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# Topological insulators and superconductors: tenfold way and dimensional hierarchy

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**Abstract.** It has recently been shown that in every spatial dimension there exist precisely five distinct classes of topological insulators or superconductors. Within a given class, the different topological sectors can be distinguished, depending on the case, by a $\mathbb{Z}$ or a $\mathbb{Z}_2$ topological invariant. This is an exhaustive classification. Here we construct representatives of topological insulators and superconductors for all five classes and in arbitrary spatial dimension $d$, in terms of Dirac Hamiltonians. Using these representatives we demonstrate how topological insulators (superconductors) in different dimensions and different classes can be related via 'dimensional reduction' by compactifying one or more spatial dimensions (in 'Kaluza–Klein'-like fashion). For $\mathbb{Z}$-topological insulators (superconductors) this proceeds by descending by one dimension at a time into a different class. The $\mathbb{Z}_2$-topological insulators (superconductors), on the other hand, are shown to be lower-dimensional descendants of parent $\mathbb{Z}$-topological insulators in the same class, from which they inherit their topological properties. The eightfold periodicity in dimension $d$ that exists for topological insulators (superconductors) with Hamiltonians satisfying at least one reality condition (arising from time-reversal or charge-conjugation/particle–hole symmetries)

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is a reflection of the eightfold periodicity of the spinor representations of the orthogonal groups SO($N$) (a form of Bott periodicity). Furthermore, we derive for general spatial dimensions a relation between the topological invariant that characterizes topological insulators and superconductors with chiral symmetry (i.e., the winding number) and the Chern–Simons invariant. For lower-dimensional cases, this formula relates the winding number to the electric polarization ($d = 1$ spatial dimensions) or to the magnetoelectric polarizability ($d = 3$ spatial dimensions). Finally, we also discuss topological field theories describing the spacetime theory of linear responses in topological insulators (superconductors) and study how the presence of inversion symmetry modifies the classification of topological insulators (superconductors).

## Contents

## 1. Introduction

Topological insulators (superconductors) are gapped phases of non-interacting fermions which exhibit topologically protected boundary modes. These boundary states are gapless, with extended wavefunctions, and protected against arbitrary deformations (or perturbations) of the Hamiltonian, as long as the generic symmetries (such as e.g. time-reversal symmetry) of the Hamiltonian are preserved and the bulk gap is not closed[7]. The different phases within a given topological insulator (superconductor) are characterized by a topological invariant, which is either an integer Chern/winding number or a $\mathbb{Z}_2$ quantity. The integer quantum Hall effect (IQHE) is the best-known example of such a phase. In the IQHE, the transverse (Hall) electrical conductance $\sigma_{xy}$ carried by edge states is quantized and is proportional to the topologically invariant Chern number [1, 2][8]. As a consequence of the quantization of the Hall conductance $\sigma_{xy}$, two different quantum Hall states with different values of $\sigma_{xy}$ cannot be adiabatically connected without closing the energy gap in the bulk. They therefore represent distinct 'topologically ordered' phases that are separated by a quantum phase transition (figure 1(a)).

Other examples of gapped topological phases are the (spinless) chiral $p_x + \mathrm{i}p_y$ superconductor [8], which breaks time-reversal symmetry ($\mathcal{T}$), and the quantum spin Hall (QSH) states [9]–[15], which are time-reversal invariant. In the former case, the topological features in question are those of the fermionic quasiparticle excitations deep in the superconducting phase, whose dynamics is described by the Bogoliubov–de Gennes (BdG) Hamiltonian[9]. The BdG Hamiltonian of any superconductor has, by construction, a 'built-in' charge-conjugation (or particle–hole) symmetry ($\mathcal{C}$). In analogy to the IQHE, the different topological phases of the $p_x + \mathrm{i}p_y$ superconductor can be labeled by an integer ($\mathbb{Z}$) topological invariant [16]. The corresponding quantized conductance is the transverse (Hall) thermal or 'Leduc-Righi' conductance (divided by temperature). The quantum spin Hall effect (QSHE), on the other hand, which occurs in two-dimensional (2D) and 3D time-reversal invariant insulators, is characterized by a $\mathbb{Z}_2$ topological number $\nu_0$ [9], [12]–[14]. This binary quantity distinguishes the nontrivial state ($\nu_0 = 1$), whose boundary modes consist of an odd number of Dirac fermion modes (i.e. odd number of Kramers' pairs), from the trivial state ($\nu_0 = 0$), which is characterized by an even number of Kramers' pairs of boundary (surface or edge) states (figure 1(b)). A physical realization of the QSHE was theoretically predicted [17] and experimentally observed [18, 19] in HgTe/(Hg,Ce)Te semiconductor quantum wells. Subsequently, based on both theoretical considerations [15, 20] and experimental measurements [21]–[25], the 3D $\mathbb{Z}_2$ topological insulator phase was shown to occur in bismuth-related materials, such as the BiSb alloys $Bi_2Se_3$ and $Bi_2Te_3$.

The key difference among the IQHE, the QSHE and the 3D $\mathbb{Z}_2$ topological insulator, and the chiral $p_x + \mathrm{i}p_y$ superconductor lies in their generic symmetry properties (discussed in more

[7] In the presence of disorder (= lack of translational symmetry), a sufficient condition is that all bulk states near the Fermi energy are localized [3].

[8] A profound implication of a non-vanishing Chern number is that exponentially localized Wannier wavefunctions cannot be constructed [4]–[6]. Yet another manifestation of the nontrivial nature of the band structure when $\sigma_{xy} \neq 0$ appears in the scaling of the entanglement entropy (and the entanglement entropy spectrum) [7].

[9] Physically, the quasiparticles are responsible for heat (energy) transport and not for the electrical transport properties of the superconductor.

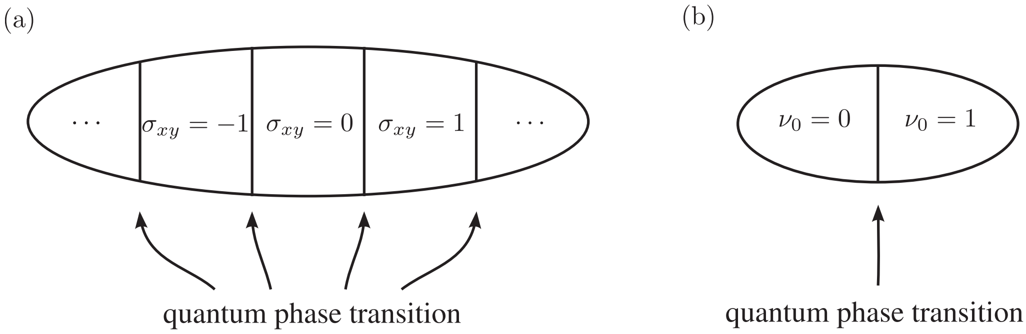


**Figure 1.** Topological distinction among quantum ground states. (a) $\mathbb{Z}$ classification and (b) $\mathbb{Z}_2$ classification.

detail below). All these states are topological in the sense that they cannot be continuously deformed into a trivial insulating state (i.e. a state without any gapless boundary modes) while keeping the generic symmetries of the system intact and without closing the bulk energy gap. The key property of the QSH states, for example, is the spin–orbit interaction in combination with time-reversal symmetry ($\mathcal{T}$). The latter protects the boundary states from acquiring a gap or becoming localized in the presence of disorder (= terms added to the Hamiltonian which break translational symmetry). The chiral $p_x + \mathrm{i}p_y$ superconductor, on the other hand, is characterized by $\mathcal{C}$ but the lack of $\mathcal{T}$.

The aforementioned examples of 'symmetry protected' topological states are part of a larger scheme[10] that fully classifies [26, 27] all topological insulators (superconductors) in terms of symmetry and spatial dimension. This classification scheme is summarized in table 3. The first column in this table provides the complete list of all possible 'symmetry classes' of single-particle Hamiltonians. There are precisely ten such 'symmetry classes', a fundamental result due to Zirnbauer [29] and Altland and Zirnbauer [30][11]. These authors recognized that there is a one-to-one correspondence between single-particle Hamiltonians and the set of ('large') symmetric spaces, of which there are precisely ten, a classic result obtained in 1926 by the mathematician Élie Cartan. The work of Altland and Zirnbauer extends, indeed completes, the much earlier work by Wigner and Dyson that is well known in the context of random matrix theory as the three 'unitary, orthogonal and symplectic' symmetry classes [32]. Before discussing in more detail the result of the classification in table 3, we will first briefly explain the notion of 'symmetry class' and the tenfold list of Hamiltonians, which is the framework within which the classification scheme in table 3 is formulated. The reader familiar with this topic may skip this subsection.

[10] A complete classification of all topological insulators (superconductors) in dimensionalities up to $d = 3$ was given in [26]. A systematic regularity (periodicity) of the classification as the dimensionality is varied was discovered by Kitaev in [27] for all dimensions through the use of $K$-theory. A certain systematic pattern as the dimensionality is varied was discovered for some of the topological insulators by Qi *et al* in [28] using a Chern–Simons action in extended space. Below we will use a version of the ideas of 'dimensional reduction' employed in [28].
[11] See, e.g., [31] for a more recent discussion.

### *1.1. Review: classification of generic Hamiltonians—'the tenfold way'*

Consider the gapped first-quantized Hamiltonian describing the topological insulator (superconductor) in the bulk ($d$ spatial dimensions). The topological features of this Hamiltonian, which we are interested in characterizing, are (by definition) not changed if we modify (deform) the Hamiltonian by adding terms (or perturbations) to it that break any translational symmetry that may be present. Thus, the topological features must be properties of a translationally *not* invariant Hamiltonian. Seeking a classification scheme, one must have some framework within which to classify such translationally *not* invariant Hamiltonians. Such a classification cannot involve the notion of ordinary symmetries, i.e. of *unitary* operators that commute with the Hamiltonian. Consider e.g. (Pauli-)spin rotation symmetry, ubiquitous in condensed matter systems. The notion of spin-rotation invariance can be eliminated by writing the Hamiltonian in block form and by focusing attention on a block of the Hamiltonian. Such a block decomposition can be performed for any symmetry that commutes with the Hamiltonian. The notion of 'symmetry classes' mentioned above refers to the properties of these blocks of symmetry-less 'irreducible' Hamiltonians: as it turns out, there are only ten of them. The basic idea why this is the case is simple to understand. The only properties that the blocks can satisfy are certain reality conditions that follow from the 'extremely generic symmetries' of time reversal and charge conjugation (or particle–hole symmetry). These are not symmetries in the above sense, since they are both represented by *anti*-unitary operators, when acting on the single-particle Hilbert space. Specifically, consider a general system of non-interacting fermions described by a 'second-quantized' Hamiltonian $H$. For a non-superconducting system, e.g., this reads

$$H = \sum_{A,B} \psi_A^\dagger \mathcal{H}_{A,B} \psi_B, \tag{1}$$

with fermion creation and annihilation operators satisfying canonical anti-commutation relations

$$\{\psi_A, \psi_B^\dagger\} = \delta_{A,B}. \tag{2}$$

Here, we imagine, for convenience of notation, that we have 'regularized' the system on a lattice, and $A$ and $B$ are combined labels for the lattice sites $i$ and $j$, and if relevant, of additional quantum numbers such as e.g. a Pauli-spin quantum number (e.g. $A = (i, a)$ with $a, b = \pm 1/2$). Then $\mathcal{H}_{A,B}$ is an $N \times N$ matrix, the 'first quantized' Hamiltonian. (Similarly, a superconducting system is described by a BdG Hamiltonian for which we use the Nambu spinor instead of complex fermion operators $\psi_A$ and $\psi_A^\dagger$ and whose first quantized form is again a matrix $\mathcal{H}$ when discretized on a lattice.)

Now, time-reversal symmetry can be expressed in terms of $\mathcal{H}$: the system is invariant under time-reversal symmetry if and only if the complex conjugate of the first quantized Hamiltonian $\mathcal{H}^*$ is equal to $\mathcal{H}$ up to a unitary rotation $U_T$, i.e.

$$\mathcal{T}: \quad U_T^\dagger \mathcal{H}^* U_T = +\mathcal{H}. \tag{3}$$

Moreover, the system is invariant under charge-conjugation (or particle–hole) symmetry if and only if the complex conjugate of the Hamiltonian $\mathcal{H}^* = \mathcal{H}^T$ is equal to *minus* $\mathcal{H}$ up to a unitary rotation $U_C$, i.e.

$$\mathcal{C}: \quad U_C^\dagger \mathcal{H}^* U_C = -\mathcal{H}. \tag{4}$$

(This property may be less familiar, but it is easy to check [26] that it is a characterization of charge-conjugation (particle–hole) symmetry for non-interacting systems of fermions). A look at equations (3) and (4) reveals that $\mathcal{T}$ and $\mathcal{C}$, when acting on the single-particle Hilbert space, are not unitary symmetries, but rather reality conditions on the Hamiltonian $\mathcal{H}$ modulo unitary rotations[12, 13].

Now it is easy to see that there are only ten possible ways for a system to respond to time-reversal and charge-conjugation (particle–hole symmetry) operations. As for time-reversal symmetry ($\mathcal{T}$), the Hamiltonian can either be (i) not time-reversal invariant, in which case we write $\mathrm{T} = 0$ or (ii) it may be time-reversal invariant and the anti-unitary time-reversal symmetry operator $\mathcal{T}$ squares to plus the identity operator, in which case we write $\mathrm{T} = +1$ or (iii) it may be time-reversal invariant and the anti-unitary time-reversal symmetry operator $\mathcal{T}$ squares to minus the identity, in which case we write $\mathrm{T} = -1$. Similarly, there are three possible ways for the Hamiltonian $\mathcal{H}$ to respond to charge-conjugation (particle–hole symmetry) $\mathcal{C}$ (again, $\mathcal{C}$ may square to plus or minus the identity operator). For these three possibilities we write $\mathrm{C} = 0, +1, -1$. Hence, there are $3 \times 3 = 9$ possible ways for a Hamiltonian $\mathcal{H}$ to respond to time-reversal and charge-conjugation (particle–hole transformation). These are not yet all ten cases because it is also necessary to consider the behavior of the Hamiltonian under the product $\mathcal{S} = \mathcal{T} \cdot \mathcal{C}$, which is a unitary operation. A moment's thought (see table 1) shows that for 8 of the 9 possibilities the behavior of the Hamiltonian under the product $\mathcal{S} = \mathcal{T} \cdot \mathcal{C}$ is uniquely fixed[14]. (We write $\mathrm{S} = 0$ if the operation $\mathcal{S}$ is not a symmetry of the Hamiltonian, and $\mathrm{S} = 1$ if it is.)

[12] In second-quantized language, time-reversal and particle–hole operations can be written in terms of their action on the canonical fermion creation and annihilation operators,

$$\mathcal{T}\psi_A\mathcal{T}^{-1} = \sum_B (U_T)_{A,B}\ \psi_B, \quad \mathcal{C}\psi_A\mathcal{C}^{-1} = \sum_B (U_C^*)_{A,B}\ \psi_B^\dagger. \tag{5}$$

While the particle–hole transformation is unitary, the time-reversal operation is anti-unitary, $\mathcal{T}\mathrm{i}\mathcal{T}^{-1} = -\mathrm{i}$. The system is time-reversal invariant (particle–hole symmetric) if and only if $\mathcal{T}H\mathcal{T}^{-1} = H$ ($\mathcal{C}H\mathcal{C}^{-1} = H$). This leads directly to conditions (3) and (4) for the first quantized Hamiltonian. Note that $\mathcal{T}H\mathcal{T}^{-1} = H$ implies $\mathcal{T}\psi_A(t)\mathcal{T}^{-1} = \mathcal{T}\mathrm{e}^{+\mathrm{i}Ht}\psi_A\mathrm{e}^{-\mathrm{i}Ht}\mathcal{T}^{-1} = \sum_B (U_T)_{A,B}\ \psi_B(-t)$. Iterating $\mathcal{T}$ and $\mathcal{C}$ twice, one obtains $\mathcal{T}^2\psi_A\mathcal{T}^{-2} = \sum_B (U_T^*U_T)_{A,B}\ \psi_B$, and $\mathcal{C}^2\psi_A\mathcal{C}^{-2} = \sum_B (U_C^*U_C)_{A,B}\ \psi_B$. When acting on the first quantized Hamiltonian this reads $(U_T^*U_T)^\dagger\mathcal{H}(U_T^*U_T) = \mathcal{H}$ and $(U_C^*U_C)^\dagger\mathcal{H}(U_C^*U_C) = \mathcal{H}$, respectively. The first quantized Hamiltonians $\mathcal{H}$ are seen (below) to run over an irreducible representation space, and thus $(U_T^*U_T)$ and $(U_C^*U_C)$ are both multiples of the identity matrix $I_N$ (by Schur's lemma). Since $U_T$ and $U_C$ are unitary matrices, there are only two possibilities for each, i.e. $U_T^*U_T = \pm I_N$ and $U_C^*U_C = \pm I_N$. The time-reversal operation $\mathcal{T}$ and the particle–hole transformation $\mathcal{C}$ can then each square to plus or to minus the identity, $\mathcal{T}^2 = \pm 1$ and $\mathcal{C}^2 = \pm 1$.

[13] It may also be worth noting that we may assume without loss of generality that there is only a *single* time-reversal operator $\mathcal{T}$ and a *single* charge-conjugation operator $\mathcal{C}$. If the (first quantized) Hamiltonian $\mathcal{H}$ was invariant under, say, *two* charge-conjugation operations $\mathcal{C}_1$ and $\mathcal{C}_2$, then the composition $\mathcal{C}_1 \cdot \mathcal{C}_2$ of these two symmetry operations would be a *unitary* symmetry when acting on the first quantized Hamiltonian $\mathcal{H}$, i.e. the product $U_{C_1} \cdot U_{C_2}^*$ would *commute* with $\mathcal{H}$. By bringing the Hamiltonian $\mathcal{H}$ in block form, $U_{C_1} \cdot U_{C_2}^*$ would then be constant on each block. Thus, on each block $U_{C_1}$ and $U_{C_2}$ would then be trivially related to each other, and it would suffice to consider one of the two charge conjugation operations. On the other hand, note that the product $\mathcal{T} \cdot \mathcal{C}$ corresponds to a *unitary* symmetry operation when acting on the first quantized Hamiltonian $\mathcal{H}$. But in this case the unitary matrix $U_T \cdot U_C^*$. does not commute but *anti*-commutes with $\mathcal{H}$. Therefore, $\mathcal{T} \cdot \mathcal{C}$ does not correspond to an 'ordinary' symmetry of $\mathcal{H}$. It is for this reason that we need to consider the product $\mathcal{T} \cdot \mathcal{C}$ (called 'chiral' or 'sublattice' symmetry $\mathcal{S}$ below) as an additional essential ingredient for the classification of the blocks, besides time-reversal $\mathcal{T}$ and charge-conjugation (particle–hole) symmetries $\mathcal{C}$.

[14] The symmetry operation $\mathcal{S}$ is sometimes called 'sublattice symmetry', hence the notation $\mathcal{S}$. However, in many instances, $\mathcal{S}$ is not realized as a sublattice symmetry, but is simply the product of $\mathcal{T}$ and $\mathcal{C}$. Therefore the term 'chiral symmetry' to describe the symmetry operation $\mathcal{S}$ is sometimes more appropriate.

**Table 1.** Listed are the ten generic symmetry classes of single-particle Hamiltonians $\mathcal{H}$, classified according to their behavior under time-reversal symmetry ($\mathcal{T}$), charge-conjugation (or particle–hole) symmetry ($\mathcal{C}$), as well as 'sublattice' (or 'chiral') symmetry ($\mathcal{S}$). The labels T, C and S represent the presence/absence of time-reversal, particle–hole and chiral symmetries, respectively, as well as the types of these symmetries. The column entitled 'Hamiltonian' lists, for each of the ten symmetry classes, the symmetric space of which the quantum mechanical time-evolution operator $\exp(\mathrm{i}t\mathcal{H})$ is an element. The column 'Cartan label' is the name given to the corresponding symmetric space listed in the column 'Hamiltonian' in Élie Cartan's classification scheme (dating back to the year 1926). The last column entitled '$G/H$ (ferm. NL$\sigma$M)' lists the (compact sectors of the) target space of the NL$\sigma$M describing Anderson localization physics at long wavelength in this given symmetry class.

| Cartan label | T | C | S | Hamiltonian | $G/H$ (ferm. NL$\sigma$M) |
|---|---|---|---|---|---|
| A (unitary) | 0 | 0 | 0 | $\mathrm{U}(N)$ | $\mathrm{U}(2n)/\mathrm{U}(n)\times\mathrm{U}(n)$ |
| AI (orthogonal) | +1 | 0 | 0 | $\mathrm{U}(N)/\mathrm{O}(N)$ | $\mathrm{Sp}(2n)/\mathrm{Sp}(n)\times\mathrm{Sp}(n)$ |
| AII (symplectic) | −1 | 0 | 0 | $\mathrm{U}(2N)/\mathrm{Sp}(2N)$ | $\mathrm{O}(2n)/\mathrm{O}(n)\times\mathrm{O}(n)$ |
| AIII (ch. unit.) | 0 | 0 | 1 | $\mathrm{U}(N+M)/\mathrm{U}(N)\times\mathrm{U}(M)$ | $\mathrm{U}(n)$ |
| BDI (ch. orth.) | +1 | +1 | 1 | $\mathrm{O}(N+M)/\mathrm{O}(N)\times\mathrm{O}(M)$ | $\mathrm{U}(2n)/\mathrm{Sp}(2n)$ |
| CII (ch. sympl.) | −1 | −1 | 1 | $\mathrm{Sp}(N+M)/\mathrm{Sp}(N)\times\mathrm{Sp}(M)$ | $\mathrm{U}(2n)/\mathrm{O}(2n)$ |
| D (BdG) | 0 | +1 | 0 | $\mathrm{SO}(2N)$ | $\mathrm{O}(2n)/\mathrm{U}(n)$ |
| C (BdG) | 0 | −1 | 0 | $\mathrm{Sp}(2N)$ | $\mathrm{Sp}(2n)/\mathrm{U}(n)$ |
| DIII (BdG) | −1 | +1 | 1 | $\mathrm{SO}(2N)/\mathrm{U}(N)$ | $\mathrm{O}(2n)$ |
| CI (BdG) | +1 | −1 | 1 | $\mathrm{Sp}(2N)/\mathrm{U}(N)$ | $\mathrm{Sp}(2n)$ |

The only case when the behavior under the combined transformation $\mathcal{S}=\mathcal{T}\cdot\mathcal{C}$ is not determined by the behavior under $\mathcal{T}$ and $\mathcal{C}$ is the case where $\mathrm{T}=0$ and $\mathrm{C}=0$. In this case, either $\mathrm{S}=0$ or $\mathrm{S}=1$ is possible. This then yields $(3\times 3-1)+2=10$ possible types of behavior of the Hamiltonian.

The list of ten possible types of behavior of the first quantized Hamiltonian under $\mathcal{T}$, $\mathcal{C}$ and $\mathcal{S}$ is given in table 1. These are the ten generic symmetry classes (the 'tenfold way'), which are the framework within which the classification scheme of topological insulators (superconductors) is formulated.

Let us first point out a very general structure seen in table 1. This is listed in the column entitled 'Hamiltonian'. When the first quantized Hamiltonian $\mathcal{H}$ is 'regularized' (or 'put on') a finite lattice, it becomes an $N\times N$ matrix (as discussed above). The entries in the column 'Hamiltonian' specify the type of $N\times N$ matrix that the quantum mechanical time-evolution operator $\exp(\mathrm{i}t\mathcal{H})$ is. For example, for systems that have no time-reversal or charge-conjugation symmetry properties at all, i.e. for which $\mathrm{T}=0$, $\mathrm{C}=0$, $\mathrm{S}=0$, which are listed in the first row of the table, there are no constraints on the Hamiltonian except for Hermiticity. Thus, $\mathcal{H}$ is a generic Hermitian matrix and the time-evolution operator is a generic unitary matrix, so that $\exp(\mathrm{i}t\mathcal{H})$ is an element of the unitary group $\mathrm{U}(N)$ of unitary $N\times N$ matrices. By imposing time-reversal symmetry (for a system that has, e.g., no other degree of freedom such as, e.g., spin), there exists a basis in which $\mathcal{H}$ is represented by a real symmetric $N\times N$ matrix. This, in turn, can be expressed as saying that the time-evolution operator is an element of the coset of groups, $U(N)/O(N)$. All other entries of the column 'Hamiltonian' can be obtained from analogous considerations[15]. What is interesting about this column is that its entries run precisely over what is known as the complete set of ten ('large') symmetric spaces[16], classified in 1926 in fundamental work by the mathematician Élie Cartan. Thus, as the first quantized Hamiltonian runs over all ten possible symmetry classes, the corresponding quantum mechanical time-evolution operator runs over all ten symmetric spaces. Thus, the appearance of the Cartan symmetric spaces is a reflection of fundamental aspects of (single-particle) quantum mechanics. We will discuss the last column entitled '$G/H$ (ferm. NL$\sigma$M)' in the following subsection.

### *1.2. Review: classification of topological insulators (superconductors)*

The approach used in [26] to classify all possible topological insulators (superconductors) rested on the existence of protected extended degrees of freedom at the system's boundary. These are, in particular, also protected in the presence of arbitrarily strong perturbations at the boundary which break translational symmetry (commonly referred to as 'random' or 'disordered'). The existence of extended, gapless degrees of freedom even in strongly random fermionic systems is highly unusual, because of the phenomenon of Anderson localization[17]. Thus, the degrees of freedom at the boundary of topological insulators (superconductors) must be of a very special kind, in that they entirely evade the phenomenon of Anderson localization. Our approach consists in classifying precisely all those problems of (non-interacting) fermionic systems which completely evade the phenomenon of Anderson localization. We have completed this task in [26]. Thus, we have reduced the problem of classifying all topological insulators (superconductors) in $d$ spatial bulk dimensions to a classification problem of Anderson localization at the $(d-1)$-dimensional boundary. By solving the mentioned problem of Anderson localization, we have thereby solved the problem of classifying all topological insulators (superconductors).

We will now focus our attention on the above-mentioned problem of Anderson localization at the $(d-1)$-dimensional boundary of a $d$-dimensional topological insulator (superconductor). Specifically, we will now review a solution of this problem [26],[18] that allows us to see directly the dependence on dimensionality $d$ of the classification of topological insulators (superconductors). In the later, main part of this paper, we will present another point of view on this dependence on dimensionality $d$ (using 'dimensional reduction').

The theoretical description of problems of Anderson localization is well known to be very systematic and geometrical [36, 37]. A problem of Anderson localization is in general described by a random Hamiltonian (i.e. one that lacks translational symmetry). That Hamiltonian will

[15] Possible realizations of the chiral symmetry classes AIII, BDI and CII possessing time-evolution operators in table 1 with $N \neq M$ are tight-binding models on bipartite graphs whose two (disjoint) subgraphs contain $N$ and $M$ lattice sites.

[16] A symmetric space is a finite-dimensional Riemannian manifold of constant curvature (its Riemann curvature tensor is covariantly constant) which has only one parameter, its radius of curvature. There are also so-called exceptional symmetric spaces, which, however, are not relevant for the problem at hand, because for them the number $N$ would be a fixed finite number, which would prevent us from being able to take the thermodynamic (infinite-volume) limit of interest for all the physical systems under consideration.

[17] This is the phenomenon that, at least for sufficiently strong disorder potentials, spatially extended (= delocalized) eigenstates of the Hamiltonian tend to become localized (i.e. exponentially decaying in space) [33]–[36].

[18] See especially footnote 22 of the 2nd article of [26].

be in one of the ten symmetry classes listed in table 1 and we are currently focusing on Hamiltonians describing the boundary of the topological insulator (superconductor). Now, as it turns out, at long length scales (much larger than the 'mean free path') a description in terms of a 'nonlinear-sigma-model' (NL$\sigma$M) emerges. An NL$\sigma$M is a system like that describing the classical statistical mechanics of a Heisenberg magnet. The only difference is that while the magnet is formulated in terms of unit vector spins, pointing to the surface of a 2D sphere, for a general NL$\sigma$M that spin is replaced[19] by an element of one of the ten symmetric spaces listed in the last column of table 1, called the 'target space' of the NL$\sigma$M, denoted by $G/H$.[20] For a given symmetry class of the original Hamiltonian, whose time-evolution operator is characterized by the penultimate column, the specific 'target space' that needs to be used for the NL$\sigma$M describing Anderson localization in this symmetry class is listed in the last column of table 1 (see also appendix A).

Now, the NL$\sigma$M on the $(d-1)$-dimensional boundary of the $d$-dimensional topological insulator (superconductor) completely evades Anderson localization if a certain extra *term of topological origin* can be added to the action of the NL$\sigma$M which has *no adjustable parameter* ([26], see footnote 17 of the present article). Whether such an extra term is allowed depends on (i) the 'target space' of the NL$\sigma$M in the symmetry class in question[21], and (ii) the dimensionality $\bar{d} := (d-1)$ of the boundary on which the NL$\sigma$M is defined. There are only three *terms of topological origin* that can possibly be added to the action of the NL$\sigma$M: these are a $\theta$-term (Pruisken term) [38], a $\mathbb{Z}_2$ topological term (see, e.g., [39]) and a Wess–Zumino–Witten (WZW) term [40, 41]. It is the homotopy groups of the NL$\sigma$M target spaces $G/H$ that determine whether it is possible to add such a topological term to a given NL$\sigma$M action (see table 2). Specifically, a $\theta$-term (Pruisken term) can appear when $\pi_{\bar{d}}(G/H) = \mathbb{Z}$. Similarly, a $\mathbb{Z}_2$ topological term is allowed when $\pi_{\bar{d}}(G/H) = \mathbb{Z}_2$, and a WZW term can be included[22] when $\pi_{\bar{d}+1}(G/H) = \mathbb{Z}$. Note that, on the one hand, one obtains, upon addition of a $\theta$-term (Pruisken term), a one-parameter family of theories (on the boundary) depending on the value of $\theta$, all of which reside in the same symmetry class. On the other hand, however, it is known that only for a special value of the parameter $\theta$, is Anderson localization avoided; for generic values of $\theta$, this is not the case. It is for this reason that the ability to add a $\theta$-term (Pruisken term) is not of interest for the question we are asking. One is therefore left with only a $\mathbb{Z}_2$ topological term and a WZW term as the only terms of topological origin that have no freely adjustable parameter and that are thus of relevance here.

The homotopy groups for all ten NL$\sigma$M target spaces $G/H$ listed in the last column of table 1 are well known from the literature (see e.g. [42] and references therein for a summary) and this information is summarized in table 2 for the convenience of the reader. In order to make a certain regular structure of this table apparent, the rows of table 1 have been re-ordered

[19] The 2D sphere $S^2$ is a particularly simple example of a symmetric space, namely it can be written as the space $S^2 = \mathrm{U}(2)/\mathrm{U}(1)\times\mathrm{U}(1)$, i.e. the first row in the last column of table 1, when $n = 1$.

[20] Both $G$ and $H$ are classical Lie groups, and $H$ is a maximal subgroup of $G$.

[21] The relevant 'target space' is, as already mentioned above, listed in the last column of table 1.

[22] Observe that, while the homotopy group determines if a term of topological origin for a given NL$\sigma$M action is allowed in principle, it depends on the specific disorder model considered, whether such a term is actually present. In any case, if a term of topological origin is possible in a specific dimension and symmetry class, then a corresponding topological insulator (superconductor) can exist in this symmetry class (in one dimension higher).

**Table 2.** Table of homotopy groups $\pi_{\bar{d}}(G/H)$ for symmetric spaces $G/H$, taken from the standard mathematical literature (see e.g. [42] and references therein for a summary). (Here, $N$ must be sufficiently large for a given $\bar{d}$. Cartan labels of those symmetry classes invariant under the chiral symmetry operation $\mathcal{S} = \mathcal{T} \cdot \mathcal{C}$ from table 1 are indicated by boldface letters.). The pattern continues for higher $\bar{d}$, with periodicity 2 for the complex case and 8 for the real case. The entries corresponding to $\mathbb{Z}$ topological insulators (superconductors) in $(\bar{d}+1)$ dimensions (see e.g. table 3) are indicated by blue color boldface symbols. There is a $(\bar{d}+1)$-dimensional $\mathbb{Z}_2$ topological insulator whenever $\pi_{\bar{d}}(G/H) = \mathbb{Z}_2$ (also indicated in blue). A $(\bar{d}+1)$-dimensional $\mathbb{Z}$ topological insulator, on the other hand, can be realized whenever $\pi_{\bar{d}+1}(G/H) = \mathbb{Z}$. This is one way ([26], see footnote 17 of the present article) to directly relate the classification of topological insulators (superconductors) to the table of homotopy groups.

| AZ | $G/H$ | $\bar{d}=0$ | $\bar{d}=1$ | $\bar{d}=2$ | $\bar{d}=3$ | $\bar{d}=4$ | $\bar{d}=5$ | $\bar{d}=6$ | $\bar{d}=7$ |
|---|---|---|---|---|---|---|---|---|---|
| *Complex case:* | | | | | | | | | |
| A | $\mathrm{U}(N+M)/\mathrm{U}(N)\times\mathrm{U}(M)$ | $\longleftarrow \mathbb{Z}$ | **0** | $\longleftarrow \mathbb{Z}$ | **0** | $\longleftarrow \mathbb{Z}$ | **0** | $\longleftarrow \mathbb{Z}$ | **0** $\longleftarrow$ |
| **AIII** | $\mathrm{U}(N)$ | **0** | $\longleftarrow \mathbb{Z}$ | **0** | $\longleftarrow \mathbb{Z}$ | **0** | $\longleftarrow \mathbb{Z}$ | **0** | $\longleftarrow \mathbb{Z}$ |
| *Real case:* | | | | | | | | | |
| AI | $\mathrm{Sp}(N+M)/\mathrm{Sp}(N)\times\mathrm{Sp}(M)$ | $\longleftarrow \mathbb{Z}$ | 0 | 0 | **0** | $\longleftarrow \mathbb{Z}$ | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | **0** $\longleftarrow$ |
| **BDI** | $\mathrm{U}(2N)/\mathrm{Sp}(2N)$ | **0** | $\longleftarrow \mathbb{Z}$ | 0 | 0 | **0** | $\longleftarrow \mathbb{Z}$ | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ |
| D | $\mathrm{O}(2N)/\mathrm{U}(N)$ | $\mathbb{Z}_2$ | **0** | $\longleftarrow \mathbb{Z}$ | 0 | 0 | **0** | $\longleftarrow \mathbb{Z}$ | $\mathbb{Z}_2$ |
| **DIII** | $\mathrm{O}(N)$ | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | **0** | $\longleftarrow \mathbb{Z}$ | 0 | 0 | **0** | $\longleftarrow \mathbb{Z}$ |
| AII | $\mathrm{O}(N+M)/\mathrm{O}(N)\times\mathrm{O}(M)$ | $\longleftarrow \mathbb{Z}$ | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | **0** | $\longleftarrow \mathbb{Z}$ | 0 | 0 | **0** $\longleftarrow$ |
| **CII** | $\mathrm{U}(N)/\mathrm{O}(N)$ | **0** | $\longleftarrow \mathbb{Z}$ | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | **0** | $\longleftarrow \mathbb{Z}$ | 0 | 0 |
| C | $\mathrm{Sp}(2N)/\mathrm{U}(N)$ | 0 | **0** | $\longleftarrow \mathbb{Z}$ | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | **0** | $\longleftarrow \mathbb{Z}$ | 0 |
| **CI** | $\mathrm{Sp}(2N)$ | 0 | 0 | **0** | $\longleftarrow \mathbb{Z}$ | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | **0** | $\longleftarrow \mathbb{Z}$ |

in a specific way[23]. Part of this re-ordering is a subdivision of all symmetry classes into what is called '*complex case*' and '*real case*' in table 2. The physical origin of this subdivision is simple to understand. In the category '*complex case*' appear precisely those symmetry classes in which there is no reality condition ($\mathcal{T}$ or $\mathcal{C}$) whatsoever imposed on the Hamiltonian. We see from table 1 that these are the classes that carry Cartan labels A and AIII. The Hamiltonians in these symmetry classes are therefore 'complex' (in this sense). The other category called '*real case*' in table 2 consists precisely of all the other eight symmetry classes which have the property that there is at least one reality condition [$\mathcal{T}$ or $\mathcal{C}$—cf equations (3) and (4)] imposed on the Hamiltonian (see table 1). In this sense the Hamiltonians in these symmetry classes are therefore 'real'.

Table 2 now tells us directly in which symmetry class there exist topological insulators or superconductors (and of which type, $\mathbb{Z}_2$ or $\mathbb{Z}$): according to the above discussion, we know that a topological insulator (superconductor) exists in a given symmetry class in $d = \bar{d}+1$ spatial

[23] We were first made aware by A Kitaev of the existence of a regularity in dimensionality in the classification of topological insulators (superconductors) [27], which, as reviewed below (see the second article in [26] and also footnote 17 of the present article) can be seen as a consequence of the regularity of the present table of homotopy groups.

**Table 3.** Classification of topological insulators and superconductors as a function of spatial dimension $d$ and symmetry class, indicated by the 'Cartan label' (first column). The definition of the ten generic symmetry classes of single particle Hamiltonians (due to Altland and Zirnbauer [29, 30]) is given in table 1. The symmetry classes are grouped into two separate lists, the complex and real cases, depending on whether the Hamiltonian is complex or whether one (or more) reality conditions (arising from time-reversal or charge-conjugation symmetries) are imposed on it; the symmetry classes are ordered in such a way that a periodic pattern in dimensionality becomes visible [27]. (See also the discussion in subsection 1.1 and table 2.) The symbols $\mathbb{Z}$ and $\mathbb{Z}_2$ indicate that the topologically distinct phases within a given symmetry class of topological insulators (superconductors) are characterized by an integer invariant ($\mathbb{Z}$) or a $\mathbb{Z}_2$ quantity, respectively. The symbol '0' denotes the case when there exists no topological insulator (superconductor), i.e. when all quantum ground states are topologically equivalent to the trivial state.

| | $d$ | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Cartan | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | ... |
| *Complex case:* | | | | | | | | | | | | | |
| A | $\mathbb{Z}$ | 0 | $\mathbb{Z}$ | 0 | $\mathbb{Z}$ | 0 | $\mathbb{Z}$ | 0 | $\mathbb{Z}$ | 0 | $\mathbb{Z}$ | 0 | ... |
| AIII | 0 | $\mathbb{Z}$ | 0 | $\mathbb{Z}$ | 0 | $\mathbb{Z}$ | 0 | $\mathbb{Z}$ | 0 | $\mathbb{Z}$ | 0 | $\mathbb{Z}$ | ... |
| *Real case:* | | | | | | | | | | | | | |
| AI | $\mathbb{Z}$ | 0 | 0 | 0 | $2\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 | 0 | 0 | ... |
| BDI | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 | 0 | 0 | $2\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 | 0 | ... |
| D | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 | 0 | 0 | $2\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 | ... |
| DIII | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 | 0 | 0 | $2\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | ... |
| AII | $2\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 | 0 | 0 | $2\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | ... |
| CII | 0 | $2\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 | 0 | 0 | $2\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ | ... |
| C | 0 | 0 | $2\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 | 0 | 0 | $2\mathbb{Z}$ | 0 | ... |
| CI | 0 | 0 | 0 | $2\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 | 0 | 0 | $2\mathbb{Z}$ | ... |

dimensions if and only if the target space of the NL$\sigma$M on the $\bar{d}$-dimensional boundary allows for either (i) a $\mathbb{Z}_2$ topological term, which is the case when $\pi_{\bar{d}}(G/H) = \pi_{d-1}(G/H) = \mathbb{Z}_2$, or (ii) a WZW term, which is the case when $\pi_d(G/H) = \pi_{\bar{d}+1}(G/H) = \mathbb{Z}$. By using this rule in conjunction with table 2 of homotopy groups, we arrive with the help of table 1 at table 3 of topological insulators and superconductors[24].

A look at table 3 reveals that in each spatial dimension there exist five distinct classes of topological insulators (superconductors), three of which are characterized by an integral ($\mathbb{Z}$) topological number, while the remaining two possess a binary ($\mathbb{Z}_2$) topological quantity[25].

[24] To be explicit, one has to move all the entries $\mathbb{Z}$ in table 2 into the locations indicated by the arrows, and replace the column label $\bar{d}$ by $d = \bar{d} + 1$. The result is table 3.

[25] Note that while $d = 0, 1, 2, 3$-dimensional systems are of direct physical relevance, higher-dimensional topological states might be of interest indirectly, because, for example, some of the additional components of momentum in a higher-dimensional space may be interpreted as adiabatic parameters (external parameters on which the Hamiltonian depends and which can be changed adiabatically, traversing closed paths in parameter space—sometimes referred to as adiabatic 'pumping processes').

The topological insulators (superconductors) appear in table 3 along diagonal lines. That is, as the spatial dimension is increased by one, the locations where the topological insulators (superconductors) appear in the table shift down by one column. This entire pattern descends directly from an analogous one appearing in the table 2 of homotopy groups.

In the main part of the present paper, we will give another derivation of this periodicity structure of table 3, by 'dimensional reduction' and by considering the Dirac Hamiltonian representatives in each of the symmetry classes in which there exist topological insulators (superconductors) in a given spatial dimension. By running the argument backwards, this can then, in turn, also be viewed as another route to obtain table 2 of homotopy groups.

Let us pause for a moment to point out a few interesting aspects relating to table 3. Firstly, it is interesting to note that the periodic structure of table 3 is quite analogous to the dimensional hierarchy of anomalies ('anomaly ladder') known in gauge theories, e.g. the (3+1)-dimensional Abelian anomaly, the (2+1)-dimensional parity anomaly and the (1+1)-dimensional non-Abelian anomaly [43]–[45]. This does not appear to be completely unexpected, considering that the IQHE is known as a condensed matter realization of the parity 'anomaly'[26].

Secondly, we want to draw the reader's attention to the fact that for a given symmetry class in table 3 any $\mathbb{Z}_2$ topological insulator (superconductor) always appears as part of a 'triplet' that consists of a $d$-dimensional $\mathbb{Z}$ topological insulator (superconductor) and two $\mathbb{Z}_2$ topological insulators (superconductors) in $(d-1)$ and $(d-2)$ dimensions. This suggests that the topological characteristics of the members of such a 'triplet' are closely related and, indeed, it was shown in [28] that the $\mathbb{Z}_2$ classification in symmetry class AII in $d=2$ and 3 can be derived from the 4D $\mathbb{Z}$ topological insulator by a process of 'dimensional reduction'. The same procedure has been applied [28] to derive $\mathbb{Z}_2$ classifications in those symmetry classes that do not possess a form of chiral symmetry (i.e. for which $\mathrm{S}=0$)—there are five of them. In section 4, we will extend this approach to the $\mathbb{Z}_2$ topological insulators (superconductors) in the remaining five symmetry classes that possess a form of chiral symmetry (i.e. for which $\mathrm{S}=1$).

Let us now discuss explicit forms of the 'terms of topological origin' that can be added to the action of the NL$\sigma$M with 'target space' $G/H$, at the boundary of the topological insulator (superconductor).

*1.2.1. Terms of WZW type.* Here there is a pattern, alternating in the dimension $\bar{d}$ of the boundary, for the way these topological terms can be constructed. (i) For a $\bar{d}=$ odd-dimensional boundary and for the NL$\sigma$Ms that describe the Anderson-delocalized boundary of the topological bulk, the field (denoted by $Q\in G/H$ below[27]—cf the last column of table 1) of the NL$\sigma$M field theory is a Hermitian matrix field that satisfies certain constraints. The WZW term responsible for the lack of Anderson localization takes on the form of the $\bar{d}$-dimensional integral over the boundary of the $\bar{d}$-dimensional Chern–Simons form (compare equation (22) of the main text below). Alternatively, it can be also written as an integral over

[26] The IQHE is not quite an anomaly in the sense that the parity and $\mathcal{T}$ are explicitly broken. However, the quantization of $\sigma_{xy}$ in the IQHE can be viewed as essentially the same phenomenon as the appearance of the Chern–Simons term in QED in $D=2+1$-dimensional spacetime, where massless Dirac fermions are coupled with the electromagnetic U(1) gauge field.

[27] While looking similar, the field $Q$ in the NL$\sigma$M has nothing to do with the spectral projector in momentum space defined in equation (7).

a $(\bar{d}+1)$-dimensional region whose boundary coincides with the physical $\bar{d}$-dimensional space, by smoothly interpolating the NL$\sigma$M field configuration $Q$ into one dimension higher. The fact that $\pi_{\bar{d}+1}(G/H) = \mathbb{Z}$ guarantees that different ways of interpolation do not matter, and the action depends only on the physical field configurations in $\bar{d}$-dimensional space. (ii) For a $\bar{d}$ = even-dimensional boundary and for the NL$\sigma$Ms that describe the Anderson-delocalized boundary of the topological bulk, the field in the NL$\sigma$M field theory is either a group element or a unitary matrix field (denoted by $g \in G/H$ below—cf the last column of table 1), which may, depending on the case, be subject to certain constraints. The WZW term responsible for the lack of Anderson localization takes on the form of a $(\bar{d}+1)$-dimensional integral of the winding number density, as defined in equation (20) of the main text below.

To illustrate these terms, we will now give explicit examples for them in low dimensionalities:

- $\underline{d=2}$: For the $d=2$-dimensional topological insulator of the IQHE, the $\bar{d}=1$-dimensional NL$\sigma$M describing the edge states is the one on $\mathrm{U}(2n)/\mathrm{U}(n)\times\mathrm{U}(n)$. The field $Q$ of the NL$\sigma$M field theory can be parameterized as $Q = U^\dagger \Lambda U \in \mathrm{U}(2n)/\mathrm{U}(n)\times\mathrm{U}(n)$, where $U \in \mathrm{U}(2n)$ and $\Lambda = \mathrm{diag}\,(I_n, -I_n)$. The term of relevance for the absence of Anderson localization at the edges of the integer quantum Hall insulator is $\propto \sigma_{xy}\int \mathrm{d}x\, \mathrm{tr}[A_x]$, where $A_x := U^\dagger\partial_x U$; this is a $\bar{d}=1$-dimensional analogue of the 3D Chern–Simons term. This term can also be rewritten as a WZW-type two-dimensional integral $\propto \sigma_{xy}\int_D \mathrm{d}x\mathrm{d}u\, \epsilon^{\mu\nu}\mathrm{tr}[Q\partial_\mu Q\partial_\nu Q]$ $(\mu,\nu = x,u)$. Here, we have extended the original $\bar{d}=1$-dimensional space to a 2D region $D$ by adding a fictitious space direction, parameterized by $u\in[0,1]$. The boundary $\partial D$ of the 2D region coincides with the original $\bar{d}=1$-dimensional space. Accordingly, the original NL$\sigma$M field $Q(x)$ is smoothly extended to $Q(x,u)$ such that it coincides with $Q(x)$ when $u=0$. Since $\pi_2\,[\mathrm{U}(2n)/\mathrm{U}(n)\times\mathrm{U}(n)] = \mathbb{Z}$ the 2D integral turns out to depend only on the field configuration on $\partial D$. Note that when we specialize to the case of $n=1$, all these expressions are well known from the coherent state path integral of an SU(2) quantum spin whose path integral is described by a $d=1$-dimensional NL$\sigma$M on the target space $\mathrm{O}(3)=\mathrm{U}(2)/\mathrm{U}(1)\times\mathrm{U}(1)$.
- $\underline{d=3}$: For $d=3$ topological insulators (superconductors) in classes AIII, DIII and CI, the relevant NL$\sigma$Ms at their $\bar{d}=2$-dimensional boundary (surface) are the ones with a group manifold as target manifold ($\mathrm{U}(n)$, $\mathrm{O}(n)$ and $\mathrm{Sp}(n)$ for classes AIII, DIII, and CI, respectively). The relevant WZW-type term can be written as a 3D integral, $\int_D \mathrm{d}^2x\,\mathrm{d}u\,\epsilon^{\mu\nu\lambda}\mathrm{tr}[(g^{-1}\partial_\mu g)(g^{-1}\partial_\nu g)(g^{-1}\partial_\lambda g)]$, where $g\in \mathrm{U}(n)$, $\mathrm{O}(n)$, $\mathrm{Sp}(n)$ [40]. Here again, the original $\bar{d}=2$-dimensional space is smoothly extended to the 3D region $D$, in such a way that $\partial D$ coincides with the physical $\bar{d}=2$-dimensional space. Accordingly, the field configuration $g(x,y)$ defined on the $\bar{d}=2$- dimensional space is smoothly extended to the 3D one $g(x,y,u)$ such that $g(x,y,u=0)=g(x,y)$.
- $\underline{d=4}$: For the $d=4$ topological insulators in classes A, AII and AI, the relevant $\bar{d}=3$ NL$\sigma$Ms have target spaces $G/H = \mathrm{G}(2n)/\mathrm{G}(n)\times\mathrm{G}(n)$ with $\mathrm{G}=\mathrm{U}$, O and Sp, respectively. The field of the NL$\sigma$M can be parameterized by $Q=U^\dagger\Lambda U$, where $U\in \mathrm{G}(2n)$. The relevant 'term of topological origin' is the Chern–Simons term $\propto \int \mathrm{d}^3x\,\epsilon^{\mu\nu\lambda}\mathrm{tr}[A_\mu\partial_\nu A_\lambda + (2/3)A_\mu A_\nu A_\lambda]$, where $A_\mu = U^\dagger\partial_\mu U$ $(\mu = x,y,z)$. The appearance of this term at the boundary of the $d=4$ topological insulators in class AII was discussed in [46].

- $\underline{d=5}$: For the $d=5$ topological insulators in symmetry classes AIII, BDI and CII, the $\bar{d}=4$-dimensional NL$\sigma$Ms have target spaces with a matrix field $g$, which is an element of $G/H = \mathrm{U}(n)$, $\mathrm{U}(2n)/\mathrm{Sp}(2n)$, $\mathrm{U}(2n)/\mathrm{O}(2n)$, respectively. For these spaces the WZW term takes the form of the $\bar{d}+1=5$-dimensional integral (with boundary) of the winding number density defined in equation (21) of the main text below.

Note that those entries in table 2 of homotopy groups that are integers, $\pi_{\bar{d}}(G/H)=\mathbb{Z}$, have a periodicity in $\bar{d}$ equal to four. Therefore, the forms of the 'terms of topological origin' of WZW type listed in the above low-dimensional cases will repeat, with the appropriate replacement of $\bar{d}$.

*1.2.2. Terms of topological origin of $\mathbb{Z}_2$ type.* The $\mathbb{Z}_2$ topological term for the NL$\sigma$M at the $\bar{d}=2$-dimensional surface of the $d=3$-dimensional $\mathbb{Z}_2$ topological insulators in symmetry class AII was discussed in [46]–[48]. Similarly, at the $\bar{d}=2$-dimensional surface of the $d=3$-dimensional $\mathbb{Z}_2$ topological insulators in symmetry class CII, the $\mathbb{Z}_2$ topological term is added to the NL$\sigma$M [49].

*1.2.3. Classifying space.* There is a third way in which the set of Cartan symmetric spaces listed in table 1 appears in the context of the classification of topological insulators (superconductors). This arises from Fermi statistics, which allows for distinguishing between the states of the (first quantized) Hamiltonian $\mathcal{H}$ with energies that lie above and those with energies that lie below the Fermi energy $E_{\mathrm{F}}$. In a topological insulator (superconductor) there is always an energy gap between the Fermi energy $E_{\mathrm{F}}$ and the eigenstates of $\mathcal{H}$ lying above as well as those lying below $E_{\mathrm{F}}$. Therefore one may, *without closing the bulk gap*, *continuously deform* the Hamiltonian $\mathcal{H}$ into one in which all eigenstates below the Fermi energy $E_{\mathrm{F}}$ have the same energy (say) $E=-1$, and all eigenstates above the Fermi energy have the same energy (say) $E=+1$. By construction, the resulting 'simplified Hamiltonian'[28], which we often denote by $Q$, has the same topological properties as the original Hamiltonian. The structure of $Q$ for all symmetry classes is listed in table III (second column) of the first article of [26] for systems with translational symmetry. ($Q$ will also be used again in the present paper.) If we were to consider a 'zero-dimensional' topological insulator (superconductor) where 'space consisted of a single point', then for each of the ten symmetry classes we obtain[29] a matrix $Q$ of a certain kind. It turns out that the so-obtained matrix $Q$ for each symmetry class is again an element of one of the ten symmetric spaces listed in table 1, except that the order in which these spaces appear is different from the order in the two columns of table 1. The resulting assignment is listed[30] in the last column in table A.1. The symmetric spaces to which the matrices $Q$ belong are what is called the 'classifying space' in the classification scheme of [27] employing $K$-theory[31]. In appendix A, we present a number of interesting relationships between these three lists of the

[28] This 'simplified Hamiltonian' $Q$ is often referred to in the first article of [26] and in the present paper as a 'projector', since it is trivially related to the projection operator $P$ onto all filled (with $E < E_{\mathrm{F}}$) eigenstates of $\mathcal{H}$ by $Q = 1-2P$. (The matrix in subsection 1.2.1 that is denoted by the same letter $Q$ is an entirely different object, not to be confused with $Q=1-2\,P$ appearing here.)
[29] From table III of the first article of [26], by setting the wavevector $k \to 0$.
[30] The last row, titled 'classifying space' in table A.1, is nothing but a list of the matrices $Q$, and this list follows from the second column of table III of the first article of [26] by letting $k=0$.
[31] The list of 'classifying spaces' was obtained in [27] through the use of Clifford algebras.

ten symmetric spaces: (i) the unitary time evolution operator, (ii) the NL$\sigma$M target space and (iii) the classifying space.

We end this subsection by commenting on additional information that can be read off from our main results, listed in table 3. This pertains to the existence of so-called *weak* topological insulators (superconductors), as well as of zero-energy or extended modes localized on topological defects in topological insulators (superconductors).

*1.2.4. Weak topological insulators and superconductors.* Table 3 classifies topological features of gapped free fermion Hamiltonians that do not depend on the presence of translational symmetries of a crystal lattice[32]. In particular, these properties are not destroyed when translation symmetry is broken, e.g., by the introduction of positional disorder. Systems that exhibit such robust topological properties are often also referred to as *strong* topological insulators (superconductors). This is to contrast them with so-called *weak* topological insulators (superconductors), which only possess topological features when translational symmetry is present. As soon as translational symmetry is broken, such *weak* topological features are no longer guaranteed to exist, and the system is allowed to become topologically trivial. For example, systems defined on a $d$-dimensional lattice whose momentum space is the $d$-dimensional torus $T^d$, allow for weak topological insulators that are not strong topological insulators. Such systems are topologically equivalent to parallel stacks of lower-dimensional strong topological insulators (superconductors). Specifically, the 3D 'weak' integer quantum Hall insulator on a lattice, discussed in [50], is essentially a layered version of the 2D integer quantum Hall insulator. Hence, it is characterized by a triplet of Chern numbers, each describing the winding of a map from the 2D torus $T^2$, which is a subspace of the 3D momentum space $T^3$, onto the complex Grassmannian, $G_{m,m+n}(\mathbb{C})$. Similarly, in symmetry class AII, there exists a 3D weak topological insulator [12]–[15], which consists of layered 2D $\mathbb{Z}_2$ topological quantum states, and whose weak topological features are described by a triplet of $\mathbb{Z}_2$ invariants.

The 3D 'weak' integer quantum Hall insulators, as well as the weak topological insulators of [12]–[15], are both examples of $d = 3$-dimensional weak topological insulators of 'codimension' one, i.e. they can be viewed as 1D arrays of $d = 2$-dimensional strong topological insulators. The existence of these states can be read from the $d = 2$-column and the rows of table 3 labeled A and AII, respectively. In general, $d$-dimensional weak topological states can be of any 'codimension' $k$, with $0 < k \leqslant d$. The existence of weak topological insulators and superconductors in $d$ spatial dimensions and for a given symmetry class can be readily inferred from table 3. That is, $d$-dimensional weak topological insulators (superconductors) of 'codimension' $k$ can occur whenever there exists a strong topological state in the same symmetry class, but in $d$–$k$ dimensions. Specifically, the topological order (characterized by elements in $\mathbb{Z}$ or in $\mathbb{Z}_2$) can be specified for each of the $\binom{d}{k}$ 'orientations' of the submanifold. Moreover, it is also possible that in addition 'strong' topological order, i.e. in the full space dimension $d$, exists. In the $K$-theory description of [27], the presence of weak topological features is described by additional summands in the Abelian group of topological invariants (i.e. $\mathbb{Z}$ or $\mathbb{Z}_2$), which appears when homotopy classes of maps from the sphere (strong topological insulators) are replaced by maps from the torus $T^d$ (weak and strong topological insulators).

[32] As we will explain below, in order to classify such so-called 'strong topological insulators' it is sufficient to only consider *continuous* Hamiltonians with momentum space $S^d$, the $d$-dimensional sphere.

*1.2.5. Zero modes localized on topological defects.* Another interesting application of table 3 is to determine whether $r$-dimensional topological defects in topological insulators (superconductors) can support localized (isolated) zero modes. For example, let us first consider a point-like defect (i.e. $r = 0$), which is embedded in a $d$-dimensional system ($d \geqslant 1$) of any symmetry class. Furthermore, let us assume that at the defect time-reversal symmetry is broken ($T = 0$) but particle–hole symmetry is preserved with $\mathrm{C} = +1$, i.e. we are dealing with symmetry class D. From table 3 we infer that in symmetry class D in $d = r + 1 = 1$ dimensions, there is a $\mathbb{Z}_2$ classification, which implies that the ($r = 0$)-dimensional boundary can support gapless states and, therefore, a point-like defect with the symmetries of class D can bind zero modes. This situation is realized, e.g., for a vortex core in a $(p \pm \mathrm{i}p)$-wave superconductor, which can bind isolated Majorana modes. In general, whether it is possible for a $r$-dimensional topological defect of a given symmetry class to support gapless states or not is determined by the entry of table 3 at the intersection of column $d = r + 1$ and the row of the given symmetry class. An application of this general statement can for example be found in the work of reference [51], where a dislocation line ($r = 1$) in a $d = 3$-dimensional lattice hosting a weak topological insulator in symmetry class AII was found to bind an extended gapless zero mode. (This corresponds in table 3 to the intersection of the row denoting symmetry class AII with the column $d = r + 1 = 1 + 1 = 2$, the latter representing the $d = 3$-dimensional weak topological insulator, which corresponds to a strong topological insulator in 'codimension' $k = 1$.) To illustrate the use of table 3, we can for example predict that a similar binding of extended zero modes to lattice dislocation lines ($r = 1$) can also occur in weak $d = 3$-dimensional topological insulators of 'codimension' $k = 1$ in symmetry classes A, D, DIII, and C.

### *1.3. Outline of the present paper*

In this paper, we discuss in detail the mechanism behind the dimensional periodicity and shift property appearing in table 3. We first demonstrate that there exists, for all five symmetry classes of topological insulators or superconductors, and in all dimensions $d$, a representative of the Hamiltonian in this class which has the form of a Dirac Hamiltonian, by constructing explicitly such a representative. We use these Dirac Hamiltonian representatives in the five symmetry classes with topological insulators (superconductors) to obtain relationships between these five symmetry classes in different dimensions. First, we construct dimensional hierarchies ('dimensional ladders') relating $\mathbb{Z}$ topological insulators (superconductors) in different dimensions and symmetry classes (see sections 2 and 3). This is done by using a process of 'dimensional reduction' in which spatial dimensions are compactified (in a 'Kaluza–Klein-like' fashion), thus relating higher- to lower-dimensional theories. By employing the same dimensional reduction process, we derive in section 4 the topological classification of the $\mathbb{Z}_2$ topological insulators (superconductors) from their higher-dimensional parent $\mathbb{Z}$ topological insulators (superconductors) in the same symmetry class. Sections 2–4 taken together provide a complete, independent derivation of table 3 of topological insulators (superconductors).

In section 2.2, we establish the connection between the topological invariant (winding number) defined for topological insulators and superconductors with chiral symmetry and yet another topological invariant, the Chern–Simons invariant, for general dimensions (equation (43)). For lower-dimensional cases, formula (43) relates the winding number to the electric polarization ($d = 1$ spatial dimensions) and the magnetoelectric polarizability ($d = 3$ spatial dimensions).

In section 2.6, we list, for topological insulators in symmetry classes A and AIII, the topological field theory describing the spacetime theory of linear responses in all spacetime dimensions $D = d + 1$. For symmetry class A, this is the Chern–Simons action, and in class AIII it is the theta term with theta angle $\theta = \pi$. (Generalizations to topological singlet superconductors with SU(2) spin-rotation symmetry are mentioned in section 5.)

Finally, as already mentioned in subsection 1.2, we have discussed, for all dimensionalities, the 'terms of topological origin' of WZW type that can be added to NL$\sigma$M field theories on symmetric spaces. In particular, in odd dimensions, these are the Chern–Simons terms.

In Appendix A, we collect a number of interesting relationships between the Cartan classification of generic Hamiltonians due to Altland and Zirnbauer, the NL$\sigma$M target space of Anderson localization, and the classifying space appearing in the K-theory approach to topological insulators. The representation theory of the spinor representations of the orthogonal groups SO($N$) is briefly reviewed in Appendix B. Furthermore, we study in Appendix C the influence of inversion symmetry on the classification of topological insulators (superconductors), combined with either time-reversal or charge-conjugation (particle–hole) symmetry.

## 2. Dimensional hierarchy: the complex case (A → AIII)

In this section, we consider the relationship between the $2n$-dimensional class A topological insulator and the $(2n-1)$-dimensional class AIII topological insulator. (Recall from table 1 that Hamiltonians in symmetry classes A and AIII are not invariant under time-reversal and charge-conjugation symmetries ($\mathcal{T}$ and $\mathcal{C}$), but Hamiltonians in class AIII possess 'chiral symmetry' called $\mathcal{S}$ in the table, i.e. they *anti*-commute with a unitary operator.) Firstly we present a general discussion about class A and AIII topological insulators (sections 2.1 and 2.2) and then we will focus on Dirac Hamiltonian representatives in these symmetry classes (sections 2.3, 2.4 and 2.5). The insights gained from the study of these Dirac Hamiltonian examples are applicable to a wider class of insulators. Finally, in section 2.6 we discuss effective topological field theories describing topological response functions of class A and AIII topological insulators.

### 2.1. Class A in $d = 2n + 2$ dimensions

The class of problems that we will consider below is non-interacting fermionic systems with translation invariance. For such systems, the eigenvalue problem at each momentum $k$ in the Brillouin zone (BZ) is described by

$$\mathcal{H}(k)|u_a(k)\rangle = E_a(k)|u_a(k)\rangle, \quad a = 1, \ldots, N_{\text{tot}}. \tag{6}$$

Here, $\mathcal{H}(k)$ is an $N_{\text{tot}} \times N_{\text{tot}}$ single-particle Hamiltonian in momentum space, and $|u_a(k)\rangle$ is the $a$th Bloch wavefunction with energy $E_a(k)$. We assume that there is a finite gap at the Fermi level, and therefore, we obtain a unique ground state by filling all states below the Fermi level. (In this paper, we always adjust $E_a(k)$ in such a way that the Fermi level is at zero energy.)

We assume there are $N_-$ ($N_+$) occupied (unoccupied) Bloch wavefunctions for each $k$ with $N_+ + N_- = N_{\text{tot}}$. We call the set of filled Bloch wavefunctions $\{|u^-_{\hat{a}}(k)\rangle\}$, where hatted indices $\hat{a} = 1, \ldots, N_-$ label the occupied bands only. We introduce the spectral projector onto the filled Bloch states and the '$Q$-matrix' by

$$P(k) = \sum_{\hat{a}} |u^-_{\hat{a}}(k)\rangle\langle u^-_{\hat{a}}(k)|, \qquad Q(k) = 1 - 2P(k). \tag{7}$$

The ground state (filled Fermi sea) is characterized at each $k$ by the set of normalized vectors $\{|u^-_{\hat{a}}(k)\rangle\}$, which is a member of $\mathrm{U}(N_{\mathrm{tot}})$ or, equivalently, by $Q(k)$, up to basis transformations within occupied and unoccupied bands. Thus $Q(k)$ can be viewed as an element of the complex Grassmannian $G_{N_+,N_++N_-}(\mathbb{C}) = \mathrm{U}(N_+ + N_-)/[\mathrm{U}(N_+)\times \mathrm{U}(N_-)]$. For a given system, $Q(k)$ defines a map from BZ into the complex Grassmannian, and hence classifying topological classes of band insulators is equivalent to counting how many distinct classes there are for the space of all such mappings. The answer to this question is given by the homotopy group $\pi_d(G_{m,m+n}(\mathbb{C}))$, which is nontrivial in even dimensions $d = 2n+2$.

Define, for the occupied bands, the non-Abelian Berry connection [52]

$$\mathcal{A}^{\hat{a}\hat{b}}(k) = A^{\hat{a}\hat{b}}_\mu(k)\mathrm{d}k_\mu = \langle u^-_{\hat{a}}(k)|\mathrm{d}u^-_{\hat{b}}(k)\rangle, \quad \mu = 1,\ldots,d, \quad \hat{a},\hat{b} = 1,\ldots,N_-, \tag{8}$$

where $A^{\hat{a}\hat{b}}_\mu = -(A^{\hat{b}\hat{a}}_\mu)^*$. The Berry curvature is defined by

$$\mathcal{F}^{\hat{a}\hat{b}}(k) = \mathrm{d}\mathcal{A}^{\hat{a}\hat{b}} + \left(\mathcal{A}^2\right)^{\hat{a}\hat{b}} = \tfrac{1}{2}F^{\hat{a}\hat{b}}_{\mu\nu}(k)\mathrm{d}k_\mu\wedge\mathrm{d}k_\nu. \tag{9}$$

Class A insulators in even spatial dimensions $d = 2n+2$ $(n = 0, 1, 2, \ldots)$ can be characterized by the Chern form of the Berry connection in momentum space. The $(n+1)$th Chern character is

$$\mathrm{ch}_{n+1}(\mathcal{F}) = \frac{1}{(n+1)!}\,\mathrm{tr}\left(\frac{\mathrm{i}\mathcal{F}}{2\pi}\right)^{n+1}. \tag{10}$$

The integral of the Chern character in $d = 2n+2$ dimensions is an integer, the $(n+1)$st Chern number,

$$\mathrm{Ch}_{n+1}[\mathcal{F}] = \int_{\mathrm{BZ}^{d=2n+2}} \mathrm{ch}_{n+1}(\mathcal{F}) = \int_{\mathrm{BZ}^{d=2n+2}} \frac{1}{(n+1)!}\,\mathrm{tr}\left(\frac{\mathrm{i}\mathcal{F}}{2\pi}\right)^{n+1} \in \mathbb{Z}. \tag{11}$$

Here, $\int_{\mathrm{BZ}^d}$ denotes the integration over $d$-dimensional $k$-space. For lattice models, it can be taken as a Wigner–Seitz cell in the reciprocal lattice space. On the other hand, for continuum models, it can be taken as $\mathbb{R}^d$. Assuming that the asymptotic behavior of the Bloch wavefunctions approaches a $k$-independent value as $|k|\to\infty$, the domain of integration can be regarded as $S^d$.[33]

When $d = 2$ $(n = 0)$, $\mathrm{Ch}_1[\mathcal{F}]$ is the TKNN integer [1],

$$\mathrm{Ch}_1[\mathcal{F}] = \frac{\mathrm{i}}{2\pi}\int_{\mathrm{BZ}^{d=2}} \mathrm{tr}(\mathcal{F}) = \frac{\mathrm{i}}{2\pi}\int \mathrm{d}^2k\,\mathrm{tr}(F_{12}), \tag{12}$$

which is nothing but the quantized Hall conductance $\sigma_{xy}$ in units of $(e^2/h)$. The second Chern number $(n = 1)$, given by $\mathrm{Ch}_2[\mathcal{F}]$,

$$\mathrm{Ch}_2[\mathcal{F}] = \frac{-1}{8\pi^2}\int_{\mathrm{BZ}^{d=4}} \mathrm{tr}\left(\mathcal{F}^2\right) = \frac{-1}{32\pi^2}\int \mathrm{d}^4k\,\epsilon^{\kappa\lambda\mu\nu}\,\mathrm{tr}\left(F_{\kappa\lambda}F_{\mu\nu}\right), \tag{13}$$

[33] For Dirac insulators with linear dispersion, discussed below, this assumption is not entirely correct. If the $k$-linear behavior of the Dirac spectrum persists to infinitely large momentum, the behavior of the wavefunctions at $|k|\to\infty$ is not trivial: the one-point compactification thus does not work. In this case, the domain of integration becomes effectively half of $S^d$, and accordingly, integer topological numbers become half-integers. However, the Dirac spectrum can be properly regularized, in such a way that the behavior of the wavefunctions becomes trivial at larger $k$; see for example equation (50). This is also the case when the Dirac Hamiltonians are formulated on a lattice (see equation (82)).

can be used to describe a topological insulator in $d = 4$ or, alternatively, a certain adiabatic 'pumping process' in lower spatial dimension [28].

The Chern character $\mathrm{ch}_{n+1}$ can be written in terms of its Chern–Simons form,

$$\mathrm{ch}_{n+1}(\mathcal{F}) = \mathrm{d}Q_{2(n+1)-1}(\mathcal{A}, \mathcal{F}). \tag{14}$$

Here the Chern–Simons form is defined as

$$Q_{2n+1}(\mathcal{A}, \mathcal{F}) := \frac{1}{n!}\left(\frac{\mathrm{i}}{2\pi}\right)^{n+1}\int_0^1 \mathrm{d}t\ \mathrm{tr}\big(\mathcal{A}\mathcal{F}_t^n\big)\,, \tag{15}$$

where

$$\mathcal{F}_t = t\mathrm{d}\mathcal{A} + t^2\mathcal{A}^2 = t\mathcal{F} + (t^2 - t)\mathcal{A}^2. \tag{16}$$

For example,

$$Q_1\,(\mathcal{A}, \mathcal{F}) = \frac{\mathrm{i}}{2\pi}\,\mathrm{tr}\,\mathcal{A}, \qquad Q_3\,(\mathcal{A}, \mathcal{F}) = \frac{-1}{8\pi^2}\,\mathrm{tr}\left(\mathcal{A}\mathrm{d}\mathcal{A} + \frac{2}{3}\mathcal{A}^3\right). \tag{17}$$

### 2.2. *Class AIII in $d = 2n + 1$ dimensions*

*2.2.1. Winding number.* We now discuss band insulators in symmetry class AIII. By definition, for all class AIII band insulators, we can find a unitary matrix $\Gamma$ that anticommutes with the Hamiltonians,

$$\{\mathcal{H}(k), \Gamma\} = 0, \qquad \Gamma^2 = 1. \tag{18}$$

It follows that the spectrum is symmetric with respect to zero energy and $N_+ = N_- =: N$. As a consequence of the chiral symmetry (18), all class AIII Hamiltonians, as well as their $Q$-matrix (7), can be brought into block off-diagonal form,

$$Q(k) = \begin{pmatrix} 0 & q(k) \\ q^\dagger(k) & 0 \end{pmatrix}, \qquad q \in \mathrm{U}(N), \tag{19}$$

in the basis in which $\Gamma$ is diagonal. The off-diagonal component $q(k)$ defines a map from BZ onto $\mathrm{U}(N)$, and classifying class AIII topological insulators reduces to considering the homotopy group $\pi_d(\mathrm{U}(N))$. The homotopy group is nontrivial in odd spatial dimensions $d = 2n + 1$, while it is trivial in even spatial dimensions, i.e. there is no nontrivial topological insulator in class AIII in even spatial dimensions.

In odd spatial dimensions $d = 2n + 1$, class AIII topological insulators are characterized by the winding number [26]

$$\nu_{2n+1}[q] := \int_{\mathrm{BZ}^{d=2n+1}} \omega_{2n+1}[q], \tag{20}$$

where the winding number density is given by

$$\begin{aligned}\omega_{2n+1}[q] &:= \frac{(-1)^n n!}{(2n+1)!}\left(\frac{\mathrm{i}}{2\pi}\right)^{n+1} \mathrm{tr}\big[(q^{-1}\mathrm{d}q)^{2n+1}\big] \\ &= \frac{(-1)^n n!}{(2n+1)!}\left(\frac{\mathrm{i}}{2\pi}\right)^{n+1} \epsilon^{\alpha_1\alpha_2\cdots}\,\mathrm{tr}\big[q^{-1}\partial_{\alpha_1}q\cdot q^{-1}\partial_{\alpha_2}q\cdots\big]\,\mathrm{d}^{2n+1}k. \end{aligned} \tag{21}$$

*2.2.2. The Chern–Simons invariant.* Although derived from the Chern form, the Chern–Simons forms, introduced in equation (15), themselves define a characteristic class for an odd-dimensional manifold. This suggests that the Chern–Simons forms can be used to characterize also AIII topological insulators in $d=2n+1$ dimensions. Integrating the Chern–Simons form over the BZ, we introduce

$$\mathrm{CS}_{2n+1}[\mathcal{A},\mathcal{F}] := \int_{\mathrm{BZ}^{2n+1}} Q_{2n+1}(\mathcal{A},\mathcal{F}). \tag{22}$$

Unlike the winding number, $\mathrm{CS}_{2n+1}[\mathcal{A},\mathcal{F}]$ is defined without assuming chiral symmetry and can be used for non-chiral topological insulators (superconductors).

Before discussing how useful Chern–Simons forms are, however, observe that they are not gauge invariant. Neither are the integrals of the Chern–Simons forms over the BZ. However, for two different choices of gauge $\mathcal{A}$ and $\mathcal{A}'$, which are connected by a gauge transformation

$$\mathcal{A}' = g^{-1}\mathcal{A}g + g^{-1}\mathrm{d}g, \qquad \mathcal{F}' = g^{-1}\mathcal{F}g, \tag{23}$$

we have

$$Q_{2n+1}(\mathcal{A}',\mathcal{F}') - Q_{2n+1}(\mathcal{A},\mathcal{F}) = Q_{2n+1}(g^{-1}\mathrm{d}g,0) + \mathrm{d}\alpha_{2n}, \tag{24}$$

where $\alpha_{2n}$ is some $2n$ form [44]. We note that

$$\begin{aligned} Q_{2n+1}\left(g^{-1}\mathrm{d}g,0\right) &= \frac{1}{n!}\left(\frac{\mathrm{i}}{2\pi}\right)^{n+1}\int_0^1 \mathrm{d}t\ \mathrm{tr}\left(\mathcal{A}(t^2-t)^n\mathcal{A}^{2n}\right) \\ &= \frac{1}{n!}\left(\frac{\mathrm{i}}{2\pi}\right)^{n+1}\mathrm{tr}\left[(g^{-1}\mathrm{d}g)^{2n+1}\right]\int_0^1 \mathrm{d}t\ (t^2-t)^n \\ &= \omega_{2n+1}[g]. \end{aligned} \tag{25}$$

This is nothing but the winding number density, and its integral

$$\nu_{2n+1}[g] := \int_{\mathrm{BZ}^{2n+1}} Q_{2n+1}\left(g^{-1}\mathrm{d}g,0\right) = \int_{\mathrm{BZ}^{2n+1}} \omega_{2n+1}[g] \tag{26}$$

is an integer, which counts the nontrivial winding of the map $g(k):\mathrm{BZ}^{2n+1}\to \mathrm{U}(N)$. Note that $\pi_{2n+1}\left[\mathrm{U}(N)\right]=\mathbb{Z}$ (for large enough $N$). We thus conclude

$$\mathrm{CS}_{2n+1}\left[\mathcal{A}',\mathcal{F}'\right] - \mathrm{CS}_{2n+1}\left[\mathcal{A},\mathcal{F}\right] = \text{integer}, \tag{27}$$

and hence the exponential

$$W_{2n+1} := \exp\{2\pi\mathrm{i}\,\mathrm{CS}_{2n+1}\left[\mathcal{A},\mathcal{F}\right]\} \tag{28}$$

is a well-defined, gauge invariant quantity, although it is not necessarily quantized.

The discussion so far has been general. In particular, it is *not* restricted to *chiral* topological insulators. We now compute the Chern–Simons invariant for class AIII topological insulators in $d=2n+1$. We first explicitly write down the Berry connection for chiral symmetric Hamiltonians. To this end, we observe that for unoccupied and occupied bands, the Bloch wavefunctions satisfy

$$Q(k)|u^{+}_{\hat{a}}(k)\rangle = +|u^{+}_{\hat{a}}(k)\rangle, \qquad Q(k)|u^{-}_{\hat{a}}(k)\rangle = -|u^{-}_{\hat{a}}(k)\rangle, \tag{29}$$

respectively. Introducing

$$|u^{\epsilon}_{\hat{a}}(k)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}\chi^{\epsilon}_{\hat{a}}(k)\\ \eta^{\epsilon}_{\hat{a}}(k)\end{pmatrix}, \qquad \epsilon=\pm, \tag{30}$$

we rewrite (29) as

$$\begin{pmatrix} 0 & q(k) \\ q^\dagger(k) & 0 \end{pmatrix} \begin{pmatrix} \chi_{\hat{a}}^{\pm}(k) \\ \eta_{\hat{a}}^{\pm}(k) \end{pmatrix} = \pm \begin{pmatrix} \chi_{\hat{a}}^{\pm}(k) \\ \eta_{\hat{a}}^{\pm}(k) \end{pmatrix}. \tag{31}$$

We can then construct a set of eigen Bloch functions as

$$|u_{\hat{a}}^{\epsilon}(k)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} \chi_{\hat{a}}^{\epsilon} \\ \epsilon q^\dagger(k) \chi_{\hat{a}}^{\epsilon} \end{pmatrix}. \tag{32}$$

The $N$-dimensional space spanned by the occupied states $\{|u_{\hat{a}}^{-}(k)\rangle\}$ can be obtained by first choosing $N$ independent orthonormal vectors $n_{\hat{a}}^{\epsilon}$ that are $k$-independent, and then from $n_{\hat{a}}^{\epsilon}$,

$$|u_{\hat{a}}^{\epsilon}(k)\rangle_{\mathrm{N}} = \frac{1}{\sqrt{2}} \begin{pmatrix} n_{\hat{a}}^{\epsilon} \\ \epsilon q^\dagger(k) n_{\hat{a}}^{\epsilon} \end{pmatrix}. \tag{33}$$

From these Bloch functions, the Berry connection is computed as

$$\begin{aligned} {}_{\mathrm{N}}\langle u_{\hat{a}}^{\epsilon}(k)|\partial_\mu u_{\hat{b}}^{\epsilon}(k)\rangle_{\mathrm{N}} \mathrm{d}k_\mu &= \tfrac{1}{2}\left[\langle n_{\hat{a}}^{\epsilon}|\partial_\mu|n_{\hat{b}}^{\epsilon}\rangle + \epsilon^2 \langle n_{\hat{a}}^{\epsilon} q(k)|\partial_\mu|q^\dagger(k) n_{\hat{b}}^{\epsilon}\rangle\right]\mathrm{d}k_\mu \\ &= \tfrac{1}{2}\left[0 + \epsilon^2 \langle n_{\hat{a}}^{\epsilon} q(k)|\partial_\mu|q^\dagger(k) n_{\hat{b}}^{\epsilon}\rangle\right]\mathrm{d}k_\mu \\ &= \tfrac{1}{2}[q(k)\partial_\mu q^\dagger(k)]_{\hat{a}\hat{b}}\mathrm{d}k_\mu =: \mathcal{A}_{\hat{a}\hat{b}}^{\mathrm{N}}, \end{aligned} \tag{34}$$

where we have made a convenient choice $(n_{\hat{a}}^{\epsilon})_{\hat{b}} = \delta_{\hat{a}\hat{b}}$. While this looks *almost* like a pure gauge, it is not exactly so because of the factor $1/2$. Note also that this calculation shows that the Berry connections for the occupied and unoccupied bands are identical. With equations (29)–(33), we have succeeded in constructing eigen Bloch wavefuctions of the '$Q$-matrix', equation (19), in block-off diagonal basis, that are free from any singularity. That is, we have explicitly demonstrated that there is no obstruction to constructing eigen wavefuctions globally. We emphasize that this applies to all symmetry classes with chiral symmetry (AIII, BDI, DIII, CII, CI) for any spatial dimension ($d = 2n$ as well as $d = 2n + 1$).

Alternatively, one can construct another set of eigen Bloch functions

$$|u_{\hat{a}}^{\epsilon}(k)\rangle_{\mathrm{S}} = \frac{1}{\sqrt{2}} \begin{pmatrix} \epsilon q(k) n_{\hat{a}}^{\epsilon} \\ n_{\hat{a}}^{\epsilon} \end{pmatrix}. \tag{35}$$

For these Bloch functions, the Berry connection is computed as

$$\begin{aligned} {}_{\mathrm{S}}\langle u_{\hat{a}}^{\epsilon}(k)|\partial_\mu u_{\hat{b}}^{\epsilon}(k)\rangle_{\mathrm{S}} \mathrm{d}k_\mu &= \tfrac{1}{2}\left[\epsilon^2 \langle n_{\hat{a}}^{\epsilon} q^\dagger(k)|\partial_\mu|q(k) n_{\hat{b}}^{\epsilon}\rangle + \langle n_{\hat{a}}^{\epsilon}|\partial_\mu|n_{\hat{b}}^{\epsilon}\rangle\right]\mathrm{d}k_\mu \\ &= \tfrac{1}{2}\left[\epsilon^2 \langle n_{\hat{a}}^{\epsilon} q^\dagger(k)|\partial_\mu|q(k) n_{\hat{b}}^{\epsilon}\rangle + 0\right]\mathrm{d}k_\mu \\ &= \tfrac{1}{2}[q^\dagger(k)\partial_\mu q(k)]_{\hat{a}\hat{b}}\mathrm{d}k_\mu =: \mathcal{A}_{\hat{a}\hat{b}}^{\mathrm{S}}, \end{aligned} \tag{36}$$

where we have made a convenient choice $(n_{\hat{a}}^{\epsilon})_{\hat{b}} = \delta_{\hat{a}\hat{b}}$. The two gauges are related to each other by

$$\mathcal{A}^{\mathrm{S}} = g^{-1}\mathcal{A}^{\mathrm{N}} g + g^{-1}\mathrm{d}g, \tag{37}$$

where the transition function $g$ is the block off-diagonal projector, $g=q$:

$$
\begin{aligned}
q^{\dagger}(k)\left[\tfrac{1}{2}q(k)\partial_\mu q^{\dagger}(k)\right]q(k)+q^{\dagger}(k)\partial_\mu q(k) &= \tfrac{1}{2}\left[\partial_\mu q^{\dagger}(k)\right]q(k)+q^{\dagger}(k)\partial_\mu q(k)\\
&= -\tfrac{1}{2}q^{\dagger}(k)\partial_\mu q(k)+q^{\dagger}(k)\partial_\mu q(k)\\
&= \tfrac{1}{2}q^{\dagger}(k)\partial_\mu q(k).
\end{aligned}
\tag{38}
$$

We now compute the Chern–Simons invariant for class AIII topological insulators in $d=2n+1$. In the gauge where $\mathcal{A}=\mathcal{A}^{\mathrm{S}}=(1/2)(q^{-1}\mathrm{d}q)$, we have

$$
\begin{aligned}
\mathrm{d}\mathcal{A} &= \tfrac{1}{2}\mathrm{d}(q^{-1}\mathrm{d}q) = -\tfrac{1}{2}(q^{-1}\mathrm{d}q)(q^{-1}\mathrm{d}q),\\
\mathcal{F}_t &= t\,\mathrm{d}\mathcal{A}+t^2\mathcal{A}^2 = \left(-\frac{t}{2}+\frac{t^2}{4}\right)(q^{-1}\mathrm{d}q)^2.
\end{aligned}
\tag{39}
$$

Then,

$$
\begin{aligned}
Q_{2n+1}(\mathcal{A},\mathcal{F}) &= \frac{1}{n!}\left(\frac{\mathrm{i}}{2\pi}\right)^{n+1}\int_0^1 \mathrm{d}t\ \mathrm{tr}\big(\mathcal{A}\mathcal{F}_t^n\big)\\
&= \frac{1}{n!}\left(\frac{\mathrm{i}}{2\pi}\right)^{n+1}\int_0^1 \left(-\frac{t}{2}+\frac{t^2}{4}\right)^n \frac{\mathrm{d}t}{2}\ \mathrm{tr}\big[(q^{-1}\mathrm{d}q)^{2n+1}\big]\\
&= \frac{1}{n!}\left(\frac{\mathrm{i}}{2\pi}\right)^{n+1}\frac{1}{2}\int_0^1 u^n(u-1)^n\mathrm{d}u\ \mathrm{tr}\big[(q^{-1}\mathrm{d}q)^{2n+1}\big],
\end{aligned}
\tag{40}
$$

which is half of the winding number density,

$$
Q_{2n+1}(\mathcal{A}^{\mathrm{S}},\mathcal{F}^{\mathrm{S}}) = \tfrac{1}{2}\omega_{2n+1}[q]. \tag{41}
$$

Hence, we conclude

$$
\mathrm{CS}_{2n+1}\left[\mathcal{A}^{\mathrm{S}},\mathcal{F}^{\mathrm{S}}\right] = \int_{\mathrm{BZ}^{d=2n+1}} Q_{2n+1}(\mathcal{A}^{\mathrm{S}},\mathcal{F}^{\mathrm{S}}) = \frac{1}{2}\nu_{2n+1}[q]. \tag{42}
$$

As a corollary,

$$
W_{2n+1} = \exp\{2\pi\mathrm{i}\,\mathrm{CS}_{2n+1}[\mathcal{A},\mathcal{F}]\} = \exp\{\pi\mathrm{i}\,\nu_{2n+1}[q]\}. \tag{43}
$$

Thus, while in general the quantity $W_{2n+1}$ is not quantized, for class AIII Hamiltonians in $d=2n+1$, $W_{2n+1}$ can take only two values, $W_{2n+1}=\pm1$.

Physically, $\mathrm{CS}_{2n+1}[\mathcal{A},\mathcal{F}]$ in $d=1$ ($n=0$) spatial dimension takes the form of the U(1) Wilson loop defined for $\mathrm{BZ}^{d=1}\simeq S^1$. It is quantized for chiral symmetric systems [54]. Also, the logarithm of $W_1$ represents the electric polarization [55, 56]. For a lattice system, the non-invariance of $\mathrm{CS}_1[\mathcal{A},\mathcal{F}]$ (i.e. it can change under a gauge transformation, $\mathrm{CS}_1[\mathcal{A},\mathcal{F}]\to\mathrm{CS}_1[\mathcal{A},\mathcal{F}]+$ (integer)) has a clear meaning: since the system is periodic, the displacement of electron coordinates has a meaning only within a unit cell, and two electron coordinates that differ by an integer multiple of the lattice constant should be identified.

In $d=3$ ($n=1$) spatial dimensions, $\mathrm{CS}_3$ represents the magnetoelectric polarizability [28, 57, 58]. While this was discussed originally for 3D $\mathbb{Z}_2$ topological insulators in symplectic symmetry (class AII), the magnetoelectric polarizability is also quantized for class AIII.

### *2.3. Dirac insulators and dimensional reduction*

We start from a $d = 2n+3$-dimensional *gapless* Dirac Hamiltonian defined in momentum space,

$$\mathcal{H}^{d=2n+3}_{(2n+3)}(k) = \sum_{a=1}^{d=2n+3} k_a \Gamma^a_{(2n+3)}. \tag{44}$$

Here, $k_{a=1,\dots,d}$ are $d$-dimensional momenta, and $\Gamma^{a=1,\dots,2n+3}_{(2n+3)}$ are $(2^{n+1} \times 2^{n+1})$-dimensional Hermitian matrices that satisfy $\{\Gamma^a_{(2n+3)}, \Gamma^b_{(2n+3)}\} = 2\delta_{a,b}$. Some results for the gamma matrices, on which the following discussion is based, are summarized in Appendix B. The massless Dirac Hamiltonian $\mathcal{H}^{d=2n+3}_{(2n+3)}(k)$ cannot be realized on a lattice in a naive way because of the fermion doubling problem.

By replacing $k_{2n+3}$ by a mass term, we obtain a $d = 2n+2$-dimensional class A topological Dirac insulator,

$$\mathcal{H}^{d=2n+2}_{(2n+3)}(k, m) = \sum_{a=1}^{d=2n+2} k_a \Gamma^a_{(2n+3)} + m\Gamma^{2n+3}_{(2n+3)}. \tag{45}$$

The topological character of this Dirac insulator will be further discussed below.

By setting in addition $k_{2n+2} = 0$, we obtain an insulator in one dimension lower,

$$\mathcal{H}^{d=2n+1}_{(2n+3)}(k, m) = \sum_{a=1}^{d=2n+1} k_a \Gamma^a_{(2n+3)} + m\Gamma^{2n+3}_{(2n+3)}. \tag{46}$$

By construction, $\mathcal{H}^{d=2n+1}_{(2n+3)}(k, m)$ anticommutes with $\Gamma^{2n+2}_{(2n+3)}$,

$$\left\{\mathcal{H}^{d=2n+1}_{(2n+3)}(k, m),\ \Gamma^{2n+2}_{(2n+3)}\right\} = 0, \tag{47}$$

and hence it is a member of class AIII.

This construction of the lower-dimensional models from their higher-dimensional 'parent' is an example of the Kaluza–Klein dimensional reduction. To obtain $\mathcal{H}^{d=2n+1}_{(2n+3)}(k, m)$ from $\mathcal{H}^{d=2n+2}_{(2n+3)}(k, m)$, one can first compactify the $(2n+2)$th spatial direction into a circle $S^1$. The $(2n+2)$th component of the momentum is then quantized, $k_{2n+2} = 2\pi N_{2n+2}/\ell$, where $N_{2n+2} \in \mathbb{Z}$, and $\ell$ is the radius of $S^1$. The energy eigenvalues now carry the integral label $N_{2n+2}$, in addition to the continuous label, $k_{i=1,\dots,2n+1}$. By making the radius of the circle very small, all levels with $N_{2n+2} \neq 0$ have very large energies, while the levels with $N_{2n+2} = 0$ are not affected by the small radius limit. In this way, in the limit $\ell \to 0$, there is a separation of energy scales, and we only keep the states with $N_{2n+2} = 0$, while neglecting all states with $N_{2n+2} \neq 0$ (the Kaluza–Klein modes).

Similarly, $\mathcal{H}^{d=2n+2}_{(2n+3)}(k, m)$ is naturally obtained from $\mathcal{H}^{d=2n+3}_{(2n+3)}(k)$ by dimensional reduction if we also include a U(1) gauge field. We can introduce an (external, electromagnetic) U(1) gauge field $a_{i=1,\cdots,2n+3}$ by minimal coupling, $\mathcal{H}^{d=2n+3}_{(2n+3)}(k) \to \mathcal{H}^{d=2n+3}_{(2n+3)}(k+a)$. In the $S^1$ compactification of the $(2n+3)$th spatial coordinate, we again keep modes with $k_{2n+3} = 0$ only while neglecting all the Kaluza–Klein modes with $k_{2n+3} \neq 0$. The vector field (gauge field) $a_{i=1,\dots,2n+3}$ in $d = 2n+3$ dimensions can be decomposed into a vector field $(a_{i=1,\dots,2n+2})$ and a scalar field $(a_{2n+3} \equiv \varphi)$ in $d = 2n+2$, leading to

$$\mathcal{H}^{d=2n+2}_{(2n+3)}(k+a, \varphi) = \sum_{i=1}^{d=2n+2} (k_i + a_i)\Gamma^i_{(2n+3)} + \varphi\Gamma^{2n+3}_{(2n+3)}. \tag{48}$$

Switching off the $d = 2n + 2$-dimensional gauge field and assuming the scalar field is constant $\varphi = m$, we obtain $\mathcal{H}^{d=2n+2}_{(2n+3)}(k, m)$.

For the massive Dirac insulator (45) in class A in $2n + 2$ dimensions, the $n$th Chern number $\mathrm{Ch}_{n+1}$ is non-vanishing [59]. Accordingly, for the massive Dirac insulator (46) in class AIII in $2n + 1$ dimensions, the winding number and the Chern–Simons form are nonzero.

As the Chern–Simons form can be derived from its higher-dimensional parent, the Chern form, one may wonder if there is a connection between $\mathrm{CS}_{2n+1} = \frac{1}{2}\nu_{2n+1}$ of a class AIII Dirac topological insulator in $d = 2n + 1$ and $\mathrm{Ch}_{n+1}$ of a class A Dirac topological insulator in $d = 2n + 2$. We now try to answer this question.

Let us start from

$$\mathcal{H}^{d=2n+2}_{(2n+3)}(k, m) = \sum_{a=1}^{d=2n+2} k_a \Gamma^a_{(2n+3)} + m(k)\Gamma^{2n+3}_{(2n+3)}. \tag{49}$$

Here we have regularized the Dirac spectrum by making the mass term $k$ dependent,

$$m(k) = m - Ck^2 \quad \text{with} \quad \mathrm{sgn}(C) = \mathrm{sgn}(m). \tag{50}$$

With this regularization, as $|k| \to \infty$, $\mathcal{H}^{d=2n+2}_{(2n+3)}(k, m) \propto \Gamma^{2n+3}_{(2n+3)}$, and hence the wavefunctions become $k$ independent (i.e., the BZ is topologically $S^d$). The sign choice of the constant $C$, $\mathrm{sgn}(C) = \mathrm{sgn}(m)$, makes the Chern invariant for the Dirac insulator nonzero.

By dropping $k_{2n+2}$, we obtain the (regularized) Dirac insulator in one dimension lower,

$$\mathcal{H}^{d=2n+1}_{(2n+3)}(\tilde{k}, m) = \sum_{a=1}^{d=2n+1} k_a \Gamma^a_{(2n+3)} + m(\tilde{k}, 0)\Gamma^{2n+3}_{(2n+3)}, \tag{51}$$

where $\tilde{k} = (k_1, \ldots, k_{2n+1})$. As mentioned before, $\mathcal{H}^{d=2n+1}_{(2n+3)}(\tilde{k}, m)$ is chiral symmetric, $\{\mathcal{H}^{d=2n+1}_{(2n+3)}(\tilde{k}, m), \Gamma^{2n+2}_{(2n+3)}\} = 0$. We work in the basis where $\Gamma^{2n+2}_{(2n+3)}$ is diagonal. In this basis, $\mathcal{H}^{d=2n+1}_{(2n+3)}$ is block off-diagonal,

$$\mathcal{H}^{d=2n+1}_{(2n+3)}(\tilde{k}, m) = \begin{pmatrix} 0 & \tilde{D}(\tilde{k}) \\ \tilde{D}^\dagger(\tilde{k}) & 0 \end{pmatrix}. \tag{52}$$

Correspondingly,

$$\mathcal{H}^{d=2n+2}_{(2n+3)}(k) = \begin{pmatrix} \Delta(k_{2n+2}) & D(k) \\ D^\dagger(k) & -\Delta(k_{2n+2}) \end{pmatrix}, \tag{53}$$

where $\Delta(k_{2n+2}) = k_{2n+2}$ and $D(k) = D(\tilde{k}, k_{2n+2})$ satisfies

$$D(\tilde{k}, k_{2n+2}) = \tilde{D}(\tilde{k}), \quad \text{when} \quad k_{2n+2} = 0. \tag{54}$$

We now look for eigenfunctions of $\mathcal{H}^{d=2n+2}_{(2n+3)}$ with negative eigenvalues,

$$\begin{pmatrix} \Delta(k_{2n+2}) & D(k) \\ D^\dagger(k) & -\Delta(k_{2n+2}) \end{pmatrix} \begin{pmatrix} \chi \\ \eta \end{pmatrix} = -\lambda(k) \begin{pmatrix} \chi \\ \eta \end{pmatrix}. \tag{55}$$

To this end, we first solve the following auxiliary eigenvalue problem:

$$\begin{pmatrix} 0 & D(k) \\ D^\dagger(k) & 0 \end{pmatrix} \begin{pmatrix} \chi \\ \eta \end{pmatrix} = -\tilde{\lambda}(k) \begin{pmatrix} \chi \\ \eta \end{pmatrix}, \tag{56}$$

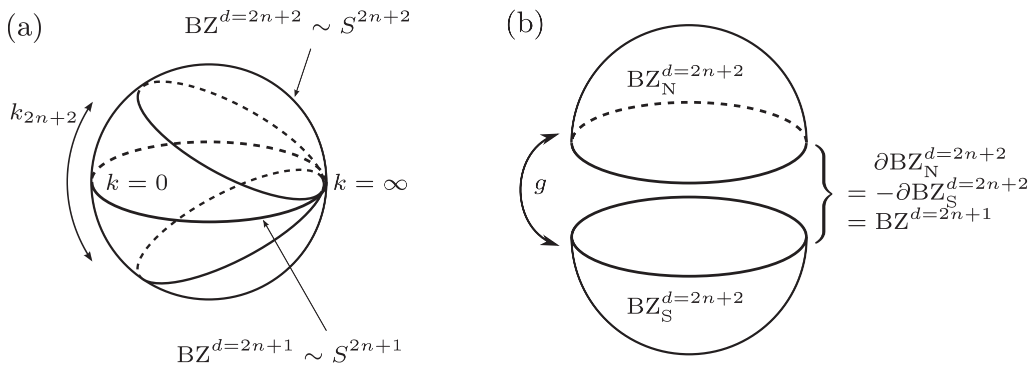


**Figure 2.** (a) The $d=2n+2$-dimensional BZ, $\mathrm{BZ}^{d=2n+2} \sim S^{2n+2} = S^{2n+1} \wedge S^1$ and its $d=2n+1$-dimensional descendant $\mathrm{BZ}^{d=2n+1} \sim S^{2n+1}$ located at the equator of $S^{2n+2}$. (b) Splitting the $d=2n+2$-dimensional BZ in half, or embedding $d=2n+1$-dimensional BZ into a higher-dimensional one.

where $\tilde{\lambda} = \sqrt{\tilde{k}^2 + [m(k)]^2}$. We see from (33) and (35) that the solutions are given by

$$\frac{1}{\sqrt{2}}\begin{pmatrix} -n_{\hat{a}} \\ q^{\dagger}(k) n_{\hat{a}} \end{pmatrix} \quad \text{or} \quad \frac{1}{\sqrt{2}}\begin{pmatrix} q(k) n_{\hat{a}} \\ -n_{\hat{a}} \end{pmatrix}, \tag{57}$$

where $q(k)$ and $q^{\dagger}(k)$ are the off-diagonal blocks of the $Q$-matrix derived from the auxiliary Hamiltonian. If we specialize to the case where $k=(\tilde{k},0)$, the projector of $\mathcal{H}^{d=2n+1}_{(2n+3)}(\tilde{k})$ is given in terms of $q(\tilde{k})$ and $q^{\dagger}(\tilde{k})$. We then construct two different sets of normalized eigenfunctions of $\mathcal{H}^{d=2n+2}_{(2n+3)}$,

$$|u^{-}_{\hat{a}}(k)\rangle_{\mathrm{N}} = \frac{1}{\sqrt{2\lambda(\lambda+\Delta)}}\begin{pmatrix} -\tilde{\lambda} n_{\hat{a}} \\ (\lambda+\Delta) q^{\dagger} n_{\hat{a}} \end{pmatrix} \tag{58}$$

and

$$|u^{-}_{\hat{a}}(k)\rangle_{\mathrm{S}} = \frac{1}{\sqrt{2\lambda(\lambda-\Delta)}}\begin{pmatrix} (\Delta-\lambda) q n_{\hat{a}} \\ \tilde{\lambda} n_{\hat{a}} \end{pmatrix}, \tag{59}$$

with the eigenvalue $-\lambda = -\sqrt{\tilde{\lambda}^2+\Delta^2}$. When specialized to $k=(\tilde{k},0)$, these wavefunctions yield the eigenfunctions (57) of the chiral Dirac Hamiltonian $\mathcal{H}^{d=2n+1}_{(2n+3)}$.

Since the Hamiltonian $\mathcal{H}^{d=2n+2}(k)$ is characterized by the nonzero Chern number, $\mathrm{Ch}_{n+1}[\mathcal{F}] \neq 0$, it is not possible to define wavefunctions globally. We thus need to split the BZ ($\mathrm{BZ}^{d=2n+2}$) into two parts, $\mathrm{BZ}^{d=2n+2}_{\mathrm{N}}$ and $\mathrm{BZ}^{d=2n+2}_{\mathrm{S}}$. We choose the interface of these two patches as $\partial\mathrm{BZ}^{d=2n+2}_{\mathrm{N}} = -\partial\mathrm{BZ}^{d=2n+2}_{\mathrm{S}} = \mathrm{BZ}^{d=2n+1}$, on which a lower-dimensional Hamiltonian 'lives'. For each patch, $\mathrm{BZ}^{d=2n+2}_{\mathrm{N,S}}$, we can choose a global gauge. Observe that the wavefunction $|u^{-}_{\hat{a}}(k)\rangle_{\mathrm{N}}$ is well defined for $k_{2n+2}>0$ and has a singularity at $(\tilde{k},k_{2n+2}) = (0,-\sqrt{m/C})$. Similarly, $|u^{-}_{\hat{a}}(k)\rangle_{\mathrm{S}}$ is well defined for $k_{2n+2}<0$ and singular at $(\tilde{k},k_{2n+2}) = (0,\sqrt{m/C})$.

The two gauges are thus complementary and at the boundary $\partial\mathrm{BZ}^{d=2n+2}_{\mathrm{N}} = -\partial\mathrm{BZ}^{d=2n+2}_{\mathrm{S}}$, they are glued by the transition function

$$\mathcal{A}^{\mathrm{S}} = g^{-1}\mathcal{A}^{\mathrm{N}} g + g^{-1}\mathrm{d}g, \tag{60}$$

where $g(\tilde{k}) \in \mathrm{U}(N_-)$ with $\tilde{k} \in \partial \mathrm{BZ}^{d=2n+2}_{\mathrm{N}}$. Then,

$$\begin{aligned}\mathrm{Ch}_{n+1}[\mathcal{F}] &= \int_{\mathrm{BZ}^{d=2n+2}} \mathrm{ch}_{n+1}(\mathcal{F}) = \int_{\mathrm{BZ}^{d=2n+2}} \mathrm{d}Q_{2n+1}(\mathcal{A},\mathcal{F}) \\ &= \int_{\mathrm{BZ}^{d=2n+2}_{\mathrm{N}}} \mathrm{d}Q_{2n+1}(\mathcal{A}^{\mathrm{N}},\mathcal{F}) + \int_{\mathrm{BZ}^{d=2n+2}_{\mathrm{S}}} \mathrm{d}Q_{2n+1}(\mathcal{A}^{\mathrm{S}},\mathcal{F}) \\ &= \int_{\partial\mathrm{BZ}^{d=2n+2}_{\mathrm{N}}} Q_{2n+1}(\mathcal{A}^{\mathrm{N}},\mathcal{F}) - \int_{\partial\mathrm{BZ}^{d=2n+2}_{\mathrm{N}}} Q_{2n+1}(\mathcal{A}^{\mathrm{S}},\mathcal{F}),\end{aligned} \tag{61}$$

where we have used the Stokes theorem. From formula (24), it follows that

$$\mathrm{Ch}_{n+1}[\mathcal{F}] = \int_{\partial\mathrm{BZ}^{d=2n+1}_{\mathrm{N}}} Q_{2n+1}\left(g^{-1}\mathrm{d}g, 0\right). \tag{62}$$

By the use of equation (25), we conclude that the rhs of the above equation is nothing but the winding number. Thus, the Chern number can be expressed as a winding number of the transition function $g$. For the case we are interested in, i.e. when a $d = 2n+1$ topological insulator 'lives' on $\partial\mathrm{BZ}^{d=2n+1}_{\mathrm{N}}$, the transition function is given by the off-diagonal block of the projector, $g(\tilde{k}) = q(\tilde{k})$. This is how two topological insulators in $d = 2n+2$ and $d = 2n+1$ are related.

### 2.4. Example: $d = 3 \to 2 \to 1$

Consider three mutually anticommuting, Hermitian matrices

$$\Gamma^{a=1,2,3}_{(3)} = \{\sigma_x,\ \sigma_y,\ \sigma_z\}, \tag{63}$$

where $\sigma_{x,y,z}$ are the $2\times 2$ Pauli matrices. These matrices can be used to construct a $d = 3$ gapless (Weyl) chiral fermion

$$\mathcal{H}^{d=3}_{(3)}(k) = \sum_{a=1}^{3} k_a \Gamma^a_{(3)}. \tag{64}$$

By replacing the third component of the momentum by a mass term, $k_{a=3} \to m$, we get a $d =$ 2-dimensional Dirac Hamiltonian,

$$\begin{aligned}\mathcal{H}^{d=2}_{(3)}(k,m) &= \sum_{a=1}^{2} k_a \Gamma^a_{(3)} + m\Gamma^3_{(3)} \\ &= k_x\sigma_x + k_y\sigma_y + m\sigma_z.\end{aligned} \tag{65}$$

This is a class A Hamiltonian. The Bloch wavefunctions are given by $[\lambda(k) := \sqrt{k^2+m^2}]$

$$\begin{aligned}|u^+(k)\rangle &= \frac{1}{\sqrt{2\lambda\,(\lambda-m)}}\begin{pmatrix} k_x - \mathrm{i}k_y \\ \lambda - m\end{pmatrix}, \\ |u^-(k)\rangle &= \frac{1}{\sqrt{2\lambda\,(\lambda+m)}}\begin{pmatrix} -k_x + \mathrm{i}k_y \\ \lambda + m\end{pmatrix}.\end{aligned} \tag{66}$$

We note that $|u^-(k)\rangle$ is well defined for all $k$ when $m > 0$. (When $m < 0$, by choosing a gauge properly, we can obtain a similar well-defined wavefunction.) Assuming $m > 0$, we adopt $|u^-(k)\rangle$, for which we obtain the Berry connection

$$A_x(k,m) = +\frac{\mathrm{i}k_y}{2\lambda\,(\lambda+m)}, \qquad A_y(k,m) = -\frac{\mathrm{i}k_x}{2\lambda\,(\lambda+m)}, \tag{67}$$

and the Berry curvature

$$F_{xy}(k,m) = \partial_{k_x} A_y - \partial_{k_y} A_x = -\frac{\mathrm{i}m}{2\lambda^3}. \tag{68}$$

The Chern number is nonzero,

$$\mathrm{Ch}_1[\mathcal{F}] = \frac{\mathrm{i}}{2\pi}\int \mathrm{d}^2k\, F_{xy} = \frac{\mathrm{i}}{2\pi}\int \mathrm{d}^2k \frac{-\mathrm{i}m}{2\lambda^3} = \frac{1}{2}\frac{m}{|m|}, \tag{69}$$

which is nothing but the Hall conductance $\sigma_{xy}$. This model can be realized, at low energies, in the honeycomb lattice model introduced by Haldane [60].

Finally, setting $k_2 = 0$, we get a $d = 1$-dimensional Dirac Hamiltonian,

$$\mathcal{H}^{d=1}_{(3)}(k,m) = k_x\sigma_x + m\sigma_z. \tag{70}$$

This is nothing but the chiral topological Dirac insulator in class AIII, as it anticommutes with $\sigma_y$. A topological invariant can be defined for the $d = 1$-dimensional Dirac Hamiltonian as follows. We first go to the canonical form by $(\sigma_x, \sigma_y, \sigma_z) \to (\sigma_x, \sigma_z, -\sigma_y)$, $\mathcal{H}^{d=1}_{(3)}(k,m) \to k_x\sigma_x - m\sigma_y$. This $d = 1$-dimensional Hamiltonian describes the physics of polyacetylene (see for example [61, 62].) The Bloch wavefunction with negative eigenvalue is

$$|u^-(k_x)\rangle = \frac{1}{\sqrt{2(k_x^2+m^2)}}\begin{pmatrix} -k_x - \mathrm{i}m \\ \lambda \end{pmatrix}. \tag{71}$$

The off-diagonal block of the projection operator $Q(k)$ in this basis is

$$q(k) = -\frac{k_x + \mathrm{i}m}{\sqrt{k_x^2+m^2}}, \tag{72}$$

and the winding number is given by

$$\nu_1[q] = \frac{\mathrm{i}}{2\pi}\int_{\mathrm{BZ}} q^{-1}\mathrm{d}q = \frac{\mathrm{i}}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}k_x \frac{-\mathrm{i}m}{k_x^2+m^2} = \frac{1}{2}\frac{m}{|m|}. \tag{73}$$

From equation (71) the Berry connection is obtained,

$$\mathcal{A}(k_x) = \langle u^-(k_x)|\mathrm{d}u^-(k_x)\rangle = \frac{1}{2}\frac{-\mathrm{i}m}{k_x^2+m^2}\mathrm{d}k_x. \tag{74}$$

Then, we find

$$\mathrm{CS}_1[\mathcal{A},\mathcal{F}] = \frac{\mathrm{i}}{2\pi}\int_{\mathrm{BZ}} \mathrm{tr}\,\mathcal{A} = \frac{\mathrm{i}}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}k_x \frac{1}{2}\frac{-\mathrm{i}m}{k_x^2+m^2} = \frac{1}{4}\frac{m}{|m|}. \tag{75}$$

This is half of the winding number $\nu_1[q]$ as expected. Hence, the Wilson 'loop' is given by

$$W_1 = \exp\{2\pi\mathrm{i}\mathrm{CS}_1[\mathcal{A},\mathcal{F}]\} = \exp\int_{\mathrm{BZ}} \mathrm{tr}\,\mathcal{A} = \mathrm{e}^{\pm\pi\mathrm{i}/2}. \tag{76}$$

Here, we mention, however, that there is a subtlety in computing the Wilson loop. In the basis where the Hamiltonian in momentum space is real, $\mathcal{H}^{d=1}_{(3)}(k,m) = k_x\sigma_x + m\sigma_z$ (70), the Bloch wavefunction is real for a given $k$, and as a consequence the Berry connection $\mathcal{A}(k_x)$ vanishes identically. One would then conclude $W_1 = 1$, not $W_1 = -1$, although $\nu_1 = \frac{1}{2}\mathrm{sgn}(m)$. This puzzle can be solved by properly regularizing the Dirac insulator. For simplicity, let us replace $k_x$ by $\sin k_x$, and $m$ by $m - 1 + \cos(k_x)$. With such a regularization, the BZ is topologically $S^1$, and one finds a singularity in the wavefunction at $k_x = \pi$, where the phase of the wavefunction jumps by $\pi$ (i.e. there is a Dirac string at $k_x = \pi$). If, on the other hand, we use a different basis (71), we can avoid having a Dirac string in the BZ, and the Wilson loop can be obtained by integrating the Berry connection over the BZ.

### *2.5. Example: $d=5\to 4\to 3$*

Consider five mutually anticommuting, Hermitian matrices

$$\Gamma^{a=1,\ldots,5}_{(5)} = \{\alpha_x,\ \alpha_y,\ \alpha_z,\ \beta,\ -\mathrm{i}\beta\gamma^5\}, \tag{77}$$

where we are using the Dirac representation,

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \gamma^5 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{78}$$

Observe that $\alpha_x\alpha_y\alpha_z\beta = -\mathrm{i}\beta\gamma_5$. These matrices can be used to construct a $(d=5)$-dimensional gapless chiral fermion

$$\mathcal{H}^{d=5}_{(5)}(k) = \sum_{a=1}^{5} k_a \Gamma^a_{(5)}. \tag{79}$$

By replacing the fifth component of the momentum by a mass term, $k_{a=5}\to m_5$, we obtain a $d=4$-dimensional Dirac Hamiltonian,

$$\mathcal{H}^{d=4}_{(5)}(k, m_5) = \sum_{a=1}^{4} k_a \Gamma^a_{(5)} + m_5 \Gamma^5_{(5)}. \tag{80}$$

It is known that for this gapped Hamiltonian, the second Chern number is nonzero [28, 59].

Finally, setting $k_4=0$, we obtain a $d=3$-dimensional Dirac Hamiltonian,

$$\mathcal{H}^{d=3}_{(5)}(k, m_5) = \sum_{a=1}^{3} k_a \Gamma^a_{(5)} + m_5 \Gamma^5_{(5)} = \sum_{a=1}^{3} k_a \alpha_a - m_5 \mathrm{i}\beta\gamma^5. \tag{81}$$

This is nothing but the chiral topological Dirac insulator in class AIII discussed in [26]. The tight-binding version of this model for a simple cubic lattice is given by

$$\mathcal{H}^{d=3}_{(5)}(k, m_5) = \sum_{a=1}^{3} \sin k_a \Gamma^a_{(5)} + \left(m_5 + \sum_{a=1}^{3} \cos k_a\right) \Gamma^5_{(5)}. \tag{82}$$

By taking open boundary conditions in the $z$-direction and periodic boundary conditions in the $x$- and $y$-directions, we can study the surface states of this model. When the winding number $\nu_3$ is non-vanishing, there are $|\nu_3|$ surface Dirac states, which cross the bulk band gap (see figure 3).

We now study the Berry connection of the above class A $(d=4)$ and class AIII $(d=3)$ Dirac insulators. To treat these two cases in a unified fashion, let us consider the following $d=4$ Dirac Hamiltonian:

$$\mathcal{H}(k, m_0) = \sum_{a=1}^{3} k_a \alpha_a + m_0 \beta + k_w(-\mathrm{i}\beta\gamma^5). \tag{83}$$

Upon identification $k_w \to m_5$, it can also be viewed as a $d=3$-dimensional Dirac Hamiltonian with two masses. The four eigenvalues are

$$E(k) = \pm\lambda(k), \quad \lambda(k) = \sqrt{k^2 + m_0^2}. \tag{84}$$

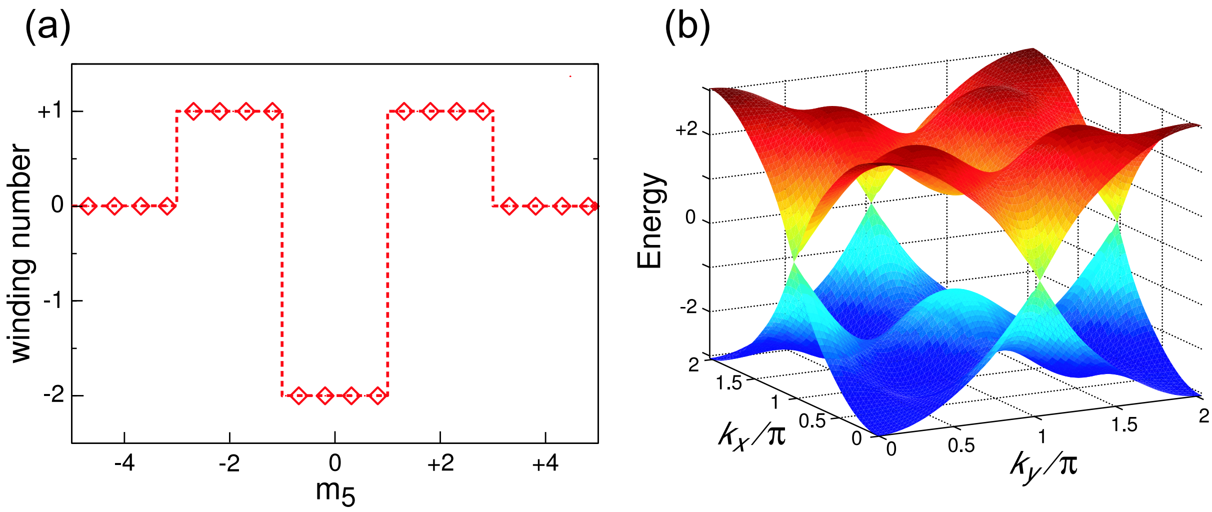


**Figure 3.** (a) Winding number $\nu_3$ for Hamiltonian (82) as a function of $m_5$. (b) 2D energy spectrum of the surface states of model (82) with mass $m_5 = +0.5$. There are two inequivalent surface modes in agreement with the winding number $\nu_3(m_5 = +0.5) = -2$.

The two normalized negative energy eigenstates with $E(k) = -\lambda(k)$ are

$$|u_1^-(k)\rangle = \frac{1}{\sqrt{2\lambda(\lambda+m_0)}} \begin{pmatrix} -k_x + \mathrm{i}k_y \\ \mathrm{i}k_w + k_z \\ 0 \\ \lambda + m_0 \end{pmatrix}, \qquad |u_2^-(k)\rangle = \frac{1}{\sqrt{2\lambda(\lambda+m_0)}} \begin{pmatrix} -k_z + \mathrm{i}k_w \\ -k_x - \mathrm{i}k_y \\ \lambda + m_0 \\ 0 \end{pmatrix}. \tag{85}$$

The two normalized positive energy eigenstates with $E(k) = +\lambda(k)$ are

$$|u_1^+(k)\rangle = \frac{1}{\sqrt{2\lambda(\lambda-m_0)}} \begin{pmatrix} k_x - \mathrm{i}k_y \\ -\mathrm{i}k_w - k_z \\ 0 \\ \lambda - m_0 \end{pmatrix}, \qquad |u_2^+(k)\rangle = \frac{1}{\sqrt{2\lambda(\lambda-m_0)}} \begin{pmatrix} -\mathrm{i}k_w + k_z \\ k_x + \mathrm{i}k_y \\ \lambda - m_0 \\ 0 \end{pmatrix}. \tag{86}$$

Note that if $m_0 > 0$, $|u_{1,2}^+(k)\rangle$ are not well defined at $\lambda(k) = m_0$ (i.e. $k = 0$). Observe that when $m_0 > 0$, $|u_{1,2}^-(k)\rangle$ have the form of wavefunctions expected from the general consideration (corresponding to the $\mathcal{A}^{\mathrm{N}}$ gauge choice).

When $m_0 = 0$, the Hamiltonian anticommutes with $\beta$ and is block off-diagonal. The off-diagonal component of the $Q$-matrix is given by

$$q(k) = \frac{-1}{\lambda}\,(k\cdot\sigma - \mathrm{i}m_5)\,. \tag{87}$$

By noting ($\mu = 1, 2, 3$)

$$\partial_\mu q = \frac{k_\mu}{\lambda^3}\,(k\cdot\sigma - \mathrm{i}m_5) - \frac{1}{\lambda}\sigma_\mu, \quad q^\dagger\partial_\mu q = \frac{-1}{\lambda^2}\left(k_\mu - k\cdot\sigma\sigma_\mu - \mathrm{i}m\sigma_\mu\right), \tag{88}$$

and also

$$\begin{aligned}
&\int \mathrm{d}^3k\,\epsilon^{\mu\nu\rho}\,\mathrm{tr}\left[q^\dagger\partial_\mu q q^\dagger\partial_\nu q q^\dagger\partial_\rho q\right]\\
&= \int \mathrm{d}^3k\,\frac{-\epsilon^{\mu\nu\rho}}{\lambda^6}\,\mathrm{tr}\left[-3\mathrm{i}m_5(k\cdot\sigma)\sigma_\mu(k\cdot\sigma)\sigma_\nu\sigma_\rho + \mathrm{i}m_5^3\sigma_\mu\sigma_\nu\sigma_\rho\right]\\
&= (-3\mathrm{i}m_5)\epsilon_{\mu\nu\rho}\frac{2\mathrm{i}}{3}\int \mathrm{d}^3k\,\frac{\epsilon^{\mu\nu\rho}k^2}{(k^2+m_5^2)^3} + \mathrm{i}m_5^3 2\mathrm{i}\epsilon_{\mu\nu\rho}\int \mathrm{d}^3k\,\frac{-\epsilon^{\mu\nu\rho}}{(k^2+m_5^2)^3}\\
&= 12m_5\int \mathrm{d}^3k\,\frac{1}{(k^2+m_5^2)^2},
\end{aligned} \tag{89}$$

the winding number is given by

$$\nu_3[q] = \frac{12}{24\pi^2}m_5\int_0^\infty \mathrm{d}k\,\frac{4\pi k^2}{(k^2+m_5^2)^2} = \frac{1}{2\pi^2}4\pi\times\frac{\pi}{4}\frac{m_5}{|m_5|} = \frac{1}{2}\frac{m_5}{|m_5|}. \tag{90}$$

We now compute the Chern–Simons invariant (magnetoelectric polarizability) for the massive Dirac Hamiltonian. For the lower two occupied bands, we can introduce a U(2) gauge field by $A^{\hat{a}\hat{b}}_\mu(k)\mathrm{d}k_\mu = \langle u^-_{\hat{a}}(k)|\mathrm{d}u^-_{\hat{b}}(k)\rangle$ ($\hat{a}, \hat{b} = 1, 2$). The U(2) gauge field is given by, in the matrix notation,

$$\begin{aligned}
A_x &= \frac{\mathrm{i}}{2\lambda(\lambda+m_0)}\begin{pmatrix} +k_y & k_w + \mathrm{i}k_z\\ k_w - \mathrm{i}k_z & -k_y\end{pmatrix},\\
A_y &= \frac{\mathrm{i}}{2\lambda(\lambda+m_0)}\begin{pmatrix} -k_x & \mathrm{i}k_w - k_z\\ -\mathrm{i}k_w - k_z & +k_x\end{pmatrix},\\
A_z &= \frac{\mathrm{i}}{2\lambda(\lambda+m_0)}\begin{pmatrix} -k_w & -\mathrm{i}k_x + k_y\\ \mathrm{i}k_x + k_y & +k_w\end{pmatrix}.
\end{aligned} \tag{91}$$

The gauge field can be decomposed into U(1) ($a^0$) and SU(2) ($a^{j=x,y,z}$) parts as

$$A_\mu(k) = a^0_\mu(k)\frac{\sigma_0}{2} + a^j_\mu(k)\frac{\sigma_j}{2}. \tag{92}$$

The U(1) part of the Berry connection is trivial, whereas the SU(2) part is given by

$$\begin{aligned}
a^x_x &= \mathrm{i}\frac{k_w}{\lambda(\lambda+m_0)}, & a^y_x &= \mathrm{i}\frac{-k_z}{\lambda(\lambda+m_0)}, & a^z_x &= \mathrm{i}\frac{+k_y}{\lambda(\lambda+m_0)},\\
a^x_y &= \mathrm{i}\frac{-k_z}{\lambda(\lambda+m_0)}, & a^y_y &= \mathrm{i}\frac{-k_w}{\lambda(\lambda+m_0)}, & a^z_y &= \mathrm{i}\frac{-k_x}{\lambda(\lambda+m_0)},\\
a^x_z &= \mathrm{i}\frac{+k_y}{\lambda(\lambda+m_0)}, & a^y_z &= \mathrm{i}\frac{+k_x}{\lambda(\lambda+m_0)}, & a^z_z &= \mathrm{i}\frac{-k_w}{\lambda(\lambda+m_0)}.
\end{aligned} \tag{93}$$

The Chern–Simons form can be computed as

$$\begin{aligned}\mathrm{CS}_3 &= \frac{-1}{8\pi^2}\int \mathrm{d}^3k\epsilon^{\mu\nu\rho}\,\mathrm{tr}\left(A_\mu\partial_\nu A_\rho + \frac{2}{3}A_\mu A_\nu A_\rho\right)\\ &= \frac{1}{8\pi^2}\int \mathrm{d}^3k\frac{m_5(2\lambda+m_0)}{\lambda^3(\lambda+m_0)^2}\\ &= \frac{1}{\pi}\frac{m_5}{|m_5|}\arctan\left[\frac{(m_5^2+m_0^2)^{1/2}-m_0}{(m_5^2+m_0^2)^{1/2}+m_0}\right]^{1/2}. \end{aligned} \tag{94}$$

When $m_0 = 0$,

$$\mathrm{CS}_3 = \frac{1}{4}\frac{m_5}{|m_5|}. \tag{95}$$

As the CS term is determined only modulo 1, the fractional part $\frac{1}{4}\mathrm{sgn}(m_5)$ is an intrinsic property. On a lattice, as there are two copies of the $4\times 4$ Dirac Hamiltonians, the total Chern–Simons invariant is given by $\mathrm{CS}_3 = \frac{1}{2}\mathrm{sgn}(m_5)$, and $\mathrm{e}^{2\pi\mathrm{i}\mathrm{CS}_3} = -1$.

There is a subtlety in computing $\mathrm{CS}_3$ and $W_3$, which is similar to the case of the Wilson loop $W_1$. When $m_0 \neq 0$ and $m_5 = 0$, the Chern–Simons form is zero identically, and one would conclude $W_3 = 1$, while chiral symmetry for the case of $m_0 \neq 0$ and $m_5 = 0$ allows us to define $\nu_3$, and $\nu_3 = \frac{1}{2}\mathrm{sgn}(m)$. As before, this puzzle can be solved by properly regularizing the Dirac insulator. With such a regularization, the BZ is topologically $S^3$, and one finds a singularity in the wavefunctions. If, on the other hand, we use a different basis, we can avoid having a Dirac string in the BZ.

### *2.6. Description in terms of field theory for the linear responses in $D = d+1$ spacetime dimensions*

For class A and AIII topological insulators or superconductors, there is always a conserved U(1) quantity; either electric charge or one component (the $z$-component, say) of spin is conserved [63]. Transport properties of these conserved quantities in these topological insulators or superconductors in $d$ spatial dimensions can be described in terms of an effective field theory for the linear responses in $D = d+1$ spacetime dimensions, which can be obtained by coupling an external spacetime-dependent gauge field $a_\mu$ to the topological insulator or superconductor (we will choose the Dirac representative; see the discussion near (48)), and by integrating out the gapped fermions. One can then read off the theory of the linear responses from the so obtained (classical) effective action for $a_\mu$.

The theory for the linear responses of a topological insulator in symmetry class A and in $d$ spatial dimensions is then given by the Chern–Simons action in $D = d+1$ spacetime dimensions,

$$S_{\mathrm{CS}}^{D=2n+1}[a] = 2\pi\mathrm{i}k\int_{\mathbb{R}^{D=2n+1}} Q_{2n+1}[a], \quad k = \mathrm{Ch}_n. \tag{96}$$

Here, $Q[a]$ is the Chern–Simons form of the U(1) gauge field $a_\mu$ defined in $D = 2n+1$-dimensional (Euclidean) spacetime, and the level $k$ of the Chern–Simons term is given in terms of $\mathrm{Ch}_n$, which is the Chern invariant computed from the Bloch wavefunctions in $d=2n$ space dimensions.

On the other hand, the theory of linear responses of a topological insulator in symmetry class AIII in $d=2n-1$ spatial dimensions is given by a theta term in $D=2n$ spacetime dimensions,

$$S_{\theta}^{D=2n}[a]=\mathrm{i}\theta\int_{\mathbb{R}^{D=2n}}\mathrm{ch}_n[f],\qquad \theta=\pi\nu_{2n-1}, \tag{97}$$

where $f$ is the field strength of the external gauge field $a_\mu$ and the theta angle $\theta$ is related to the winding number $\nu_{2n-1}$, which can be computed from the Bloch wavefunctions. The integration of fermions in $D=2n$ dimensions is trickier than in $D=2n+1$ dimensions; while a simple derivative expansion of the fermion determinant would appear to yield the Chern–Simons action (96), a more careful evaluation yields in fact the theta term, which is obtained from the Fujikawa Jacobian [64].

The theta angle in the theta term (97) can take on *a priori* any value if there is no discrete symmetry that pins its value. In class AII $\mathbb{Z}_2$ topological insulators in $D=4n$ dimensions, time-reversal symmetry demands $\theta$ to be an integer multiple of $\pi$. Similarly, in class AIII, chiral symmetry pins $\theta$ to be an integer multiple of $\pi$. This can be seen from the symmetry properties of the Chern–Simons and theta terms,

$$\begin{aligned}\mathcal{T}: S_{\mathrm{CS}}^{D=2n+1}&\to(-1)^n S_{\mathrm{CS}}^{D=2n+1},\qquad S_{\theta}^{D=2n}\to(-1)^{n+1}S_{\theta}^{D=2n},\\ \mathcal{C}: S_{\mathrm{CS}}^{D=2n+1}&\to(-1)^{n+1} S_{\mathrm{CS}}^{D=2n+1},\qquad S_{\theta}^{D=2n}\to(-1)^{n}S_{\theta}^{D=2n}.\end{aligned} \tag{98}$$

Here, the (anti-unitary) time-reversal symmetry operation $\mathcal{T}$ may either square to plus or minus the identity. Similarly, the charge-conjugation symmetry operation $\mathcal{C}$ may either square to plus or minus the identity. Since the chiral symmetry $\mathcal{S}$ can be expressed as the product of these two symmetry operations, i.e. $\mathcal{S}=\mathcal{T}\cdot\mathcal{C}$, one obtains

$$\mathcal{S}: S_{\theta}^{D=2n}\to -S_{\theta}^{D=2n}. \tag{99}$$

Together with the $2\pi$ periodicity of $\theta$, it follows that $\theta$ is either 0 or $\pi$.

## 3. Dimensional hierarchy for $\mathbb{Z}$ topological insulators: the real case

### *3.1. Dimensional reduction*

We now consider eight 'real' symmetry classes. In particular, we consider topological insulators (superconductors) with integer classification, $\mathbb{Z}$ or $2\mathbb{Z}$. ($\mathbb{Z}_2$ cases will be discussed in section 4.) A connection similar to the one between classes A and AIII can be established.

The massive Dirac Hamiltonians relevant to this section are all obtained from the following massless Dirac Hamiltonian:

$$(0):\quad \mathcal{H}_{(2n+3)}^{d=2n+3}(k)=\sum_{a=1}^{d=2n+3}k_a\Gamma_{(2n+3)}^{a}, \tag{100}$$

**Table 4.** Symmetry class of Dirac Hamiltonians $\mathcal{H}^{d=2n+3}_{(2n+3)}(k)$ (100), $\mathcal{H}^{d=2n+2}_{(2n+3)}(k,m)$ (101), $\mathcal{H}^{d=2n+1}_{(2n+3)}(k,m)$ (102), $\mathcal{H}^{d=2n}_{(2n+3)}(k,m)$ (103) and $\mathcal{H}^{d=2n-1}_{(2n+3)}(k,m)$ (104), marked by '0', '$i$', '$ii$', '$iii$', and '$iv$', respectively. Chiral and non-chiral symmetric classes are colored in blue and red, respectively.

| $AZ \backslash d$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | … |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| AI | $i$ | | | | $iii$ | | | 0 | $i$ | | | | … |
| BDI | | $ii$ | | | | $iv$ | | | | $ii$ | | | … |
| D | | 0 | $i$ | | | | $iii$ | | | 0 | $i$ | | … |
| DIII | | | | $ii$ | | | | $iv$ | | | | $ii$ | … |
| AII | $iii$ | | | 0 | $i$ | | | | $iii$ | | | 0 | … |
| CII | | $iv$ | | | | $ii$ | | | | $iv$ | | | … |
| C | | | $iii$ | | | 0 | $i$ | | | | $iii$ | | … |
| CI | | | | $iv$ | | | | $ii$ | | | | $iv$ | … |

by replacing some momenta by a mass or by simply dropping them. Specifically, we will consider

$$(i): \quad \mathcal{H}^{d=2n+2}_{(2n+3)}(k,m) = \sum_{a=1}^{d=2n+2} k_a \Gamma^a_{(2n+3)} + m\Gamma^{2n+3}_{(2n+3)}, \tag{101}$$

$$(ii): \quad \mathcal{H}^{d=2n+1}_{(2n+3)}(k,m) = \sum_{a=1}^{d=2n+1} k_a \Gamma^a_{(2n+3)} + m\Gamma^{2n+3}_{(2n+3)}, \tag{102}$$

$$(iii): \quad \mathcal{H}^{d=2n}_{(2n+3)}(k,m) = \sum_{a=1}^{d=2n} k_a \Gamma^a_{(2n+3)} + m\mathcal{M}, \tag{103}$$

$$(iv): \quad \mathcal{H}^{d=2n-1}_{(2n+3)}(k,m) = \sum_{a=1}^{d=2n-1} k_a \Gamma^a_{(2n+3)} + m\mathcal{M}, \tag{104}$$

where

$$\mathcal{M} := \mathrm{i}\Gamma^{2n+3}_{(2n+3)}\Gamma^{2n+2}_{(2n+3)}\Gamma^{2n+1}_{(2n+3)}. \tag{105}$$

The massive Dirac Hamiltonian $\mathcal{H}^{d=2n+2}_{(2n+3)}(k,m)$ is obtained from its gapless parent $\mathcal{H}^{d=2n+3}_{(2n+3)}(k)$ by replacing $k_{2n+3}$ with a mass $m$. By further removing $k_{2n+2}$, we obtain $\mathcal{H}^{d=2n+1}_{(2n+3)}(k,m)$. This is essentially the same procedure as in the previous section, where we obtained the class AIII topological Dirac Hamiltonian from its parent class A Hamiltonian. On the other hand, $\mathcal{H}^{d=2n}_{(2n+3)}(k,m)$ can be obtained from $\mathcal{H}^{d=2n+3}_{(2n+3)}(k)$ by first removing three components of the momentum $k_{2n+3,2n+2,2n+1}$ and then adding $\mathcal{M}$ as a mass term. Finally, $\mathcal{H}^{d=2n-1}_{(2n+3)}(k,m)$ is obtained from $\mathcal{H}^{d=2n}_{(2n+3)}(k,m)$ by dimensional reduction.

Here, an important difference from the dimensional reduction in the complex case is the shifting of symmetry classes. The parent Hamiltonian $\mathcal{H}^{d=2n+3}_{(2n+3)}(k)$ has one (and only one) of four discrete symmetries, $\mathcal{T}$ (squaring to plus or minus the identity) or $\mathcal{C}$ (squaring to plus or minus the identity), depending on the dimensionality $d$ (see table 4 and appendix B). That is, it is a member of any one of AI, D, AII and C.

*3.1.1. From $d = 2n+3$ to $d = 2n+2$.* When dimensionally reducing $\mathcal{H}^{d=2n+3}_{(2n+3)}(k)$ to $\mathcal{H}^{d=2n+2}_{(2n+3)}(k, m)$, the symmetry of the parent Hamiltonian $\mathcal{H}^{d=2n+3}_{(2n+3)}(k)$ is broken by the mass term: while the sign of the kinetic term is reversed under the discrete symmetry, the sign of the mass term remains unchanged. Thus, the new massive Hamiltonian is a member of a different symmetry class. By this procedure, we obtain an even-dimensional Hamiltonian $\mathcal{H}^{d=2n+2}_{(2n+3)}(k, m)$ with the 'shifted' symmetry,

$$\mathrm{AI} \to \mathrm{C}, \quad \mathrm{C} \to \mathrm{AII}, \quad \mathrm{AII} \to \mathrm{D}, \quad \mathrm{D} \to \mathrm{AI}. \tag{106}$$

This can be easily proved by taking an explicit form of gamma matrices (see appendix B). Observe that while we have chosen to remove $k_{2n+3}$ and hence $\Gamma^{2n+3}_{(2n+3)}$, any other component could have been removed instead of $k_{2n+3}$ and $\Gamma^{2n+3}_{(2n+3)}$. However, all these different choices are unitarily equivalent, as they are simply related by a permutation of Clifford generators, $\Gamma^{a}_{(2n+3)}$.

*3.1.2. From $d = 2n+2$ to $d = 2n+1$.* Further dimensionally reducing $\mathcal{H}^{d=2n+2}_{(2n+3)}(k, m)$ to $\mathcal{H}^{d=2n+1}_{(2n+3)}(k, m)$, we obtain a chiral symmetric Dirac Hamiltonian. Together with the existing discrete symmetry, this chiral symmetry yields one more discrete symmetry. One can see the symmetry of the newly generated Hamiltonian is shifted,

$$\mathrm{D} \to \mathrm{BDI}, \quad \mathrm{AII} \to \mathrm{DIII}, \quad \mathrm{C} \to \mathrm{CII}, \quad \mathrm{AI} \to \mathrm{CI}. \tag{107}$$

This again can be easily proved by taking an explicit form of gamma matrices (see appendix B).

*3.1.3. From $d = 2n+3$ to $d = 2n$.* Let us now consider $\mathcal{H}^{d=2n}_{(2n+3)}(k, m)$. One can check that this Hamiltonian belongs to the same symmetry class as its parent $\mathcal{H}^{d=2n+3}_{(2n+3)}(k)$. To study the topological properties of $\mathcal{H}^{d=2n}_{(2n+3)}(k, m)$, observe that, by construction, $\mathcal{H}^{d=2n}_{(2n+3)}(k, m)$ commutes with a product made of any two of $\Gamma^{2n+1,2n+2,2n+3}_{(2n+3)}$,

$$\left[\mathcal{H}^{d=2n}_{(2n+3)}(k, m), \Gamma^{a}_{(2n+3)}\Gamma^{b}_{(2n+3)}\right] = 0, \tag{108}$$

where $(a, b) = (2n+1, 2n+2)$, $(2n+2, 2n+3)$ or $(2n+3, 2n+1)$. This suggests that the Hamiltonian can be made block diagonal. We note that in the representation of the gamma matrices we are using, the Hamiltonian is block diagonal,

$$\begin{aligned}\mathcal{H}^{d=2n}_{(2n+3)}(k, m) &= \sum_{a=1}^{d=2n} k_a \Gamma^{a}_{(2n+1)} \otimes \sigma_3 - m\Gamma^{2n+1}_{(2n+1)} \otimes \sigma_0 \\ &= \begin{pmatrix} \mathcal{H}^{d=2n}_{(2n+1)}(k, -m) & 0 \\ 0 & -\mathcal{H}^{d=2n}_{(2n+1)}(k, m) \end{pmatrix}.\end{aligned} \tag{109}$$

By the use of a unitary transformation for the lower right block,

$$\Gamma^{2n+1}_{(2n+1)}\left[-\mathcal{H}^{d=2n}_{(2n+1)}(k, m)\right]\Gamma^{2n+1}_{(2n+1)} = \mathcal{H}^{d=2n}_{(2n+1)}(k, -m), \tag{110}$$

$\mathcal{H}^{d=2n}_{(2n+3)}(k, m)$ reduces to two copies of $\mathcal{H}^{d=2n}_{(2n+1)}(k, -m)$. On the other hand, we have already seen that each $\mathcal{H}^{d=2n}_{(2n+1)}(k, -m) = \sum_{a=1}^{d=2n} k_a \Gamma^{a}_{(2n+1)} - m\Gamma^{2n+1}_{(2n+1)}$ has a nontrivial Chern number $\pm 1$. We thus conclude that the Chern number characterizing $\mathcal{H}^{d=2n}_{(2n+3)}(k)$ is $\pm 2$.

*3.1.4. From $d = 2n$ to $d = 2n - 1$.* Finally, we discuss the topological insulators (superconductors) $\mathcal{H}^{d=2n-1}_{(2n+3)}(k, m)$ marked by '$iv$' in table 4. One can check that the symmetry class of this Hamiltonian is shifted from that of $\mathcal{H}^{d=2n}_{(2n+3)}(k, m)$ as

$$\mathrm{AI} \to \mathrm{CI}, \quad \mathrm{C} \to \mathrm{CII}, \quad \mathrm{AII} \to \mathrm{DIII}, \quad \mathrm{D} \to \mathrm{BDI}. \tag{111}$$

Just as $\mathcal{H}^{d=2n}_{(2n+3)}(k, m)$ is characterized by a nonzero Chern invariant that is even, the descendant $\mathcal{H}^{d=2n-1}_{(2n+3)}(k, m)$ is also characterized by an even winding number.

The symmetry properties of all the Dirac Hamiltonians discussed here are summarized in table 4.

### *3.2. Example: $d = 3 \to 2 \to 1$*

Consider a $d = 3$-dimensional gapless Dirac fermion

$$\mathcal{H}(k) = k_x\sigma_x + k_y\sigma_y + k_z\sigma_z. \tag{112}$$

This Hamiltonian is a member of class AII, since

$$\sigma_y\mathcal{H}(k)\sigma_y = \mathcal{H}^*(-k). \tag{113}$$

Starting from this Hamiltonian, we dimensionally reduce this Hamiltonian successively and obtain the lower-dimensional Hamiltonians with shifted symmetry classes, AII $\to$ D $\to$ BDI. We replace $k_z$ by a mass term, and consider a $d = 2$-dimensional massive Dirac fermion

$$\mathcal{H}(k, m) = k_x\sigma_x + k_y\sigma_y + m\sigma_z. \tag{114}$$

This Hamiltonian is now a member of class D since

$$\sigma_x\mathcal{H}^*(k, m)\sigma_x = -\mathcal{H}(-k, m). \tag{115}$$

As mentioned before, the Chern number is nonzero for this model, $\mathrm{Ch}_2 = \frac{1}{2}\mathrm{sgn}(m)$. This Hamiltonian is in the same universality class as the chiral $p + \mathrm{i}p$-wave topological superconductor [8, 65].

The single-particle Hamiltonian (114), of course, looks identical to (65). This degeneracy is lifted once we consider more generic types of perturbations than the mass term, which can in principle be spatially inhomogeneous. Also, because of the $\mathcal{C}$ symmetry (see equation (115)), the Hamiltonian (114) can be viewed as a single-particle Hamiltonian for real (Majorana) fermions, while this is not the case for a class AIII single-particle Hamiltonian. In other words, a class D system can be written in the second quantized form as

$$H = \frac{1}{2}\sum_{k\in \mathrm{BZ}^2} \left(a^\dagger_k, a_{-k}\right) \mathcal{H}(k, m) \begin{pmatrix} a_k \\ a^\dagger_{-k} \end{pmatrix}. \tag{116}$$

where $a^\dagger_k/a_k$ is a fermion creation/annihilation operator with momentum $k$.

By further switching off $k_y$ or by the dimensional reduction in the $y$-direction,

$$\mathcal{H}(k, m) = k_x\sigma_x + m\sigma_z. \tag{117}$$

This Hamiltonian is a member of class BDI since

$$\sigma_x\mathcal{H}^*(k, m)\sigma_x = -\mathcal{H}(-k, m), \quad \sigma_z\mathcal{H}^*(k, m)\sigma_z = \mathcal{H}(-k, m). \tag{118}$$

This model can be realized as a continuum limit of the lattice Majorana fermion model discussed in [66]. For this $d = 1$ topological massive Dirac Hamiltonian, the winding number and the Wilson loop can be computed in the same way as we did for the $d = 1$ class AIII topological Dirac insulators (70). From (73), we immediately see $\nu_1 = \frac{1}{2}\mathrm{sgn}(m)$.

### 3.3. Example: $d = 5 \to 2$

Consider $d = 2 \cdot 1 + 3$ dimensions. We can take the following five matrices as gamma matrices,

$$\Gamma_{(5)}^{a=1,\ldots,5} = \left\{ \tau_y \otimes \sigma_{x,y,z}, \quad \tau_x \otimes \sigma_0, \quad \tau_z \otimes \sigma_0 \right\}. \tag{119}$$

Note that

$$\sigma_y \left(\Gamma_{(5)}^a\right)^{\mathrm{T}} \sigma_y = +\Gamma_{(5)}^a. \tag{120}$$

Thus, the gapless Hamiltonian

$$\mathcal{H}(k) = \sum_{a=1}^{5} k_a \Gamma_{(5)}^a \tag{121}$$

is a member of class C, as seen from

$$\sigma_y k_a \left(\Gamma_{(5)}^a\right)^{\mathrm{T}} \sigma_y = -(-k_a)\Gamma_{(5)}^a. \tag{122}$$

We now remove three momenta, and add one mass term. There are four possible mass terms that are compatible with the class C symmetry

$$\tau_{x,z,0} \otimes \sigma_y, \qquad \tau_y \otimes \sigma_0. \tag{123}$$

To construct a kinetic term we pick two gamma matrices from the list (119). For any choice of two gamma matrices there is only one mass term in equation (123) that anticommutes with the chosen kinetic term. In this way, we obtain, for example, the following massive Hamiltonian:

$$\mathcal{H}(k, m) = \tau_y \otimes \sigma_x k_x + \tau_y \otimes \sigma_z k_z + m\tau_0 \otimes \sigma_y. \tag{124}$$

Observe that $\mathrm{i}(\tau_y \otimes \sigma_y)(\tau_x \otimes \sigma_0)(\tau_z \otimes \sigma_0) = \tau_0 \otimes \sigma_y$. It is easy to see that this Hamiltonian has the doubled Chern number, $\mathrm{Ch}_1 = \pm 2$. To see this, first rotate $\tau_y \to \tau_z$,

$$\begin{aligned} \mathcal{H}(k, m) &\to \tau_z \otimes \sigma_x k_x + \tau_z \otimes \sigma_z k_z + m\tau_0 \otimes \sigma_y \\ &= \begin{pmatrix} \sigma_x k_x + \sigma_z k_z + \sigma_y m & 0 \\ 0 & -\sigma_x k_x - \sigma_z k_z + \sigma_y m \end{pmatrix}, \end{aligned} \tag{125}$$

and then apply a unitary transformation,

$$\begin{aligned} &\begin{pmatrix} \sigma_0 & 0 \\ 0 & \sigma_y \end{pmatrix} \begin{pmatrix} \sigma_x k_x + \sigma_z k_z + \sigma_y m & 0 \\ 0 & -\sigma_x k_x - \sigma_z k_z + \sigma_y m \end{pmatrix} \begin{pmatrix} \sigma_0 & 0 \\ 0 & \sigma_y \end{pmatrix} \\ &= \begin{pmatrix} \sigma_x k_x + \sigma_z k_z + \sigma_y m & 0 \\ 0 & \sigma_x k_x + \sigma_z k_z + \sigma_y m \end{pmatrix}. \end{aligned} \tag{126}$$

The $d = 2$-dimensional Hamiltonian constructed here has the same topological properties as the $d = 2$-dimensional $d + \mathrm{i}d$-wave superconductor discussed in [69].

## 4. $\mathbb{Z}_2$ topological insulators and dimensional reduction

In the previous sections, we have studied $\mathbb{Z}$ topological insulators (superconductors), which are characterized by an integer—the Chern or winding number. In this section, we discuss $\mathbb{Z}_2$ topological insulators (superconductors) and show how they can be derived as lower-dimensional descendants of parent $\mathbb{Z}$ topological insulators (superconductors) (see table 5).

**Table 5.** All $\mathbb{Z}_2$ topological insulators (superconductors) can be described through dimensional reduction as lower-dimensional descendants of parent $\mathbb{Z}$ topological insulators (superconductor) in the same symmetry class, which are characterized by nontrivial winding/Chern numbers. Symmetry classes in which chiral ('sublattice') symmetry is present ($S = 1$) are colored blue (the Cartan label marked in boldface), whereas those where it is absent ($S = 0$) are colored red.

| AZ | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | ... |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| AI | $\mathbb{Z}$ | 0 | 0 | 0 | $2\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 | 0 | 0 | ... |
| **BDI** | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 | 0 | 0 | $2\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 | 0 | ... |
| D | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 | 0 | 0 | $2\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 | ... |
| **DIII** | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 | 0 | 0 | $2\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | ... |
| AII | $2\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 | 0 | 0 | $2\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | ... |
| **CII** | 0 | $2\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 | 0 | 0 | $2\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ | ... |
| C | 0 | 0 | $2\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 | 0 | 0 | $2\mathbb{Z}$ | 0 | ... |
| **CI** | 0 | 0 | 0 | $2\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 | 0 | 0 | $2\mathbb{Z}$ | ... |

Recently, Qi *et al* [28] employed this procedure to derive descendant $\mathbb{Z}_2$ topological insulators (superconductors) for those symmetry classes that break chiral symmetry. Here, we show how this approach can be generalized and applied to all eight symmetry classes of table 5. We first treat chiral symmetric systems, and then review the case of chiral symmetry breaking classes. The reasoning follows closely that of [28].

### *4.1. Topological insulators with chiral symmetry*

Four among the eight symmetry classes of table 5 (see also table 1) are invariant under chiral ('sublattice') symmetry, which is a combination of particle–hole and time-reversal symmetries. These four symmetry classes are called BDI, CI, CII and DIII. It is possible to characterize the topological properties of chiral symmetric $\mathbb{Z}$ topological insulators by a winding number (topological invariant), which is defined in terms of the block off-diagonal projector (see section 2.2.1). From this topological invariant we can derive a $\mathbb{Z}_2$ classification by imposing the constraint of additional discrete symmetries (such as $\mathcal{C}$ and $\mathcal{T}$) for the lower-dimensional descendants. For a $d$-dimensional $\mathbb{Z}$ topological insulator (superconductor) in a given symmetry class, we distinguish between first and second descendants, whose (reduced) dimensionality is $d-1$ and $d-2$, respectively.

*4.1.1. Symmetry properties of winding number.* In order to better understand the role played by $\mathcal{T}$ and $\mathcal{C}$, we first study the transformation properties of the winding number (20) and the winding number density (21) under these discrete symmetries. First of all, we note that the winding number density is purely real, $w^*_{2n+1}[q] = w_{2n+1}[q]$, which can be checked by direct calculation. Without any additional discrete symmetries, i.e. for symmetry class AIII, the off-diagonal projector $q$ and hence the winding number density (21) are not subject to additional constraints. However, for the symmetry classes BDI, DIII, CII and CI, the presence of time reversal and particle–hole symmetries relates the projector $q$ at wavevector $k$ to the one at wavevector $-k$. As a consequence, the configurations of the winding number density $w$ in momentum space are restricted by time-reversal and particle–hole symmetries. Let us now derive these symmetry constraints on the winding number density $w_{2n+1}[q]$ for any odd spatial dimension $d = 2n+1$.

*Classes DIII and CI:* First, we consider symmetry classes DIII and CI, where the block off-diagonal projector satisfies [26]

$$q^T(-k) = \epsilon q(k), \quad \epsilon = \begin{cases} -1, & \text{DIII}, \\ +1, & \text{CI}. \end{cases} \tag{127}$$

We introduce the auxiliary functions

$$v_\mu(k) := \left( q^\dagger \frac{\partial}{\partial k_\mu} q \right)(k) \quad \text{and} \quad \tilde{v}_\mu(k) := \left( q \frac{\partial}{\partial k_\mu} q^\dagger \right)(k). \tag{128}$$

From the symmetry property (127), it follows that $v_\mu(k) = -\tilde{v}^*_\mu(-k)$, irrespective of the value taken by $\epsilon$. Noting that $(\mathrm{d}q^\dagger)q = -q^\dagger \mathrm{d}q$, we find

$$\epsilon^{\alpha_1\alpha_2\cdots\alpha_{2n+1}} \mathrm{tr}\left[ v_{\alpha_1}(k) v_{\alpha_2}(k) \cdots v_{\alpha_{2n+1}}(k) \right] = \epsilon^{\alpha_1\alpha_2\cdots\alpha_{2n+1}} \mathrm{tr}\left[ v_{\alpha_1}(-k) v_{\alpha_2}(-k) \cdots v_{\alpha_{2n+1}}(-k) \right]^*. \tag{129}$$

Thus, the winding number density for symmetry class DIII and CI is subject to the constraint

$$w_{2n+1}\left[q(k)\right] = (-1)^{n+1} w^*_{2n+1}\left[q(-k)\right]. \tag{130}$$

Consequently, the winding number $\nu_{4n+1}[q]$ is vanishing in $d = 4n+1$ dimensions, i.e. there exists no nontrivial topological state characterized by an integer winding number in $(4n+1)$-dimensional systems belonging to symmetry class DIII or CI (cf table 5). Conversely, in $d = (4n+3)$ dimensions both in class DIII and CI there are topologically nontrivial states (*ii* or *iv* in table 4), and one would naively expect that for each of these states there are lower-dimensional descendants characterized by $\mathbb{Z}_2$ topological invariants. However, this is not the case, as we will explain below.

*Classes BDI and CII:* Next, we consider symmetry classes BDI and CII, where the projector satisfies [26]

$$G q^*(-k) G^{-1} = q(k), \quad G = \begin{cases} \sigma_0, & \text{BDI}, \\ \mathrm{i}\sigma_y, & \text{CII}. \end{cases} \tag{131}$$

Introducing the auxiliary function $v_\mu(k)$, equation (128), as before, we find that $v_\mu(k) = -G v^*_\mu(-k) G^{-1}$, for both classes BDI and CII. From the cyclic property of the trace it follows that

$$\epsilon^{\alpha_1\alpha_2\cdots\alpha_{2n+1}} \mathrm{tr}\left[ v_{\alpha_1}(k) v_{\alpha_2}(k) \cdots v_{\alpha_{2n+1}}(k) \right] = \epsilon^{\alpha_1\alpha_2\cdots\alpha_{2n+1}} (-1)^{2n+1} \mathrm{tr}\left[ v_{\alpha_1}(-k) v_{\alpha_2}(-k) \cdots v_{\alpha_{2n+1}}(-k) \right]^*. \tag{132}$$

Hence, the winding number density in class BDI and CII is constrained by

$$w_{2n+1}\left[q(k)\right] = (-1)^n w^*_{2n+1}\left[q(-k)\right]. \tag{133}$$

As a result, the winding number $\nu_{4n-1}[q]$ is vanishing in $d = 4n-1$ dimensions, i.e. there are no nontrivial $(4n-1)$-dimensional $\mathbb{Z}$ topological insulators belonging to symmetry class BDI or CII (see table 5). On the other hand, in $(4n+1)$ dimensions there exist $\mathbb{Z}$ topological states in both classes BDI and CII (*ii* or *iv* in table 4), and one would expect, as before, that for each of these states there are lower-dimensional topologically nontrivial descendants. Again, this expectation turns out to be incorrect, as we will explain below.

*4.1.2. $\mathbb{Z}_2$ classification of first descendants.* In this section, we show how a $\mathbb{Z}_2$ topological classification is obtained for $2n$-dimensional, chiral symmetric insulators (superconductors) under the constraint of additional discrete symmetries (i.e. $\mathcal{C}$ and $\mathcal{T}$). To uncover the $\mathbb{Z}_2$ topological characteristics of chiral symmetric systems, we study the topological distinctions among the block off-diagonal projectors $q(k)$. Let us consider two projectors $q_1(k)$ and $q_2(k)$, whose momentum space configuration is restricted by the symmetry constraint of one of the classes DIII/CI, equation (127), or BDI/CII, equation (131). We introduce a continuous interpolation $q(k,t)$, $t \in [0,\pi]$ between these two projectors (see figure 4(a)) with

$$q(k, t=0) = q_1(k) \qquad \text{and} \qquad q(k, t=\pi) = q_2(k). \tag{134}$$

Since the topological space of $2n$-dimensional class AIII insulators is simply connected, the continuous deformation $q(k,t)$ is well defined. In general, $q(k,t)$ does not satisfy the symmetry constraints encoded by equation (127) or (131), respectively. However, by combining equation (134) with its symmetry transformed partner, we can construct an interpolation that obeys the discrete symmetries of the given symmetry class (see figure 4(b)). In the case of symmetry class DIII/CI, we define for $t \in [\pi, 2\pi]$

$$q(k,t) = \epsilon q^T(-k, 2\pi - t), \quad \epsilon = \begin{cases} -1, & \text{DIII} \\ +1, & \text{CI}, \end{cases} \tag{135}$$

while, in the case of symmetry class BDI/CII, we set for $t \in [\pi, 2\pi]$

$$q(k,t) = G q^*(-k, 2\pi - t) G^{-1}, \quad G = \begin{cases} \sigma_0, & \text{BDI} \\ \mathrm{i}\sigma_y, & \text{CII}. \end{cases} \tag{136}$$

Equations (134)–(136) with the parameter $t$ replaced by the wavevector component $k_{2n+1}$ represent a $(2n+1)$-dimensional projection operator respecting the symmetry constraints of the corresponding symmetry class. Consequently, a winding number for $q(k,t)$, $\nu_{2n+1}[q(k,t)]$, can be defined in the $(k,t)$ space. Two different interpolations $q(k,t)$ and $q'(k,t)$ generally give different winding numbers, $\nu_{2n+1}[q(k,t)] \neq \nu_{2n+1}[q'(k,t)]$. However, we can show that symmetry constraint (135) or (136), respectively, leads to

$$\nu_{2n+1}[q(k,t)] - \nu_{2n+1}[q'(k,t)] = 0 \mod 2. \tag{137}$$

To prove equation (137) we introduce two new interpolations $r_1(k,t)$ and $r_2(k,t)$ that transform into each other under the discrete symmetry operations (see figure 4)

$$\begin{aligned} r_1(k,t) &= \begin{cases} q(k,t), & t \in [0,\pi], \\ q'(k, 2\pi - t), & t \in [\pi, 2\pi], \end{cases} \\ r_2(k,t) &= \begin{cases} q'(k, 2\pi - t), & t \in [0,\pi], \\ q(k,t), & t \in [\pi, 2\pi], \end{cases} \end{aligned} \tag{138}$$

These are recombinations of the deformations $q(k,t)$ and $q'(k,t)$ with

$$\nu_{2n+1}[q(k,t)] - \nu_{2n+1}[q'(k,t)] = \nu_{2n+1}[r_1(k,t)] + \nu_{2n+1}[r_2(k,t)]. \tag{139}$$

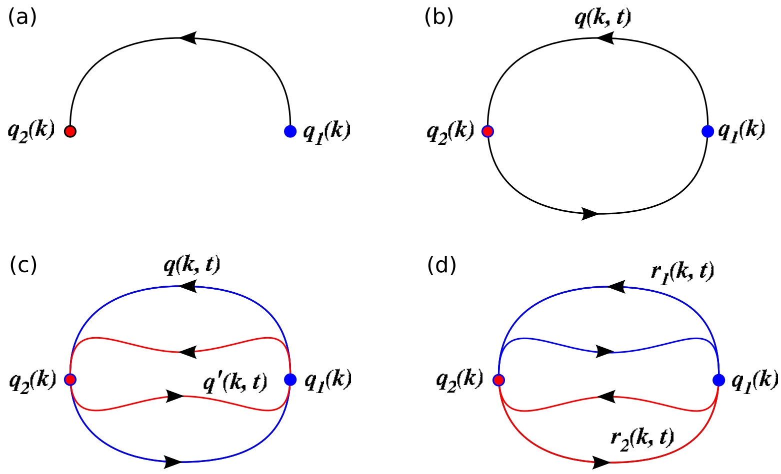


**Figure 4.** (a) One-parameter interpolation of two topological insulators represented by the projectors $q_1$ and $q_2$. In (b), the one-way interpolation (a) is extended by making use of the discrete symmetry. (c) Two different interpolations, each colored red and blue, respectively. In (d), the original interpolations are rearranged into two different interpolations.

Now, we make use of the result from section 4.1.1. Namely, for symmetry class BDI/CII we found

$$w_{4n+1}[q(k,t)] = w^*_{4n+1}[q(-k,-t)] \tag{140}$$

in $d = 4n+1$ spatial dimensions, whereas for symmetry class DIII/CI

$$w_{4n-1}[q(k,t)] = w^*_{4n-1}[q(-k,-t)] \tag{141}$$

in $d = 4n-1$ spatial dimensions. Let us first consider class BDI/CII in $d = 4n+1$ dimensions. With equations (20) and (140) we obtain

$$\begin{aligned} \nu_{4n+1}[r_1] &= \int \mathrm{d}^{4n}k\,\mathrm{d}t\; w_{4n+1}[r_1(k,t)] \\ &= \int \mathrm{d}^{4n}k\,\mathrm{d}t\; w^*_{4n+1}[r_1(-k,-t)] \\ &= \int \mathrm{d}^{4n}k\,\mathrm{d}t\; w^*_{4n+1}[r_2(k,t)] = \nu_{4n+1}[r_2], \end{aligned} \tag{142}$$

where we made use of the fact that $r_1$ transforms into $r_2$ under the discrete symmetry operations of class BDI/CII. In conclusion, we have shown that $\nu_{4n+1}[q(k,t)] - \nu_{4n+1}[q'(k,t)] = 2\nu_{4n+1}[r_1(k,t)] \in 2\mathbb{Z}$ for any two interpolations $q(k,t)$ and $q'(k,t)$ belonging to class BDI/CII. Hence, we can define a relative invariant for the $4n$-dimensional projection operators $q_1(k)$ and $q_2(k)$

$$\nu_{4n}\,[q_1(k), q_2(k)] = (-1)^{\nu_{4n+1}[q(k,t)]}, \tag{143}$$

which is independent of the particular choice of the interpolation $q(k,t)$ between $q_1(k)$ and $q_2(k)$. Once we have identified a 'vacuum' projection operator, e.g. $q_0(k) \equiv q_0$, we can construct with equation (143) a $\mathbb{Z}_2$ invariant: nontrivial Hamiltonians are characterized by $\nu_{4n}[q, q_0] = -1$, whereas trivial ones satisfy $\nu_{4n}[q, q_0] = +1$. Finally, we note that the calculation leading to the relative invariant $\nu_{4n}[q_1, q_2]$, equation (143), can be repeated for symmetry class DIII/CI in $d = 4n - 1$ dimensions yielding a relative invariant $\nu_{4n-2}[q_1, q_2]$.

For $d = 4n - 1$ ($d = 4n + 1$) the dimensional reduction seems to be possible both for class DIII and CI (BDI and CII). However, for a given $n$ the dimensional reduction seems to be meaningful only for one of them; while for one of them (corresponding to *ii* in table 4), there is a descendant $\mathbb{Z}_2$ insulator in one dimension lower, for the other (corresponding to *iv* in table 4), there are no descendant $\mathbb{Z}_2$ insulators. In other words, for a given $n =$ odd (even), there are lower-dimensional $\mathbb{Z}_2$ topological insulators for either one of class DIII and CI (BDI and CII), but not both. This is because the above procedure does not apply when the classification of topological insulator is not $\mathbb{Z}$, but $2\mathbb{Z}$.

*4.1.3. $\mathbb{Z}_2$ classification of second descendants.* The dimensional reduction procedure presented in the previous subsection can be repeated once more to obtain a $\mathbb{Z}_2$ classification of the second descendants. As before, we first focus on symmetry class BDI/CII and study the topological distinctions among the block off-diagonal projectors. We consider two $(4n - 1)$-dimensional projectors $q_1(k)$ and $q_2(k)$, which satisfy the symmetry constraints imposed by class BDI/CII. We define an adiabatic interpolation $q(k, t)$, $t \in [0, 2\pi]$

$$\begin{aligned} &q(k, t = 0) = q_1(k), \qquad\qquad q(k, t = \pi) = q_2(k), \\ &q(k, t) = Gq^*(-k, -t)G^{-1}, \quad G = \begin{cases} \sigma_0, & \text{BDI}, \\ \mathrm{i}\sigma_y, & \text{CII}. \end{cases} \end{aligned} \tag{144}$$

We can interpret $q(k, t)$ as a $4n$-dimensional projector belonging to symmetry class BDI/CII. Therefore, for two deformations $q(k, t)$ and $q'(k, t)$ of the form (144) a relative invariant $\nu_{4n}[q(k, t), q'(k, t)]$ can be defined, as discussed in section 4.1.2. It turns out that due to condition (144) the invariant $\nu_{4n}[q(k, t), q'(k, t)]$ is independent of the particular choice of interpolations, i.e. $\nu_{4n}[q(k, t), q'(k, t)] = +1$ for any two deformations $q(k, t)$ and $q'(k, t)$ satisfying condition (144). In order to prove this, we consider a continuous interpolation $r(k, t, s)$ between the two deformations $q(k, t)$ and $q'(k, t)$ with

$$\begin{aligned} &r(k, t, s = 0) = q(k, t), \qquad r(k, t, s = \pi) = q'(k, t), \\ &r(k, t = 0, s) = q_1(k), \qquad r(k, t = \pi, s) = q_2(k), \\ &r(k, t, s) = Gr^*(-k, -t, -s)G^{-1}, \quad G = \begin{cases} \sigma_0, & \text{BDI}, \\ \mathrm{i}\sigma_y, & \text{CII}. \end{cases} \end{aligned} \tag{145}$$

This represents a $(4n + 1)$-dimensional off-diagonal projector in symmetry class BDI/CII with the winding number $\nu_{4n+1}[r(k, t, s)]$. We note that $r(k, t, s)$ is not only a deformation between $q(k, t)$ and $q'(k, t)$, but can also be viewed as a continuous interpolation between $r(k, 0, s) \equiv q_1(k)$ and $r(k, \pi, s) \equiv q_2(k)$ (for any $s \in [0, 2\pi]$). Therefore, we find $\nu_{4n}[q(k, t), q'(k, t)] = \nu_{4n}[r(k, t, 0), r(k, t, \pi)] = \nu_{4n}[r(k, 0, s), r(k, \pi, s)]$. Since $r(k, 0, s) \equiv q_1(k)$ and $r(k, \pi, s) \equiv q_2(k)$ are independent of $s$, we find that $\nu_{4n}[r(k, 0, s), r(k, \pi, s)] = (-1)^{\nu_{4n+1}[r]} = +1$. Hence, we have shown that $\nu_{4n}[q(k, t), q'(k, t)]$ only depends on $q_1(k)$ and $q_2(k)$. Therefore, $\nu_{4n}[q_0, q(k, t)]$ together with a reference ('vacuum') projector $q_0$ constitutes a well-defined $\mathbb{Z}_2$ invariant in $4n - 1$ dimensions.

*4.1.4. Example: $d = 3 \to 2 \to 1$.* As an example we consider a 3D topological Dirac superconductor belonging to symmetry class DIII. Consider a $d = 3$-dimensional Dirac Hamiltonian,

$$\mathcal{H}^{d=3}_{(5)}(k, m) = k_x\alpha_x + k_y\alpha_y + k_z\alpha_z - m\mathrm{i}\beta\gamma^5. \tag{146}$$

This is nothing but the chiral topological Dirac superconductor in class DIII. This Hamiltonian is essentially identical to the BdG Hamiltonian describing the Bogoliubov quasiparticles in the B phase of superfluid $^3$He [26, 68, 69][34]. It also describes an auxiliary Majorana hopping problem for an interacting bosonic model on the diamond lattice [70]. In this basis, discrete symmetries are given by

$$\begin{aligned} \mathcal{T}: \quad & (\sigma_y \otimes \tau_x) \left[\mathcal{H}^{d=3}_{(5)}(-k, m)\right]^* (\sigma_y \otimes \tau_x) = \mathcal{H}^{d=3}_{(5)}(k, m), \\ \mathcal{C}: \quad & (\sigma_y \otimes \tau_y) \left[\mathcal{H}^{d=3}_{(5)}(-k, m)\right]^* (\sigma_y \otimes \tau_y) = -\mathcal{H}^{d=3}_{(5)}(k, m). \end{aligned} \tag{147}$$

Combining these two, we have chiral symmetry, which allows us to define the winding number $\nu_3$. From the calculations in section 2.5, the winding number is nonzero, $\nu_3 = \pm 1/2$, depending on the sign of the mass.

By dimensional reduction, we obtain the Hamiltonian in one dimension lower,

$$\mathcal{H}^{d=2}_{(5)}(k, m) = k_x \alpha_x + k_y \alpha_y - mi\beta\gamma^5. \tag{148}$$

This Hamiltonian is a 2D analogue of $^3$He-B and is unitarily equivalent to the direct product of spinless $p + ip$ and $p - ip$ wave superconductors. As this is obtained from dimensional reduction of a parent topological superconductor (146), this is a $\mathbb{Z}_2$ state. Finally, by further reducing dimensions,

$$\mathcal{H}^{d=1}_{(5)}(k, m) = k_x \alpha_x - mi\beta\gamma^5. \tag{149}$$

This is a 1D $p_x$-wave superconductor. Again, this is a $\mathbb{Z}_2$ state.

We now discuss the topological character of these states in more detail. The $\mathbb{Z}_2$ nature of the state in this $d = 2$ example can be studied by the Kane–Mele invariant [9, 15]. It can be expressed as an SU(2) Wilson loop

$$W_{\mathrm{SU}(2)}[L] := \frac{1}{2}\mathrm{tr}\, P \exp\left[\oint_L \mathcal{A}(k)\right]. \tag{150}$$

Here $\mathcal{A}(k)$ is the SU(2) Berry connection and $P$ represents the path ordering. By definition, $W_{\mathrm{SU}(2)}[L]$ is a well-defined and gauge invariant quantity for any loop $L$ in the BZ. For time-reversal invariant systems, it is useful to consider a loop $L$ that satisfies time-reversal symmetry; i.e. a loop that is mapped onto itself (up to reparameterization) under $k \to -k$. For these time-reversal invariant loops, the SU(2) Wilson loop is quantized,

$$W_{\mathrm{SU}(2)}[L] = \pm 1, \tag{151}$$

and provides a way to distinguish different $\mathbb{Z}_2$ states [9, 15, 71]. The quantization of the Wilson loop can be proved by first noting that because of $\mathcal{T}$, Bloch wavefunctions at $k$ and $-k$ are related to each other by a unitary transformation $w(k)$,

$$|\Theta u^-_{\hat{a}}(k)\rangle = w_{\hat{a}\hat{b}}(k)|u^-_{\hat{a}}(-k)\rangle, \tag{152}$$

[34] In [53], a topological invariant counting the number of gap-closing Dirac points in an extended, higher-dimensional parameter space was discussed for a four-band example (146), as opposed to $\nu_3[q]$ defined for a given topological phase. Moreover, the crucial role for the protection of topological properties arising from the combined time-reversal and charge-conjugation symmetries of symmetry class DIII was not discussed.

where $\Theta$ represents $\mathcal{T}$ operation and

$$w_{\hat{a}\hat{b}}(k) := \langle u^-_{\hat{a}}(-k)|\Theta u^-_{\hat{b}}(k)\rangle. \tag{153}$$

Accordingly, the Berry connection at $k$ is gauge equivalent to $A^{\mathrm{T}}_\mu$ at $-k$,

$$\begin{aligned} A_\mu(-k) &= +w(k)A^T_\mu(k)w^\dagger(k) - w(k)\partial_\mu w^\dagger(k) \\ &= -w(k)A^*_\mu(k)w^\dagger(k) - w(k)\partial_\mu w^\dagger(k). \end{aligned} \tag{154}$$

Because of this sewing condition (154) of the gauge field, when plugged in (150), contributions at $k$ and $-k$ in the path integral cancel pairwise, except at those momenta that are invariant under $\mathcal{T}$ by themselves. Thus,

$$W_{\mathrm{SU}(2)}[L] = \prod_K \mathrm{Pf}\,[w(K)]\,, \tag{155}$$

where $K$ is a momentum that is invariant under $k \to -k$.

We now compute the $\mathbb{Z}_2$ number for the $d = 2$ class DIII topological superconductor (148). From (85),

$$|u^-_1(k)\rangle = \frac{1}{\sqrt{2}\lambda}\begin{pmatrix} -k_x + \mathrm{i}k_y \\ \mathrm{i}m \\ 0 \\ \lambda \end{pmatrix}, \quad |u^-_2(k)\rangle = \frac{1}{\sqrt{2}\lambda}\begin{pmatrix} \mathrm{i}m \\ -k_x - \mathrm{i}k_y \\ \lambda \\ 0 \end{pmatrix}. \tag{156}$$

Then, their time-reversal counterparts are

$$|\Theta u^-_1(k)\rangle = \frac{-\mathrm{i}}{\sqrt{2}\lambda}\begin{pmatrix} \lambda \\ 0 \\ -\mathrm{i}m \\ k_x + \mathrm{i}k_y \end{pmatrix}, \quad |\Theta u^-_2(k)\rangle = \frac{-\mathrm{i}}{\sqrt{2}\lambda}\begin{pmatrix} 0 \\ -\lambda \\ -k_x + \mathrm{i}k_y \\ \mathrm{i}m \end{pmatrix}, \tag{157}$$

where $\Theta = (\sigma_y \otimes \tau_x)\mathcal{K}$ with $\mathcal{K}$ being the complex conjugation. The 'sewing matrix' $w(k)$ can then be computed as

$$w(k) := \langle u_{\hat{a}}(-k)|\Theta u_{\hat{b}}(k)\rangle = \frac{1}{\lambda(k)}\begin{pmatrix} -\mathrm{i}k_x + k_y & m(k) \\ -m(k) & +\mathrm{i}k_x + k_y \end{pmatrix}. \tag{158}$$

Here, we have regularized the Dirac Hamiltonian properly, by making the mass $k$-dependent, e.g. $m \to m(k) = m - Ck^2$. With this regularization, $k = 0$ and $k = \infty$ are the two time-reversal invariant momenta. One finds

$$\begin{aligned} \mathrm{Pf}\,w(0) &= \frac{m(0)}{\lambda(0)}\mathrm{Pf}\,(\mathrm{i}\sigma_y) = \frac{m}{|m|}\mathrm{Pf}\,(\mathrm{i}\sigma_y), \\ \mathrm{Pf}\,w(\infty) &= \frac{m(\infty)}{\lambda(\infty)}\mathrm{Pf}\,(\mathrm{i}\sigma_y) = \frac{-C}{|C|}\mathrm{Pf}\,(\mathrm{i}\sigma_y), \end{aligned} \tag{159}$$

and hence

$$W_{\mathrm{SU}(2)}[L] = -\mathrm{sign}(m)\,\mathrm{sign}(C). \tag{160}$$

That is, when $\mathrm{sign}(m) = \mathrm{sign}(C)$, the Hamiltonian (146) is a $\mathbb{Z}_2$ topological superconductor.

### *4.2. Topological insulators lacking chiral symmetry*

Four among the eight ('real') symmetry classes of table 5 break chiral ('sublattice') symmetry. The $\mathbb{Z}$ topological insulators (superconductors) that break chiral symmetry are characterized by a Chern number (see equation (11)). Using this topological invariant one can derive the $\mathbb{Z}_2$ classification for the lower-dimensional descendants. This derivation is analogous to the discussion in section 4.1 and has been performed previously in [28] for the $\mathbb{Z}_2$ topological insulators that break chiral symmetry. For these reasons we do not repeat the argument here and refer the reader to [28] for details. For the $\mathbb{Z}_2$ topological insulators (superconductors) that break chiral symmetry, one can construct a $\mathbb{Z}_2$ index similar to the one constructed by Moore and Balents [12], in all (even) dimensions [72].

## 5. Discussion

In this paper, we have performed an exhaustive study of all topological insulators and superconductors in arbitrary dimensions. The main part of this paper deals with dimensional reduction procedures, which relate topological insulators (superconductors) in different dimensions and symmetry classes. We also discussed topological field theories in $D = d + 1$ spacetime dimensions describing linear responses of topological insulators (superconductors). Furthermore, we studied how the presence of inversion symmetry modifies the classification of topological insulators (superconductors) (see appendix C). In the following we give a brief summary of the main results of the paper.

### *5.1. Dimensional reduction procedures*

We have constructed for all five symmetry classes of topological insulators or superconductors a Dirac Hamiltonian representative, in all spatial dimensions. Using these Dirac Hamiltonians as canonical examples, we have demonstrated that topological insulators (superconductors) in different spatial dimensions and symmetry classes can be related to each other by dimensional reduction procedures. These Dirac representatives have been useful for constructing string theory realization of topological insulators and superconductors: In [73], a one-to-one correspondence between the tenfold classification of topological insulators and superconductors and a $K$-theory classification of $D$-branes was established, where open string excitations between two $D$-branes of various dimensions are shown to reproduce all Dirac representatives constructed in this paper.

*5.1.1. The 'complex' case.* We first studied topological insulators (superconductors) with Hamiltonians that are complex (i.e. belonging to the 'complex case' of table 3, that is, classes A and AIII from table 1). Here, starting from a topological insulator that lacks chiral symmetry (i.e. class A) in even spatial dimensions $d = 2n$, we obtain a topological insulator (superconductor) in $d = 2n - 1$, which possesses chiral symmetry (i.e. class AIII), by dimensional reduction. In order to understand how the topological characteristics of the $d = 2n - 1$ class AIII topological insulator (characterized by the winding number $\nu_{2n-1}$) are inherited from its higher-dimensional parent, the $d = 2n$ class A topological insulator (characterized by the Chern number $\mathrm{Ch}_n$), it is important to first point out a few properties of the momentum space topology of Bloch wavefunctions in symmetry classes A and AIII. Firstly, we note that the nonzero Chern number in class A leads to an obstruction to the existence of globally defined Bloch eigenfunctions. That is, it is not possible to construct Bloch eigenfunctions for the parent class A topological insulator globally on the $d = 2n$-dimensional BZ. Hence, the Bloch eigenfunctions can only be defined locally on some suitably chosen coordinate patches. For the descendant topological insulator (superconductor) with chiral symmetry, on the other hand, since there is no Chern invariant in $d = 2n - 1$, there always exists a basis (i.e. a gauge) in which the Bloch eigenfunctions are well defined globally on the entire $d = 2n - 1$-dimensional BZ. Such a basis is provided by the one in which the Hamiltonian is block off-diagonal. The existence of such a block off-diagonal basis, in turn, is implied by the chiral symmetry of the descendant class AIII topological insulator (superconductor). As a consequence, the role played by the chiral symmetry is to guarantee that Bloch eigenfunctions of class AIII topological insulators (superconductors) can be defined globally on the entire BZ.

Now, by adopting such a block off-diagonal basis for the class AIII topological insulator, we have shown that the $d = 2n - 1$-dimensional BZ of the descendant class AIII Hamiltonian defines the boundary of two local coordinate patches of the $d = 2n$-dimensional BZ of the parent class A topological insulator. The transition function between these two coordinate patches is given by the block off-diagonal projector[35] $q$ of the descendant Hamiltonian, and the Chern number $\mathrm{Ch}_n$ of the parent Hamiltonian can be written in terms of a winding number of this transition function (see section 2.3).

*5.1.2. The 'real' case.* Also demonstrated is, using the Dirac Hamiltonian representatives, the periodicity eight shift of symmetry classes for the topological insulators (superconductors) in the eight symmetry classes in which the Hamiltonian possesses at least one reality condition (arising from $\mathcal{T}$ or $\mathcal{C}$). Once one has constructed a representative in terms of a Dirac Hamiltonian, the reality properties of the spinor representations of the orthogonal groups $\mathrm{SO}(N)$ (which are linked to the reality properties of the representations of the Clifford algebra formed by the gamma matrices) leads directly to this eightfold periodicity in the spatial dimension $d$ (see section 3). From the Dirac Hamiltonian representatives of topological insulators (superconductors) in all $d$ spatial dimensions (all of which are of course massive), one can realize a $d - 1$-dimensional boundary, by making a domain wall at which the mass term changes sign [74]. There then appears a boundary state localized at the boundary, which is a defining property of topological character in the bulk. These boundary states are of special kind, as they are protected from the appearance of a gap and from Anderson localization, by the time-reversal and charge-conjugation symmetry properties of the specific symmetry class. Indeed, one of the underlying strategies of classification adopted in [26] was to classify the properties of these boundary Hamiltonians in each symmetry class, including those of Dirac type, which must be completely gapless and delocalized when they come from a topological bulk, but can otherwise be gapped and localized for a non-topological bulk. By constructing massive Dirac Hamiltonian representatives in the bulk for all topological insulators (superconductors), which give rise to the gapless boundary Dirac Hamiltonians, we undertook here in some sense a complementary task as compared to that in [26].

[35] Of the type described in equation (34) of the first article in [26].

### *5.2. Topological field theories*

In the low-energy limit, all topological insulators (superconductors) can be described by topological field theories for the linear responses in spacetime, which characterize universal (in principle) experimentally accessible observables of the topological features, such as, e.g., in transport. For example, for symmetry class A in even spatial dimensions $d = 2n$, the topological field theory of the linear responses in $D = d + 1$ spacetime dimensions is given by the Chern–Simons action, whose coupling coefficient is the $n$th Chern number $\mathrm{Ch}_n$. For symmetry class AIII in odd spatial dimensions $d = 2n - 1$, on the other hand, the topological field theory in $D = 2n$ spacetime dimensions is given by the $\theta$ term, whose coefficient (the $\theta$ angle) is given by the winding number $\nu_{2n+1}$ (see section 2.6). For topological singlet superconductors (symmetry classes C and CI), one can couple the external SU(2) gauge field to the conserved spin current operator of the BdG quasiparticles. The spin response in topological singlet superconductors can be described by SU(2) gauge theory with Chern–Simons-type topological term in $d = 2n$ [8] and with the $\theta$-type term in $d = 2n + 1$ [75]. In passing we note that it is also possible to establish a connection among these topological field theories in various spacetime dimensions and symmetry classes via dimensional reduction procedures. The topological field theory formulation may be a good starting point to explore, more generally, topological phases in interacting systems beyond those that are currently known.

### *5.3. Topological insulators with inversion symmetry and either time-reversal or charge-conjugation symmetry*

We have also studied the restrictions imposed on ground-state properties of topological insulators (superconductors) by the presence of inversion symmetry. That is, we studied topological states that are protected by a combination of spatial inversion (denoted by $\mathcal{I}$) and an additional discrete symmetry (i.e. $\mathcal{T}$ or $\mathcal{C}$). These systems are invariant under the combined symmetry operations $\mathcal{T} \cdot \mathcal{I}$ or $\mathcal{C} \cdot \mathcal{I}$, but all three symmetries $\mathcal{T}$, $\mathcal{C}$ and $\mathcal{I}$ are assumed to be absent. We have determined the space of projectors describing these topological states. From the homotopy groups of the space of projectors follows the classification of topological states that are protected by $\mathcal{T} \cdot \mathcal{I}$ or $\mathcal{C} \cdot \mathcal{I}$ (see table C.2).

### *5.4. Directions for future work*

An important direction for future study is the search for experimental realizations of 3D topological singlet or triplet superconductors. Given how fast experimental realizations of the QSHE in $d = 2$ and the $\mathbb{Z}_2$ topological insulators in $d = 3$ have been found, we anticipate a similar development for the 3D topological singlet or triplet superconductors. For example, unconventional superconductors in heavy fermion systems, typically possessing strong spin–orbit effects, have been studied extensively over the years. They might be good candidates for topological superconductors. Moreover, the search for nontrivial topological quantum ground states is not restricted to free fermions, or BCS quasiparticles, but includes also, more generally, strongly interacting systems other than BCS with emergent free fermion behavior at low energies. Furthermore, it should be noted that the classification scheme given by table 3 is also applicable outside the realm of condensed matter physics. For example, topological properties of color superconducting phases [76, 77], which are predicted to occur in quark matter, can be discussed in terms of the present classification scheme.

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## Appendix A. Cartan symmetric spaces: generic Hamiltonians, NL$\sigma$M field theories and classifying spaces of $K$-theory

In this appendix, we review the appearance of Cartan's tenfold list of symmetric spaces in the context of (i) basic quantum mechanics: where they describe the time evolution operators $\exp(\mathrm{i}t\mathcal{H})$ of generic Hamiltonians $\mathcal{H}$, (ii) NL$\sigma$M field theories: where they describe the 'target space' manifold of the NL$\sigma$M and (iii) $K$-theory: where they describe the 'classifying space' (briefly discussed at the end of subsection 1.2 of the introduction). As reviewed in the introduction, the homotopy groups of these symmetric spaces play a key role in the classification of topological insulators and superconductors both in the approach of [26], which makes use of results from Anderson localization physics, and in the approach of [27], which is based on $K$-theory.

In table A.1, we list for each symmetry class denoted by its Cartan label in the first column, the time evolution operator in this symmetry class (penultimate column of table 1) in the second column, the target spaces[36] of the NL$\sigma$M field theories in the third column, and in the last column the classifying space appearing in $K$-theory [27].

Here we would like to re-emphasize the remarkable fact that the *same* ten Cartan symmetric spaces describe all three objects listed in the last three columns of table A.1. Furthermore, there are remarkable relations between these columns. Firstly, the second column ('time evolution operator') can be obtained from the last column ('classifying space') by shifting the entries in the last column down by one entry (modulo eight, and modulo two in the 'real' and 'complex' cases, respectively). Secondly, the third column ('NL$\sigma$M target space') is obtained from the last column by performing a reflection (modulo 8) in the last column about the entry in the row labeled D (and an exchange for the complex case). Consequently, there is then also a resulting relationship between the second and third columns [78].

As reviewed in subsection 1.2 of the introduction, the classifying spaces listed in the last column of table A.1 describe topological insulators (superconductors) in zero dimensions, i.e. at one point in space[37]. The disconnected components of this space of Hamiltonians $Q$ (which cannot be continuously deformed into each other) are labeled by $\mathbb{Z}$ or $\mathbb{Z}_2$ appearing in the $d = 0$ column of table 3, which denotes the list of zeroth homotopy groups of the spaces in the last

[36] There are three different varieties of NL$\sigma$M field theories: supersymmetric, fermionic replica and bosonic replica models. In the latter two formulations, the replica limit must be taken, where one lets the number of replicas, $N$, tend to zero at the end of the calculations. While the target spaces of fermionic replica models are compact, those of bosonic replica models are non-compact. In the supersymmetric formulation, on the other hand, the target spaces are supermanifolds with both bosonic and fermionic coordinates. The fermionic and bosonic replica NL$\sigma$Ms, with $N$ finite, can be viewed as fermion–fermion and boson–boson subsectors, respectively, of the corresponding supersymmetric NL$\sigma$Ms [36].

[37] Kitaev [27]; compare also table III (second column, with $k = 0$) of the first article of [26].

**Table A.1.** Three appearances of the list of Cartan's ten symmetric spaces. First column: unitary time evolution operator; second column: (compact) target space of NL$\sigma$Ms; third column: classifying space. (We use the convention in which $m =$ even in Sp$(m)$. Moreover, the Cartan labels of those symmetry classes invariant under the chiral symmetry operation $\mathcal{S} = \mathcal{T} \cdot \mathcal{C}$ from table 1 are indicated by boldface letters.)

| Cartan label | Time evolution operator $\exp\{\mathrm{i}t\mathcal{H}\}$ | Fermionic replica NL$\sigma$M target space | Classifying space |
|---|---|---|---|
| A | $\mathrm{U}(N)\times\mathrm{U}(N)/\mathrm{U}(N)$ | $\mathrm{U}(2n)/\mathrm{U}(n)\times\mathrm{U}(n)$ | $\mathrm{U}(N+M)/\mathrm{U}(N)\times\mathrm{U}(M)=C_0$ |
| **AIII** | $\mathrm{U}(N+M)/\mathrm{U}(N)\times\mathrm{U}(M)$ | $\mathrm{U}(n)\times\mathrm{U}(n)/\mathrm{U}(n)$ | $\mathrm{U}(N)\times\mathrm{U}(N)/\mathrm{U}(N)=C_1$ |
| AI | $\mathrm{U}(N)/\mathrm{O}(N)$ | $\mathrm{Sp}(2n)/\mathrm{Sp}(n)\times\mathrm{Sp}(n)$ | $\mathrm{O}(N+M)/\mathrm{O}(N)\times\mathrm{O}(M)=R_0$ |
| **BDI** | $\mathrm{O}(N+M)/\mathrm{O}(N)\times\mathrm{O}(M)$ | $\mathrm{U}(2n)/\mathrm{Sp}(2n)$ | $\mathrm{O}(N)\times\mathrm{O}(N)/\mathrm{O}(N)=R_1$ |
| D | $\mathrm{O}(N)\times\mathrm{O}(N)/\mathrm{O}(N)$ | $\mathrm{O}(2n)/\mathrm{U}(n)$ | $\mathrm{O}(2N)/\mathrm{U}(N)=R_2$ |
| **DIII** | $\mathrm{SO}(2N)/\mathrm{U}(N)$ | $\mathrm{O}(n)\times\mathrm{O}(n)/\mathrm{O}(n)$ | $\mathrm{U}(2N)/\mathrm{Sp}(2N)=R_3$ |
| AII | $\mathrm{U}(2N)/\mathrm{Sp}(2N)$ | $\mathrm{O}(2n)/\mathrm{O}(n)\times\mathrm{O}(n)$ | $\mathrm{Sp}(N+M)/\mathrm{Sp}(N)\times\mathrm{Sp}(M)=R_4$ |
| **CII** | $\mathrm{Sp}(N+M)/\mathrm{Sp}(N)\times\mathrm{Sp}(M)$ | $\mathrm{U}(n)/\mathrm{O}(n)$ | $\mathrm{Sp}(N)\times\mathrm{Sp}(N)/\mathrm{Sp}(N)=R_5$ |
| C | $\mathrm{Sp}(2N)\times\mathrm{Sp}(2N)/\mathrm{Sp}(2N)$ | $\mathrm{Sp}(2n)/\mathrm{U}(n)$ | $\mathrm{Sp}(2N)/\mathrm{U}(N)=R_6$ |
| **CI** | $\mathrm{Sp}(2N)/\mathrm{U}(N)$ | $\mathrm{Sp}(2n)\times\mathrm{Sp}(2n)/\mathrm{Sp}(2n)$ | $\mathrm{U}(N)/\mathrm{O}(N)=R_7$ |

column of table A.1. All higher homotopy groups of the same spaces can then be inferred from table 2 due to the dimensional periodicity and shift properties visible in that table.

## Appendix B. Spinor representations of SO($N$)

In this appendix, we review spinor representations of SO$(N)$ and their properties under reality conditions [79, 80]. It is most convenient to discuss spinor representations in terms of Clifford algebras, i.e. in terms of gamma matrices $\{\Gamma^a_{(N)}\}_{a=1,\dots,N}$ satisfying $\{\Gamma^j_{(N)},\Gamma^k_{(N)}\}=2\delta_{jk}$, with $j,k=1,\dots,N$. Given such a set of gamma matrices a spinor representation of SO$(N)$ can be readily obtained

$$M_{jk} = -\frac{\mathrm{i}}{4}\left[\Gamma^j_{(N)},\Gamma^k_{(N)}\right], \tag{B.1}$$

with the SO$(N)$ generators $M_{jk}$.

### *B.1. Spinors of* SO$(2n+1)$

In what follows, we will focus on SO$(2n+1)$, which has a $2^n$-dimensional irreducible spinor representation. The gamma matrices in the Dirac representation for $N=2n+1$ are defined recursively by

$$\begin{aligned}
\Gamma^a_{(2n+1)} &= \Gamma^a_{(2n-1)}\otimes\sigma_3, \qquad a=1,\dots,2n-2,\\
\Gamma^{2n-1}_{(2n+1)} &= I_{2^{n-1}}\otimes\sigma_1,\\
\Gamma^{2n}_{(2n+1)} &= I_{2^{n-1}}\otimes\sigma_2,\\
\Gamma^{2n+1}_{(2n+1)} &= (-\mathrm{i})^n\Gamma^1_{(2n+1)}\Gamma^2_{(2n+1)}\cdots\Gamma^{2n}_{(2n+1)},
\end{aligned} \tag{B.2}$$

where $I_{2^{n-1}}$ is the $2^{n-1}\times 2^{n-1}$ identity matrix. (The gamma matrices in the Dirac representation for $N=2n$ can be constructed by just leaving out $\Gamma^{2n+1}_{(2n+1)}$, i.e. $\Gamma^{a}_{(2n)}=\Gamma^{a}_{(2n+1)}$, with $a=1,\dots,2n$.) To be more explicit,

$$\begin{aligned}
\Gamma^{1}_{(2n+1)} &= \sigma_1\otimes\underbrace{\sigma_3\otimes\cdots\otimes\sigma_3}_{n-1},\\
\Gamma^{2}_{(2n+1)} &= \sigma_2\otimes\underbrace{\sigma_3\otimes\cdots\otimes\sigma_3}_{n-1},\\
\Gamma^{3}_{(2n+1)} &= \sigma_0\otimes\sigma_1\otimes\underbrace{\sigma_3\otimes\cdots\otimes\sigma_3}_{n-2},\\
\Gamma^{4}_{(2n+1)} &= \sigma_0\otimes\sigma_2\otimes\underbrace{\sigma_3\otimes\cdots\otimes\sigma_3}_{n-2},\\
&\vdots\\
\Gamma^{2n-1}_{(2n+1)} &= \underbrace{\sigma_0\otimes\cdots\otimes\sigma_0}_{n-1}\otimes\sigma_1,\\
\Gamma^{2n}_{(2n+1)} &= \underbrace{\sigma_0\otimes\cdots\otimes\sigma_0}_{n-1}\otimes\sigma_2,
\end{aligned} \tag{B.3}$$

and

$$\Gamma^{2n+1}_{(2n+1)} = \underbrace{\sigma_3\otimes\cdots\otimes\sigma_3}_{n}. \tag{B.4}$$

From the explicit construction of the gamma matrices, we infer that $\Gamma^{1,3,\cdots,2n+1}_{(2n+1)}$ are all real, and $\Gamma^{2,4,\cdots,2n}_{(2n+1)}$ are purely imaginary. In order to implement discrete symmetries on the space of Dirac Hamiltonians, we define the matrices

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

By use of the reality and anticommutation properties of the gamma matrices, one finds that

$$\begin{aligned}
\left[B^{1}_{(2n+1)}\right]^{*} B^{1}_{(2n+1)} &= (-1)^{n(n-1)/2},\\
\left[B^{2}_{(2n+1)}\right]^{*} B^{2}_{(2n+1)} &= (-1)^{n(n+1)/2}.
\end{aligned} \tag{B.6}$$

The operator $B^{2}_{(2n+1)}$ is used to construct Majorana (real) representations of SO$(2n+1)$. For odd $N=2n+1$, they are possible when [79, 80]

$$\begin{aligned}
&\left[B^{2}_{(2n+1)}\right]^{*} B^{2}_{(2n+1)} = (-1)^{n(n+1)/2} = 1\\
&\Longrightarrow \quad n=0,3 \mod 4 \quad (N=2n+1=1,7 \mod 8).
\end{aligned} \tag{B.7}$$

Observe that when $n$ is even, all gamma matrices can be made real and symmetric, whereas when $n$ is odd, they can be made purely imaginary and skew-symmetric.

For later use, we also introduce

$$\begin{aligned}
B^{12}_{(2n+1)} &:= \left[B^{2}_{(2n+1)}\right]^{-1} B^{1}_{(2n+1)} = (-\mathrm{i})^{n}\Gamma^{2n+1}_{(2n+1)},\\
\tilde{B}^{1}_{(2n+1)} &:= B^{1}_{(2n+1)}\Gamma^{2n}_{(2n+1)},\\
\tilde{B}^{2}_{(2n+1)} &:= B^{2}_{(2n+1)}\Gamma^{2n}_{(2n+1)}.
\end{aligned} \tag{B.8}$$

Note that these matrices satisfy

$$
\begin{aligned}
B^{1}_{(2n+1)}\Gamma^{a}_{(2n+1)}\left[B^{1}_{(2n+1)}\right]^{-1} &= \begin{cases}(-1)^{n+1}\Gamma^{a*}_{(2n+1)}, & a=1,\dots,2n,\\ (-1)^{n}\Gamma^{a*}_{(2n+1)}, & a=2n+1,\end{cases}\\
B^{2}_{(2n+1)}\Gamma^{a}_{(2n+1)}\left[B^{2}_{(2n+1)}\right]^{-1} &= (-1)^{n}\Gamma^{a*}_{(2n+1)}, \quad a=1,\dots,2n+1,\\
B^{12}_{(2n+1)}\Gamma^{a}_{(2n+1)}\left[B^{12}_{(2n+1)}\right]^{-1} &= \begin{cases}-\Gamma^{a}_{(2n+1)}, & a=1,\dots,2n,\\ +\Gamma^{a}_{(2n+1)}, & a=2n+1.\end{cases}
\end{aligned}
\tag{B.9}
$$

In the following subsection, we will use the '$B$-matrices', equations (B.5) and (B.8), as symmetry operators in order to implement discrete symmetries on the space of Dirac Hamiltonians. To identify the character of these discrete symmetries we first compute the sign $\eta_{B_{(2n+1)}}$ picked up by $B_{(2n+1)}$ under transposition, $[B_{(2n+1)}]^{\mathrm{T}} = \eta_{B_{(2n+1)}} B_{(2n+1)}$. Note that the sign $\eta_{B_{(2n+1)}}$ is independent of the choice of basis for the gamma matrices (see [79]). From equations (B.6) and (B.7) and by use of the property $[B^2_{(2n+1)}]^{\dagger} B^2_{(2n+1)} = 1$, it follows that

$$\eta_{B^2_{(2n+1)}} = (-1)^{n(n+1)/2}. \tag{B.10}$$

Similarly,

$$
\begin{aligned}
\eta_{B^1_{(2n+1)}} &= (-1)^{n(n-1)/2},\\
\eta_{\tilde{B}^1_{(2n+1)}} &= -(-1)^{n(n+1)/2},\\
\eta_{\tilde{B}^2_{(2n+1)}} &= (-1)^{n(n+3)/2}.
\end{aligned}
\tag{B.11}
$$

### *B.2. Discrete symmetries of Dirac Hamiltonians*

Let us now determine the symmetry properties of the Dirac Hamiltonians $\mathcal{H}^{d=2n+3}_{(2n+3)}(k)$, $\mathcal{H}^{d=2n+2}_{(2n+3)}(k)$, $\dots$, $\mathcal{H}^{d=2n-1}_{(2n+3)}(k,m)$, defined in equations (100)–(104). We find that these Dirac Hamiltonians satisfy the following symmetry conditions:

$$(0): B^2_{(2n+1)}\mathcal{H}^{d=2n+1}_{(2n+1)}(k)\left[B^2_{(2n+1)}\right]^{-1} = (-1)^{n+1}\left[\mathcal{H}^{d=2n+1}_{(2n+1)}(-k)\right]^{*}, \tag{B.12}$$

$$(i): B^1_{(2n+1)}\mathcal{H}^{d=2n}_{(2n+1)}(k,m)\left[B^1_{(2n+1)}\right]^{-1} = (-1)^{n}\left[\mathcal{H}^{d=2n}_{(2n+1)}(-k,m)\right]^{*}, \tag{B.13}$$

$$
\begin{aligned}
(ii): B^1_{(2n+1)}\mathcal{H}^{d=2n-1}_{(2n+1)}(k,m)\left[B^1_{(2n+1)}\right]^{-1} &= (-1)^{n}\left[\mathcal{H}^{d=2n-1}_{(2n+1)}(-k,m)\right]^{*},\\
\tilde{B}^1_{(2n+1)}\mathcal{H}^{d=2n-1}_{(2n+1)}(k,m)\left[\tilde{B}^1_{(2n+1)}\right]^{-1} &= (-1)^{n+1}\left[\mathcal{H}^{d=2n-1}_{(2n+1)}(-k,m)\right]^{*}.
\end{aligned}
\tag{B.14}
$$

$$(iii): B^2_{(2n+1)}\mathcal{H}^{d=2n-2}_{(2n+1)}(k,m)\left[B^2_{(2n+1)}\right]^{-1} = (-1)^{n+1}\left[\mathcal{H}^{d=2n-2}_{(2n+1)}(-k,m)\right]^{*}, \tag{B.15}$$

$$
\begin{aligned}
(iv): B^2_{(2n+1)}\mathcal{H}^{d=2n-3}_{(2n+1)}(k,m)\left[B^2_{(2n+1)}\right]^{-1} &= (-1)^{n+1}\left[\mathcal{H}^{d=2n-3}_{(2n+1)}(-k,m)\right]^{*},\\
\tilde{B}^2_{(2n+1)}\mathcal{H}^{d=2n-3}_{(2n+1)}(k,m)\left[\tilde{B}^2_{(2n+1)}\right]^{-1} &= (-1)^{n}\left[\mathcal{H}^{d=2n-3}_{(2n+1)}(-k,m)\right]^{*}.
\end{aligned}
\tag{B.16}
$$

A few remarks are in order.

- The Hamiltonians $\mathcal{H}^{d=2n-1}_{(2n+1)}(k,m)$ and $\mathcal{H}^{d=2n-3}_{(2n+1)}(k,m)$ satisfy two different discrete symmetry conditions and are therefore also left invariant under the combination of these two symmetries, which defines a chiral symmetry. In other words, both $\mathcal{H}^{d=2n-1}_{(2n+1)}(k,m)$ and $\mathcal{H}^{d=2n-3}_{(2n+1)}(k,m)$ anticommute with a unitary matrix

$$\begin{aligned}\left\{\mathcal{H}^{d=2n-1}_{(2n+1)}(k,m),\,\Gamma^{2n}_{(2n+1)}\right\}&=0,\\ \left\{\mathcal{H}^{d=2n-3}_{(2n+1)}(k,m),\,\Gamma^{2n-2}_{(2n+1)}\right\}&=0.\end{aligned} \tag{B.17}$$

- The Hamiltonians $\mathcal{H}^{d=2n}_{(2n+3)}(k,m)$ and $\mathcal{H}^{d=2n-1}_{(2n+3)}(k,m)$ can be made block diagonal because

$$\begin{aligned}\left[\mathcal{H}^{d=2n}_{(2n+3)}(k,m),\,\Gamma^{a}_{(2n+3)}\Gamma^{b}_{(2n+3)}\right]&=0,\\ \left[\mathcal{H}^{d=2n-1}_{(2n+3)}(k,m),\,\Gamma^{a}_{(2n+3)}\Gamma^{b}_{(2n+3)}\right]&=0,\end{aligned} \tag{B.18}$$

where $(a,b)=(2n+1,2n+2)$, $(2n+2,2n+3)$ or $(2n+3,2n+1)$.

- In the case of the massive Hamiltonian $\mathcal{H}^{d=2n}_{(2n+1)}(k,m)$, the parity transformation[38] can be implemented by $B^{12}_{(2n+1)}$

$$B^{12}_{(2n+1)}\mathcal{H}^{d=2n}_{(2n+1)}(k,m)\left[B^{12}_{(2n+1)}\right]^{-1}=\mathcal{H}^{d=2n}_{(2n+1)}(-k,m). \tag{B.19}$$

By combining the discrete symmetry $B^{1}_{(2n+1)}$ and the parity symmetry $B^{12}_{(2n+1)}$, the Hamiltonian also satisfies

$$B^{2}_{(2n+1)}\mathcal{H}^{d=2n}_{(2n+1)}(k,m)\left[B^{2}_{(2n+1)}\right]^{-1}=(-1)^{n}\left[\mathcal{H}^{d=2n}_{(2n+1)}(k,m)\right]^{*}. \tag{B.20}$$

This discrete symmetry is unique in that, unlike $\mathcal{T}$ or $\mathcal{C}$ that relates Bloch Hamiltonians at $k$ and $-k$, it constrains the form of the Hamiltonian at a given $k$. This is nothing but the real/pseudo-real condition for $\mathrm{SO}(2n+1)$. As a consequence, the Hamiltonian in $k$-space can be written as a real/pseudo-real matrix. Hence, classifying topological insulators (superconductors) satisfying the combination of $B^{1}_{(2n+1)}$ and $B^{12}_{(2n+1)}$ amounts to classifying *real* bundles. (It is not necessary to satisfy both, however.) An example of a topological insulator/superconductor satisfying the combination of $B^{1}_{(2n+1)}$ and $B^{12}_{(2n+1)}$ is constructed in appendix C.

## Appendix C. Topological insulators protected by a combination of spatial inversion and either time-reversal or charge-conjugation symmetry

In the main text, we have focused on the role of generic symmetries such as time reversal and charge conjugation, which are not related to any spatial symmetries. However, real systems often have discrete spatial symmetries, such as parity, reflection, discrete rotations, etc. Hence, it is meaningful to study the restrictions imposed by these symmetries on the Bloch wavefunctions and thus on the ground state properties. In this appendix, we briefly discuss topological states that are protected by a combination of spatial inversion and an additional discrete symmetry, such as $\mathcal{T}$ or $\mathcal{C}$.

[38] Parity here simply means $k\to -k$ symmetry. In odd spacetime dimensions, it is actually not called parity.

### *C.1. Inversion symmetry combined with another discrete symmetry*

Consider a tight-binding Hamiltonian,

$$H = \sum_{r,r'} \psi^{\dagger}(r)\, \mathcal{H}(r,r')\, \psi(r'), \quad \mathcal{H}^{\dagger}(r',r) = \mathcal{H}(r,r'), \tag{C.1}$$

where $\psi(r)$ is an $n_{\mathrm{f}}$-component fermion operator, and index $r$ labels the lattice sites. (The internal indices are suppressed.) Each block in the single-particle Hamiltonian $\mathcal{H}(r,r')$ is an $n_{\mathrm{f}}\times n_{\mathrm{f}}$ matrix, and we assume that the total size of the single-particle Hamiltonian is $n_{\mathrm{f}}V\times n_{\mathrm{f}}V$, where $V$ is the total number of lattice sites. The components in $\psi(r)$ can describe, e.g., orbitals or spin degrees of freedom, as well as different sites within a crystal unit cell centered at $r$.

Provided the system has translational symmetry,

$$\mathcal{H}(r,r') = \mathcal{H}(r-r'), \tag{C.2}$$

with periodic boundary conditions in each spatial direction (i.e. the system is defined on a torus $T^d$), we can perform the Fourier transformation and obtain in momentum space

$$H = \sum_{k\in \mathrm{BZ}} \psi^{\dagger}(k)\, \mathcal{H}(k)\, \psi(k), \tag{C.3}$$

where

$$\psi(r) = \sqrt{V}^{-1} \sum_{k\in \mathrm{BZ}} \mathrm{e}^{\mathrm{i}k\cdot r}\psi(k), \quad \mathcal{H}(k) = \sum_{r} \mathrm{e}^{-\mathrm{i}k\cdot r}\mathcal{H}(r). \tag{C.4}$$

(Here, if different components in $\psi(r)$ were to represent different sites within a unit cell centered at $r$, we could include the phase $\mathrm{e}^{\mathrm{i}k\cdot(r-r_a)}$ in the definition of $\psi(k)$, $\psi(k)\to \mathrm{diag}(\mathrm{e}^{\mathrm{i}k\cdot(r-r_a)})_{a=1,\ldots,n_{\mathrm{f}}}\psi(k)$ where $r_a$ represents a location within a unit cell.)

In the main text of this paper, we considered topological insulators (superconductors) protected by discrete symmetries, such as $\mathcal{T}$ and $\mathcal{C}$. We now focus on the effect of inversion symmetry. By definition, an inversion $\Omega$ relates fermion operators at $r$ and at $-r$,

$$\Omega\, \psi(r)\, \Omega^{-1} = U\psi(-r), \tag{C.5}$$

where $U$ is a constant $n_{\mathrm{f}}\times n_{\mathrm{f}}$ unitary matrix. (It is important to distinguish between inversion and parity symmetry. The former means $r\to -r$ for any spacetime dimension. Parity transformation in even spacetime dimension agrees with inversion, but in odd spacetime dimension, it is different from inversion.) One can imagine, for example, $U$ represents a parity eigenvalue of each orbital at site $r$ ($s$, $p$, ..., orbitals), which can be either +1 or −1. Similarly, if different components in $\psi(r)$ represent different sites in the unit cell centered at $r$, inversion transformation sends $r$ to $-r$ and, at the same time, can reshuffle locations of electron operators within a unit cell, which can be described by the unitary matrix $U$. The invariance of $H$ under $\Omega$ implies

$$U^{-1}\mathcal{H}(r,r')U = \mathcal{H}(-r,-r'), \quad U^{-1}\mathcal{H}(r)U = \mathcal{H}(-r). \tag{C.6}$$

Thus, the Bloch Hamiltonians at $k$ and $-k$ are unitarily equivalent,

$$U^{-1}\mathcal{H}(k)U = \mathcal{H}(-k). \tag{C.7}$$

To summarize, definition (C.5) implies that (i) the spectrum at $k$ is identical to the one at $-k$ and (ii) the unitary matrix $U$ relating the Hamiltonian at $k$ to the one at $-k$ is $k$ independent. This form of symmetry does not necessarily correspond to inversion symmetry verbatim, but might

**Table C.1.** The ten generic symmetry classes of single-particle Hamiltonians classified in terms of the presence (◯) or absence (×) of the time-reversal symmetry ($\epsilon_V = +1$) with T$= -1$ ($\eta_V = -1$) and T$= +1$ ($\eta_V = +1$), and the particle–hole symmetry ($\epsilon_V = -1$) with C$= -1$ ($\eta_V = -1$) and C$= +1$ ($\eta_V = +1$), as well as chiral (or sublattice) symmetry denoted by S; see table 1. For the notation of these symmetry classes in terms of $(\epsilon_V, \eta_V)$, see the main text and [26].

| $(\epsilon_V, \eta_V)$ | Cartan | S | T$=-1$ $(1,-1)$ | T$=+1$ $(1,1)$ | C$=-1$ $(-1,-1)$ | C$=+1$ $(-1,1)$ |
|---|---|---|---|---|---|---|
| Standard | A | × | × | × | × | × |
| | AI | × | × | ◯ | × | × |
| | AII | × | ◯ | × | × | × |
| Chiral | AIII | ◯ | × | × | × | × |
| (sublattice) | BDI | ◯ | × | ◯ | × | ◯ |
| | CII | ◯ | ◯ | × | ◯ | × |
| BdG | D | × | × | × | × | ◯ |
| | C | × | × | × | ◯ | × |
| | DIII | ◯ | ◯ | × | × | ◯ |
| | CI | ◯ | × | ◯ | ◯ | × |

describe an inversion symmetry that is realized as a projective symmetry (e.g. invariance of the Hamiltonian under inversion followed by a gauge transformation). The only big assumption here is that we have assumed $U$ is $k$ independent.

We now combine the inversion symmetry with another discrete symmetry,

$$V^{-1}\mathcal{H}(k)V = \epsilon_V \mathcal{H}(-k)^T, \quad \epsilon_V = \pm 1, \\ \text{with} \quad V^T = \eta_V V, \quad \eta_V = \pm 1. \tag{C.8}$$

As before we distinguish four different cases (see section 1.1 and in particular equations (3) and (4)): $(\epsilon_V, \eta_V) = (1, 1)$ corresponds to a time-reversal symmetry with T$= +1$, $(\epsilon_V, \eta_V) = (1, -1)$ denotes a time-reversal symmetry with T$= -1$, $(\epsilon_V, \eta_V) = (-1, 1)$ is a particle–hole symmetry with C$= +1$, and $(\epsilon_V, \eta_V) = (-1, -1)$ is a particle–hole symmetry with C$= -1$. These four cases together with the corresponding 'Cartan label' are summarized in table C.1. Then, for the combined transformation,

$$W^{-1}\mathcal{H}(k)W = \epsilon_W \mathcal{H}(k)^{\mathrm{T}}, \quad W := UV, \quad \text{with} \quad \epsilon_W = \epsilon_V. \tag{C.9}$$

Iterating this transformation twice,

$$\mathcal{H}(k) \to W\mathcal{H}(k)^{\mathrm{T}}W^{-1} \to W(W^{-1})^{\mathrm{T}}\mathcal{H}(k)W^{\mathrm{T}}W^{-1}, \tag{C.10}$$

which suggests, from Schur's lemma, $W^{\mathrm{T}}W^{-1} \propto I_{n_f}$. Hence, as before, for $W$, we distinguish the following two cases:

$$W^{\mathrm{T}} = \eta_W W, \quad \eta_W = \pm 1. \tag{C.11}$$

The signature $\eta_W$ is invariant under unitary transformations. It depends on the signature $\eta_V$, the signature $\eta_U$ for the inversion $U^{\mathrm{T}} = \eta_U U$, and the commutation relation of $U$ and $V$. Here, note that the signature $\eta_U$ for inversion alone is not invariant under unitary transformation, while the signature $\eta_W$ is invariant. As an illustration, let us consider spinless fermions. Time-reversal symmetry $\mathcal{T}$ for spinless fermions implies

$$\mathcal{H}(i,j)^* = \mathcal{H}(i,j). \tag{C.12}$$

Thus, when inversion and $\mathcal{T}$ are combined,

$$\mathcal{H}^*(r) = W\mathcal{H}(-r)W^{-1}, \quad \mathcal{H}^*(k) = W^{-1}\mathcal{H}(k)W, \quad \text{where} \quad W = U. \tag{C.13}$$

In this example and in this basis, the signature of $W$ solely depends on the signature of $U$, $\eta_W = \eta_U$.

Interesting examples are provided by Dirac Hamiltonians. For a massive Dirac Hamiltonian, the mass matrix itself can be taken as the unitary matrix $U$ that was introduced in equation (C.5). Put differently, any massive Dirac Hamiltonian possesses a $U$-type symmetry. These $U$-type symmetries can be, however, different from the inversion symmetry that is imposed at the microscopic level. However, if one starts from a microscopic lattice model with inversion symmetry, and arrives at a Dirac Hamiltonian with a mass in the continuum, inversion symmetry in the continuum must be implemented by a mass matrix.

Firstly, consider Hamiltonian (101)

$$(i): \quad \mathcal{H}^{d=2n}_{(2n+1)}(k,m) = \sum_{a=1}^{d=2n} k_a \Gamma^a_{(2n+1)} + m\Gamma^{2n+1}_{(2n+1)}. \tag{C.14}$$

This Hamiltonian has a $V$-type symmetry with

$$V = B^1_{(2n+1)}, \quad \epsilon_V = (-1)^n, \quad \eta_V = \eta_{B^1_{(2n+1)}} = (-1)^{n(n-1)/2}. \tag{C.15}$$

There is inversion symmetry represented by

$$U = \Gamma^{2n+1}_{(2n+1)}, \quad \eta_U = +1. \tag{C.16}$$

The combined transformation $W$ is given by

$$W = B^2_{(2n+1)}, \quad \epsilon_W = (-1)^n, \quad \eta_W = \eta_{B^2_{(2n+1)}} = (-1)^{n(n+1)/2}. \tag{C.17}$$

Secondly, we consider the massive Dirac Hamiltonian (103)

$$\begin{aligned}(iii): \quad \mathcal{H}^{d=2n-2}_{(2n+1)}(k,m) &= \sum_{a=1}^{d=2n-2} k_a \Gamma^a_{(2n+1)} + m\mathcal{M}, \\ \text{with} \quad \mathcal{M} &:= \mathrm{i}\Gamma^{2n+1}_{(2n+1)}\Gamma^{2n}_{(2n+1)}\Gamma^{2n-1}_{(2n+1)}.\end{aligned} \tag{C.18}$$

The $V$-type discrete symmetry for this is

$$V = B^2_{(2n+1)}, \quad \epsilon_V = (-1)^{n+1}, \quad \eta_V = \eta_{B^2_{(2n+1)}} = (-1)^{n(n+1)/2}. \tag{C.19}$$

The inversion symmetry is represented by

$$U = \mathcal{M}, \quad \eta_U = +1. \tag{C.20}$$

Thus, the combined transformation is

$$\begin{aligned}W &= \mathcal{M}B^2_{(2n+1)} = \mathrm{i}\Gamma^{2n+1}_{(2n+1)}\Gamma^{2n}_{(2n+1)}\Gamma^{2n-1}_{(2n+1)} \times \Gamma^2_{(2n+1)}\Gamma^4_{(2n+1)}\cdots\Gamma^{2n}_{(2n+1)}. \\ &\text{with} \quad \epsilon_W = (-1)^{n+1}, \quad \eta_W = (-1)^{n(n+1)/2}.\end{aligned} \tag{C.21}$$

where we have noted $UV = VU$.

### *C.2. Classification of gapped Hamiltonians in the presence of a combination of spatial inversion and either time-reversal or charge-conjugation symmetry*

We now classify the ground states of gapped Hamiltonians protected by a $W$-type symmetry. We distinguish four different cases, $(\epsilon_W, \eta_W) = (\pm 1, \pm 1)$.

Let us first consider the case of $(\epsilon_W, \eta_W) = (1, 1)$, in which case $W$ is a symmetric unitary matrix, $W = W^{\mathrm{T}}$ $(\eta_W = +1)$. Such a matrix is an element of $\mathrm{U}(n_{\mathrm{f}})/\mathrm{O}(n_{\mathrm{f}})$. Any element in $\mathrm{U}(n_{\mathrm{f}})/\mathrm{O}(n_{\mathrm{f}})$ can be written as $W = XX^{\mathrm{T}}$, where $X$ is a unitary matrix. One can then take a basis in which the Bloch Hamiltonian for any given $k$ is a real symmetric matrix. In other words, if we define $\tilde{\mathcal{H}} := X^{\dagger}\mathcal{H}X$, then $\tilde{\mathcal{H}}^{*} = \tilde{\mathcal{H}}$. Thus, when $(\epsilon_W, \eta_W) = (+1, +1)$, the Hamiltonian is real symmetric and hence Bloch wavefunctions can be taken real at each $k$. We assume that there are $N_-$ $(N_+)$ occupied (unoccupied) Bloch wavefunctions for each $k$ with $N_+ + N_- = N_{\mathrm{tot}} (= n_{\mathrm{f}})$. The spectral projector onto the filled Bloch states or the '$Q$-matrix' in this case can be viewed as an element of the real Grassmannian $G_{N_-,N_++N_-}(\mathbb{R}) = \mathrm{O}(N_+ + N_-)/[\mathrm{O}(N_+) \times \mathrm{O}(N_-)]$. For a given system, the '$Q$-matrix' defines a map from the BZ onto the real Grassmannian. Hence, classifying topological classes of band insulators amounts to counting the number of topologically inequivalent mappings from the BZ to $G_{N_-,N_++N_-}(\mathbb{R})$. Mathematically, this is given by the homotopy group of the space of projectors (i.e. of the real Grassmannian in the present case), which can be read from table 2.

The same reasoning can be repeated for the case $(\epsilon_W, \eta_W) = (+1, -1)$. One finds that the space of projectors is the quaternionic Grassmannian $G_{N_-,N_++N_-}(\mathbb{H}) = \mathrm{Sp}(N_+ + N_-)/[\mathrm{Sp}(N_+) \times \mathrm{Sp}(N_-)]$, whose homotopy group is again given in table 2.

When $(\epsilon_W, \eta_W) = (-1, +1)$, the Hamiltonian can be taken, in a suitable basis, as real and skew symmetric, i.e. an element of $\mathrm{so}(n_{\mathrm{f}})$. Any element of $\mathrm{so}(n_{\mathrm{f}})$ can be transformed into a canonical form by an orthogonal transformation. For the $Q$-matrix, its canonical form $\tilde{Q}$ is a matrix whose matrix elements are $\pm 1$,

$$Q = S\tilde{Q}S^{\mathrm{T}}, \qquad S \in \mathrm{SO}(n_{\mathrm{f}}),$$
$$\text{where} \quad \tilde{Q} = \begin{pmatrix} 0 & +1 & & & \cdots \\ -1 & 0 & & & \\ & & 0 & +1 & \\ & & -1 & 0 & \\ \vdots & & & & \ddots \end{pmatrix}, \tag{C.22}$$

where we have assumed that $n_{\mathrm{f}}$ is an even integer. We thus identified the space of projectors as $\mathrm{SO}(n_{\mathrm{f}})/\mathrm{U}(n_{\mathrm{f}}/2)$. Finally, when $(\epsilon_W, \eta_W) = (-1, -1)$, we identify the space of projectors as $\mathrm{Sp}(n_{\mathrm{f}})/\mathrm{U}(n_{\mathrm{f}})$.

To summarize, we have listed in table C.2, for each of the four cases of $W$-type symmetries, the space of projectors '$G/H$' together with their homotopy groups $\pi_d(G/H)$, which yields the classification of topological insulators (superconductors) protected by a combination of inversion and an additional discrete symmetry. Note that we focus here on the implication of the combination of inversion and discrete symmetries, but we do not require each symmetry separately.

*C.2.1. Example: $(\epsilon_W, \eta_W) = (1, 1)$ in $d = 2$.* We now specialize to the case of $(\epsilon_W, \epsilon_W) = (1, 1)$. The relevant space of the projection operators is the real Grassmannian $G_{N_+,N_++N_-}(\mathbb{R})$

**Table C.2.** Classification of topological insulators (superconductors) protected by a combination of spatial inversion and an additional discrete symmetry.

| | | $d$ | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| $(\epsilon_W, \eta_W)$ Projectors | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | ... |
| $(+1, -1)$ $\mathrm{Sp}(N+M)/\mathrm{Sp}(N)\times\mathrm{Sp}(M)$ | $\mathbb{Z}$ | 0 | 0 | 0 | $\mathbb{Z}$ | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | 0 | ... |
| $(-1, +1)$ $\mathrm{O}(2N)/\mathrm{U}(N)$ | $\mathbb{Z}_2$ | 0 | $\mathbb{Z}$ | 0 | 0 | 0 | $\mathbb{Z}$ | $\mathbb{Z}_2$ | ... |
| $(+1, +1)$ $\mathrm{O}(N+M)/\mathrm{O}(N)\times\mathrm{O}(M)$ | $\mathbb{Z}$ | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | 0 | $\mathbb{Z}$ | 0 | 0 | 0 | ... |
| $(-1, -1)$ $\mathrm{Sp}(N)/\mathrm{U}(N)$ | 0 | 0 | $\mathbb{Z}$ | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | 0 | $\mathbb{Z}$ | 0 | ... |

and the projection operator defines a map from the BZ onto the real Grassmannian. In particular, when $d=2$, the projector $Q(k_x, k_y)$ defines a map from $S^2$ or $T^2$ onto $G_{N_+,N_-+N_+}(\mathbb{R})$. The homotopy group $\pi_2[G_{N_+,N_-+N_+}(\mathbb{R})]=\mathbb{Z}_2$ tells us that the space of quantum ground states is partitioned into two topologically distinct sectors.

A representative $Q$-field configuration that is a nontrivial element of $\pi_2[G_{N_+,N_-+N_+}(\mathbb{R})]=\mathbb{Z}_2$ can be constructed by following [81]. For simplicity, take the case where we have four bands in total and two filled bands; take $N_+=N_-=2$. Then such a representative $Q$-matrix is given by

$$Q^{(l)}(k)=\begin{pmatrix} n_z^{(l)} & 0 & -n_x^{(l)} & -n_y^{(l)} \\ 0 & n_z^{(l)} & n_y^{(l)} & -n_x^{(l)} \\ -n_x^{(l)} & n_y^{(l)} & -n_z^{(l)} & 0 \\ -n_y^{(l)} & -n_x^{(l)} & 0 & -n_z^{(l)} \end{pmatrix},$$

$$\text{with}\quad n^{(l)}(k):=\left(n_x^{(l)}, n_y^{(l)}, n_z^{(l)}\ \right) \tag{C.23}$$

$$=(\cos(l\phi)\sin(\theta),\quad \sin(l\phi)\sin(\theta),\quad \cos\theta),$$

where $l\in\mathbb{Z}$, and $\theta$ and $\phi$ are spherical coordinates parameterizing the BZ $\simeq S^2$. The projector is a nontrivial element of the second homotopy group when $l$ is odd, while it is trivial when $l$ is even. Observe that the normalized vector $n^{(l)}(k)$ itself defines a map from $S^2$ onto $S^2$, and wraps $S^2$ integer $(=l)$ times.

We can construct a Hamiltonian that has $Q^{(l)}(k)$ as a projector. We consider the following four-band tight-binding Hamiltonian on the square lattice:

$$H=\sum_r\left[\psi^\dagger(r)\,h_0\,\psi(r)\ +\psi^\dagger(r)\,h_x\,\psi(r+\hat{x})+\text{h.c.}+\psi^\dagger(r)\,h_y\,\psi(r+\hat{y})+\text{h.c.}\right], \tag{C.24}$$

where $\hat{x}=(1,0)$ and $\hat{y}=(0,1)$, respectively, and

$$h_0=-\mu\begin{pmatrix}\sigma_0 & 0\\ 0 & -\sigma_0\end{pmatrix},\quad h_x=\begin{pmatrix} t\sigma_0 & \Delta\sigma_y \\ -\Delta\sigma_y & -t\sigma_0\end{pmatrix},\quad h_y=\begin{pmatrix} t\sigma_0 & -\mathrm{i}\Delta\sigma_0 \\ -\mathrm{i}\Delta\sigma_0 & -t\sigma_0\end{pmatrix}, \tag{C.25}$$

and $t, \Delta, \mu\in\mathbb{R}$ are parameters of the model. In $k$-space,

$$\mathcal{H}(k)=\begin{pmatrix} R_z & 0 & -R_x & -R_y \\ 0 & R_z & R_y & -R_x \\ -R_x & R_y & -R_z & 0 \\ -R_y & -R_x & 0 & -R_z \end{pmatrix}, \tag{C.26}$$

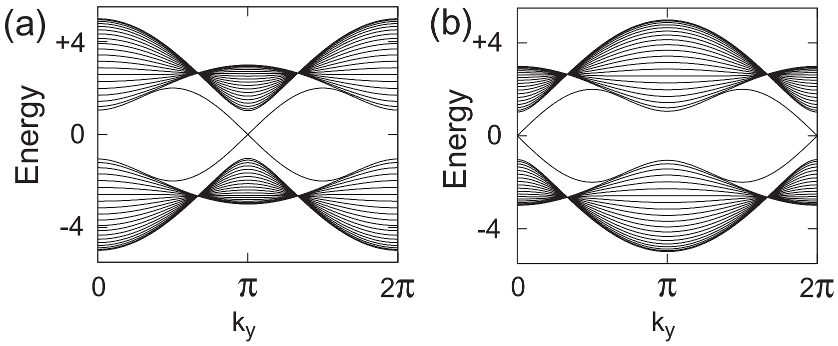


**Figure C.1.** The energy spectrum with $t = \Delta = 1$ and $\mu = -1$ (a) and $\mu = +1$ (b).

where

$$R(k) = \left(-2\Delta \sin k_y, \quad -2\Delta \sin k_x, \quad 2t\left(\cos k_x + \cos k_y\right) - \mu\right). \tag{C.27}$$

We will set $t = \Delta = 1$ henceforth. As we change $\mu$, there are four phases separated by quantum phase transitions at $\mu = \pm 4$ and $\mu = 0$. When $|\mu| > 4$, the normalized vector $R(k)/|R(k)|$ does not wrap $S^2$ as we sweep the momentum and the system is in a trivial phase. On the other hand, for $|\mu| < 4$ the normalized vector $R(k)/|R(k)|$ wraps the sphere $S^2$ $n = +1$ times (or $n = -1$ times), and hence the system is in a nontrivial phase. The projector constructed from (C.26) is topologically equivalent to $Q^{(l)}(k)$ with $l$ odd.

For topological insulators and superconductors protected by $\mathcal{T}$, $\mathcal{C}$ or a combination of both, a diagnostic of bulk topological character is the existence of gapless edge modes. For insulators and superconductors with an inversion symmetry, it is less clear if looking for edge modes is useful to characterize the bulk topological character since the boundary breaks inversion symmetry. (Nevertheless, as discussed recently in [82], for the entanglement entropy spectrum, an inversion symmetry can protect the gapless entanglement entropy spectrum.) For the present case, however, the Hamiltonian has several accidental symmetries (see below), in particular $\mathcal{T}$ (odd), which may protect the gapless nature of edge states if they exist and if the number of Kramers pairs is odd. In figure C.1, the energy spectrum for $\mu = \pm 1$ in the slab geometry is presented; here two edges along the $y$-direction (located at $x = 0$ and $x = N_x$) are created, and the energy eigenvalues are plotted as a function of $k_y$. Each eigenvalue is doubly degenerate for each $k_y$. For $\mu = \pm 1$, there are four edge modes, two of which are localized at $x = 0$ and the other two at $x = N_x$, whereas for $|\mu| > 4$, there is no edge mode.

The only symmetry we have assumed so far for ensembles of Hamiltonians is a $W$-type symmetry with $(\epsilon_W, \eta_W) = (1, 1)$. The representative Hamiltonian (C.25) and (C.26), however, accidentally has several other discrete symmetries. The Hamiltonian is invariant under the following discrete symmetries: Time-reversal symmetires $\mathcal{T}$

$$A^{-1}\mathcal{H}(-k)^* A = \mathcal{H}(k), \qquad A = \tau_z\sigma_0 \quad \text{or} \quad \tau_z\sigma_y, \tag{C.28}$$

inversion symmetries $\mathcal{I}$

$$B^{-1}\mathcal{H}(-k) B = \mathcal{H}(k), \qquad B = \tau_z\sigma_0 \quad \text{or} \quad \tau_z\sigma_y, \tag{C.29}$$

and charge-conjugation symmetries $\mathcal{C}$

$$C^{-1}\mathcal{H}(-k)^* C = -\mathcal{H}(k), \qquad C = \tau_x\sigma_x \quad \text{or} \quad \tau_x\sigma_z. \tag{C.30}$$

Although accidental, the presence of these symmetries allows us to interpret the Hamiltonian in many different ways. For example, since the Hamiltonian is invariant under $\mathcal{T}$, $A = \tau_z\sigma_y$ with $A^{\mathrm{T}} = -A$, it is a member of symmetry class AII. Furthermore, it supports two branches of modes per edge that are counterpropagating. The representative Hamiltonian so constructed is thus a $\mathbb{Z}_2$ topological insulator in class AII (i.e. it is in the QSH phase). By further imposing a $\mathcal{C}$, $C = \tau_x\sigma_z$ with $C^{\mathrm{T}} = +C$, the single particle Hamiltonian can be interpreted as a member of symmetry class DIII. Again, it is a nontrivial $\mathbb{Z}_2$ topological superconductor in class DIII. Thus, nontrivial $\mathbb{Z}_2$ topological insulators (AII) and superconductors (DIII) in $d = 2$ dimensions can be interpreted, somewhat accidentally, as a nontrivial element of $\pi_2[G_{N_+,N_-+N_+}(\mathbb{R})] = \mathbb{Z}_2$. To implement a $W$-type symmetry, $\mathcal{T}$ for symmetry classes AII and DIII ($A = \tau_z\sigma_y$ with $A^{\mathrm{T}} = -A$) can be combined with an inversion symmetry represented by $B = \tau_z\sigma_y$. This inversion symmetry is, however, an artificial symmetry in the sense that it flips spin.

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