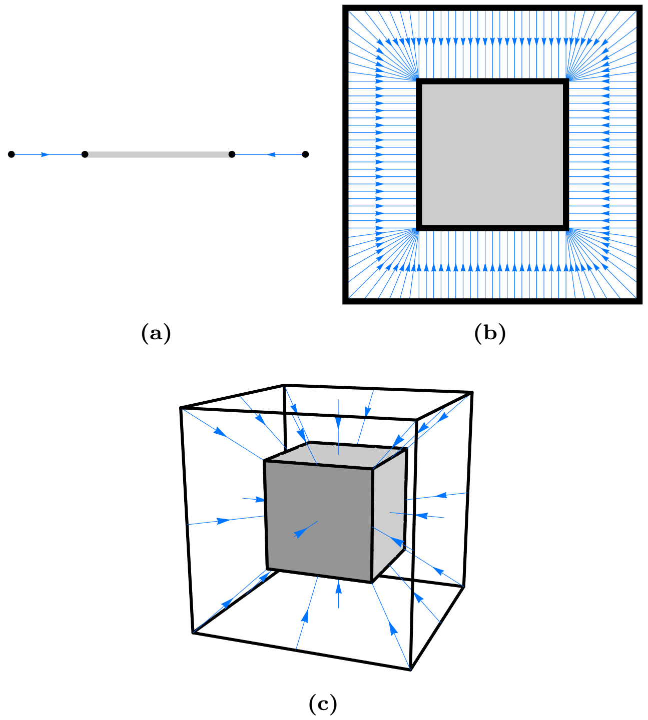

FIG. 2. (Color online) The domain of $b_d(\gamma, f)$ for (a) $d = 1$, (b) $d = 2$, and (c) $d = 3$. The loop γ is represented in blue with an arrow indicating the direction in which it is traversed and the domain of f is depicted in gray. In (a) and (b), black points are mapped to the base point $y_0 \in Y^{\mathbb{Z}_2}$. In (c), the entire surfaces of the two cubes are mapped to y_0.

following, modified form:

$$\left[(S^d,s_0),\left(Y,Y_0^{\mathbb{Z}_2}\right)\right]_{\mathbb{Z}_2} \simeq [S^d,Y]^*_{\mathbb{Z}_2}/[S^1,Y^{\mathbb{Z}_2}]^*. \tag{B2}$$

In fact, Eqs. (B1) and (B2) hold more generally with S^d replaced by any $\mathbb{Z}_2$-CW complex, though this will not be needed in the present paper.

The identifications (B1) and (B2) have a simple geometrical interpretation: the boundary of $S^d = [-\pi,\pi]^d$ is always a fixed point of the $\mathbb{Z}_2$-action and as such it has to map to $Y^{\mathbb{Z}_2}$. A loop γ representing a class in $[S^1,Y^{\mathbb{Z}_2}]^*$ now acts on a representative f of a class in $[S^d,Y]^*_{\mathbb{Z}_2}$ by moving the image point of the boundary along γ to give a map $b_d(\gamma, f) : S^d \to Y$ (see Fig. 2). In formulas,

$$b_d(\gamma,f)(x) := \begin{cases} f(2x) & \text{for } |x| \leqslant \frac{\pi}{2}, \\ \gamma(3\pi - 4|x|) & \text{for } |x| > \frac{\pi}{2}, \end{cases} \tag{B3}$$

where $|x| := \max(x_i)_{i=1\ldots d}$.

Although defined on the level of representatives, Eq. (B3) yields a well-defined action on the level of homotopy classes and the orbit of this action is identified on the right-hand side of (B1) and (B2). In the following special case, the map b_d simplifies considerably, which will later be crucial for the proof of the theorem:

Lemma 1. For $[\gamma] \in [S^1,(LY)^{\mathbb{Z}_2}]^*$ and $[f] \in [S^d,\Omega Y]^*_{\mathbb{Z}_2}$,

$$[b_d(\gamma,f)] = [b_{d+1}(\gamma(\cdot)(0),f)] \text{ in } [S^d,LY]^*_{\mathbb{Z}_2}. \tag{B4}$$

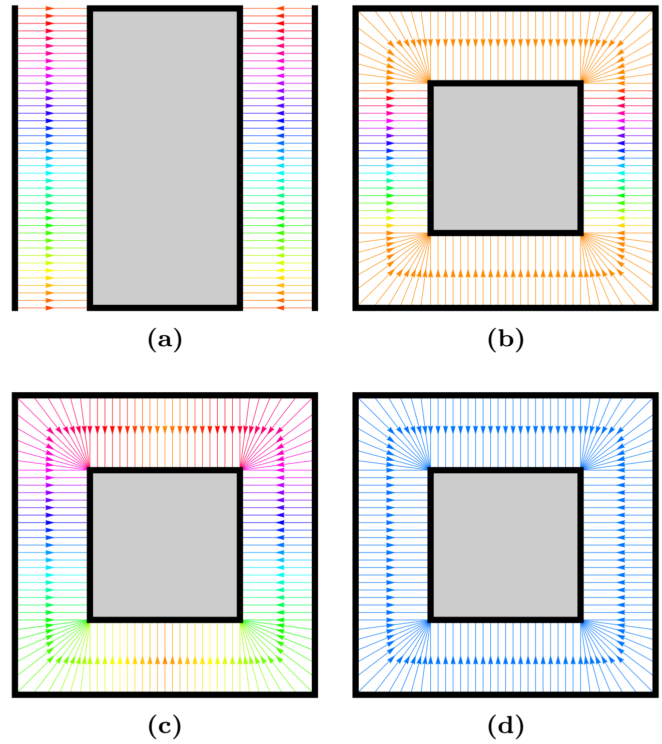

FIG. 3. (Color online) Steps in the proof of lemma 1 for $d = 1$. The gray area corresponds to the domain of $f : S^1 \to \Omega Y$ interpreted as a map $S^2 \to Y$. All black lines are mapped to the base point of Y. (a) shows the domain of $b_1(\gamma, f)$, in this case given by conjugation of f by $\gamma : S^1 \to (LY)^{\mathbb{Z}_2}$. The latter can be viewed as a free loop of based loops (colored lines) and arrows indicate the direction in which the based loops are traversed. (b) shows the result of applying the homotopy of the upper and lower sides to the constant map, giving the configuration with α_0. The stage at $\alpha_1 = \beta_0$ is shown in (c), while (d) depicts the final configuration with β_1, which corresponds to the domain of $b_2(\gamma(\cdot)(0), f)$.

On the right-hand side of the equation, f is interpreted as a map $S^{d+1} \to Y$.

Proof. The map γ is a based loop of free loops with base point being the constant loop at $y_0 \in Y$. Alternatively, it may be viewed as a free loop of based loops by switching the two loop coordinates. The latter interpretation is shown in Fig. 3(a) for $d = 1$, where lines with arrows represent based loops. The fact that this is a free loop of based loops is indicated by the color code: All these loops may be different, but there are periodic boundary conditions (the top based loop is the same as the lowest one, both being shown in orange).

The map $b_d(\gamma, f)(\cdot, \pm\pi)$ is homotopic to $f(\cdot)(\pm\pi)$, since $f(x)(\pm\pi) = y_0$ and the action fixes the neutral element. This can be seen in Fig. 3(a) for $d = 1$; the upper and lower boundaries correspond to the concatenation of the based loop $\gamma(\cdot)(\pm\pi)$ (orange), the constant loop $f(\cdot)(\pm\pi)$ (black), and the reversed version of $\gamma(\cdot)(\pm\pi)$ (orange, reversed arrow). This combination is clearly homotopic to the constant loop and this homotopy is used to arrive at Fig. 3(b).

For the next homotopies, the central part of the cube $[-\pi,\pi]^{d+1}$, which is associated with f (gray area in Fig. 3), will remain invariant. The surrounding part is equivalent to a map $S^d \to \Omega Y$, but since we will only use special homotopies that leave the part with $x_{d+1} = 0$ invariant [the blue loops in Fig. 3(b)], we will restrict to only one hemisphere of S^d, which is a disk D^d. The same homotopies will be applied to the other hemisphere.

We introduce the radial coordinate $0 \leqslant r \leqslant 1$ of D^d, which corresponds to $x_1 = \cdots = x_d = 0$ at $r = 0$ and to $x_{d+1} = 0$ at $r = 1$. The result of using the null homotopy of $b_d(\gamma, f)(\cdot, \pm\pi)$ is a map $\alpha_0 : D^d \to \Omega Y$ depicted for $d = 1$ in Fig. 3(b) and given in general by

$$\alpha_0(r) := \begin{cases} \gamma(\pi) & \text{for} \quad r \leqslant \frac{1}{2}, \\ \gamma(2\pi(1-r)) & \text{for} \quad r > \frac{1}{2}, \end{cases} \tag{B5}$$

The first homotopy is given by

$$\alpha_t(r) := \begin{cases} \gamma(\pi) & \text{for} \quad r \leqslant \frac{1-t}{2}, \\ \gamma\left(\frac{2\pi}{1+t}(1-r)\right) & \text{for} \quad r > \frac{1-t}{2}, \end{cases} \tag{B6}$$

where $0 \leqslant t \leqslant 1$. For $d = 1$, this corresponds to the step from Fig. 3(b) to Fig. 3(c); the former shows $\alpha_0 : D^1 \to \Omega Y$, which maps to the orange loop at $r = 0$ and to the blue loop at $r = 1$. The homotopy α_t pushes the orange region completely to $r = 0$ while "stretching" the remainder accordingly, which results in α_1 shown in Fig. 3(c).

Subsequently, all other loops are also pushed to $r = 0$ and "annihilate," leaving only the blue one. In formulas, this second homotopy is given by

$$\beta_t(r) := \gamma\left(\pi(1-r)(1-t)\right), \tag{B7}$$

where $\beta_0 = \alpha_1$. Since all $\mathbb{Z}_2$-actions introduced for $[-\pi,\pi]^{d+1}$ fix the radial coordinate r and all homotopies depend only on r, they all go through equivariant maps.

For the next lemma, we use lemma 1 to show that the homotopy classes of maps with periodic boundary conditions in one coordinate of $[-\pi,\pi]^d$ include the classes of maps that map to a fixed point at the edges of that interval.

Lemma 2.

$$\left[(S^d,s_0),\left(LY,(LY)_0^{\mathbb{Z}_2}\right)\right]_{\mathbb{Z}_2} \supset \left[(S^{d+1},s_0),\left(Y,Y_0^{\mathbb{Z}_2}\right)\right]_{\mathbb{Z}_2} \tag{B8}$$

Proof.

$$\begin{aligned} &\left[(S^d,s_0),\left(LY,(LY)_0^{\mathbb{Z}_2}\right)\right]_{\mathbb{Z}_2} \\ &\quad = [S^d,LY]^*_{\mathbb{Z}_2}/[S^1,(LY)^{\mathbb{Z}_2}]^* && \text{(B9)} \\ &\quad = [S^1,\Omega^d Y]_{\mathbb{Z}_2}/[S^1,(LY)^{\mathbb{Z}_2}]^* && \text{(B10)} \\ &\quad \supset \left[(S^1,s_0),\left(\Omega^d Y,(\Omega^d Y)_0^{\mathbb{Z}_2}\right)\right]_{\mathbb{Z}_2}/[S^1,(LY)^{\mathbb{Z}_2}]^* && \text{(B11)} \\ &\quad = \left([S^1,\Omega^d Y]^*_{\mathbb{Z}_2}/[S^1,(\Omega^d Y)^{\mathbb{Z}_2}]^*\right)/[S^1,(LY)^{\mathbb{Z}_2}]^* && \text{(B12)} \\ &\quad = [S^1,\Omega^d Y]^*_{\mathbb{Z}_2}/[S^1,Y^{\mathbb{Z}_2}]^* && \text{(B13)} \\ &\quad = \left[(S^{d+1},s_0),\left(Y,Y_0^{\mathbb{Z}_2}\right)\right]_{\mathbb{Z}_2}. && \text{(B14)} \end{aligned}$$

This chain of equalities and inclusions needs some explanation. We first use the relation (B2) between based and unbased homotopy classes to arrive at (B9). Then, for Eq. (B10), the perspective is changed to viewing the (free) loop parameter of LY as the domain and the d coordinates of S^d as the domain of elements in $\Omega^d Y$. Importantly, this effects a change from based homotopy classes to unbased ones. The inclusion (B11) is well defined on the quotient since $(\Omega^d Y)_0^{\mathbb{Z}_2}$ is fixed under conjugation by elements in $(LY)^{\mathbb{Z}_2}$. Having arrived at (B12) by again using (B2), we use lemma 1 to homotope the action of elements in $[S^1,(\Omega^d Y)^{\mathbb{Z}_2}]^*$ as well as $[S^1,(LY)^{\mathbb{Z}_2}]^*$ to the action of some element in $[S^1,Y^{\mathbb{Z}_2}]^*$, yielding (B13). In the last step, we use (B2) again to complete the proof.

We are now equipped to prove theorem 1. For the case without defects, if $Y^{\mathbb{Z}_2}$ is connected,

$$\begin{aligned} [T^d,Y]_{\mathbb{Z}_2} &= [S^1,L^{d-1}Y]_{\mathbb{Z}_2} \\ &\supset \left[(S^1,s_0),\left(L^{d-1}Y,(L^{d-1}Y)_0^{\mathbb{Z}_2}\right)\right]_{\mathbb{Z}_2} \\ &\supset \left[(S^2,s_0),\left(L^{d-2}Y,(L^{d-2}Y)_0^{\mathbb{Z}_2}\right)\right]_{\mathbb{Z}_2} \\ &\supset \cdots \\ &\supset \left[(S^{d-1},s_0),\left(LY,(LY)_0^{\mathbb{Z}_2}\right)\right]_{\mathbb{Z}_2} \\ &\supset \left[(S^d,s_0),\left(Y,Y_0^{\mathbb{Z}_2}\right)\right]_{\mathbb{Z}_2} \\ &= [S^d,Y]_{\mathbb{Z}_2}. \end{aligned} \tag{B15}$$

If $Y^{\mathbb{Z}_2}$ has several components $Y_n^{\mathbb{Z}_2}$, we repeat the above steps for different base points $y_0 \in Y_n^{\mathbb{Z}_2}$ to obtain

$$\begin{aligned} [T^d,Y]_{\mathbb{Z}_2} &= \coprod_n \left[(T^d,s_0),\left(Y,Y_n^{\mathbb{Z}_2}\right)\right]_{\mathbb{Z}_2} \\ &\supset \coprod_n \left[(S^d,s_0),\left(Y,Y_n^{\mathbb{Z}_2}\right)\right]_{\mathbb{Z}_2} \\ &= [S^d,Y]_{\mathbb{Z}_2}. \end{aligned} \tag{B16}$$

In the presence of defects, similar steps lead to the result of theorem 1. Assuming again that $Y^{\mathbb{Z}_2}$ is connected,

$$\begin{aligned} [S^{d_x} \times T^{d_k},Y]_{\mathbb{Z}_2} &= [S^{d_x},L^{d_k}Y]_{\mathbb{Z}_2} \\ &\supset \left[(S^{d_x},s_0),\left(L^{d_k}Y,(L^{d_k}Y)_0^{\mathbb{Z}_2}\right)\right]_{\mathbb{Z}_2} \\ &\supset \left[(S^{d_x+1},s_0),\left(L^{d_k-1}Y,(L^{d_k-1}Y)_0^{\mathbb{Z}_2}\right)\right]_{\mathbb{Z}_2} \\ &\supset \left[(S^{d_x+2},s_0),\left(L^{d_k-2}Y,(L^{d_k-2}Y)_0^{\mathbb{Z}_2}\right)\right]_{\mathbb{Z}_2} \\ &\supset \cdots \\ &\supset \left[(S^{d_x+d_k-1},s_0),\left(LY,(LY)_0^{\mathbb{Z}_2}\right)\right]_{\mathbb{Z}_2} \\ &\supset \left[(S^{d_x+d_k},s_0),\left(Y,Y_0^{\mathbb{Z}_2}\right)\right]_{\mathbb{Z}_2} \\ &= [S^{d_x+d_k},Y]_{\mathbb{Z}_2}. \end{aligned} \tag{B17}$$

By the same argument as in Eq. (B16), the result generalizes to disconnected $Y^{\mathbb{Z}_2}$ by repeating the above for base points in all different components. This completes the proof of theorem 1.

APPENDIX C: STACKED SKYRMIONS

In this part of the Appendix, we give the mathematical reasons for the following two aspects of the nonstable regime: (1) strong invariants may "break down" in the presence of weak ones and (2) phases outside the subset $[S^d,Y]_{\mathbb{Z}_2} \subset [T^d,Y]_{\mathbb{Z}_2}$ may be realized by stacking lower-dimensional insulators. We will use the example introduced in Eq. (12), which exhibits both of the above features and which can be formulated in a nonequivariant setting (hence there are no $\mathbb{Z}_2$ subscripts in the following). Its topological phases are the set $[T^2,\mathrm{Gr}_1(\mathbb{R}^3)]$, which will be determined in the following, leading to the result in Eq. (13). We first outline a procedure to compute $[T^2,Y]$ in general and then specialize to $Y = \mathrm{Gr}_1(\mathbb{R}^3)$.

Denoting by $(LY)_n$ the nth connected component of the free loop space LY, the set $[T^2,Y]$ is a disjoint union of subsets labeled (n_1,n_2), which contain classes whose representatives restrict to $(LY)_{n_1}$ on $S^1 \times \{s_0\}$ and to $(LY)_{n_2}$ on $\{s_0\} \times S^1$. Notice that the number of elements in a sector (n_1,n_2) is the same as in (n_2,n_1).

The number of elements in a subset (n_1,n_2) can be determined by computing $[S^1,(LY)_{n_1}]$ and counting the elements that map to $(LY)_{n_2}$ under the map p_* induced by the evaluation map. For our concrete example $Y = \mathrm{Gr}_1(\mathbb{R}^3)$, the free loop space LY has two connected components, which we denote by $(LY)_0$ (containing the constant map) and $(LY)_1$ [containing all nontrivial loops, which are freely homotopic to elements in the nontrivial class of $\pi_1(\mathrm{Gr}_1(\mathbb{R}^3)) = \mathbb{Z}_2$].

For our example, it will turn out that $\pi_1((LY)_1)$ is Abelian and therefore [cf. Eq. (B1)]

$$[S^1,(LY)_1] \simeq \pi_1\left((LY)_1\right). \tag{C1}$$

Choosing a base point in $(LY)_1$, the long exact sequence associated to the free loop fibration contains the right-hand side of the above equation and reads

$$\begin{array}{ccccccccc} \pi_2(Y) & \xrightarrow{\partial_2} & \pi_1\left((\Omega Y)_1\right) & \xrightarrow{i_*} & \pi_1\left((LY)_1\right) & \xrightarrow{p_*} & \pi_1(Y) & \xrightarrow{\partial_1} & \pi_0\left((\Omega Y)_1\right). \\ \| & & \| & & & & \| & & \| \\ \mathbb{Z} & & \mathbb{Z} & & & & \mathbb{Z}_2 & & 0 \end{array}$$

This exact sequence is *not* split as the one with a base point in $(LY)_0$ in Eq. (A6). This entails the fact that $[S^1,(LY)_1] \neq [S^2,Y] \times [S^1,Y] = \mathbb{N}_0 \times \mathbb{Z}_2$, since the first map ∂_2 is *not* the constant map as in the split case, but rather multiplication by -2 [28]. Indeed, exactness implies that $\pi_1((LY)_1)$ must be a group with exactly four elements, leaving only the possibilities $\mathbb{Z}_2 \times \mathbb{Z}_2$ or $\mathbb{Z}_4$. In either case, it is an Abelian group as previously claimed and therefore $[S^1,(LY)_1]$ also contains only four elements (rather than infinitely many). This explains how strong invariants can break down.

The other point, that phases outside the subset $[S^d,Y] \subset [T^d,Y]$ may be stacked, is explained by the fact that $\pi_1((LY)_1) = \mathbb{Z}_4$ rather than $\mathbb{Z}_2 \times \mathbb{Z}_2$ [27]. If $\psi : S^1 \to \mathrm{Gr}_1(\mathbb{R}^3)$ is a nontrivial topological insulator in one dimension, i.e., represents the nontrivial class in $\pi_1(\mathrm{Gr}_1(\mathbb{R}^3)) = \mathbb{Z}_2$, then the generator of $\pi_1((LY)_1) = \mathbb{Z}_4$ is represented by $\psi(k_1 + k_2)$, where k_1 is the coordinate associated to π_1 and k_2 is the free loop coordinate. Since the group structure in π_1 is concatenation of loops, the other elements in $\mathbb{Z}_4$ are represented respectively by

$$\psi(mk_1 + k_2), \tag{C2}$$

with $m = 0,1,2,3$. These configurations are illustrated in Figs. 1(b) ($m = 0$), 1(d) ($m = 2$), and 1(f) ($m = 3$). The ones with even m belong to the sector (1,0), while the ones with odd m belong to the sector (1,1). All of these maps correspond to the one-dimensional nontrivial insulator stacked along the $(-1,m)$ direction of the two-dimensional lattice $\mathbb{Z}^2$.

The above implies that the sectors (1,1), (1,0) and therefore also the sector (0,1) contain two elements, all of which can be realized by stacking. Together with the result of Appendix B, which states that the sector (0,0) is in bijection with $[S^2,\mathrm{Gr}_1(\mathbb{R}^3)] = \mathbb{N}_0$, the result (13) follows. Of the sector (0,0) only the constant map can be realized by stacking, giving a total of *seven* (rather than the naively expected *four*) stacked topological insulators. The only topological phases that cannot be realized by stacking here are precisely the nontrivial elements in the subset $\mathbb{N}_0 = [S^2,\mathrm{Gr}_1(\mathbb{R}^3)] \subset [T^2,\mathrm{Gr}_1(\mathbb{R}^3)]$.

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