

**Week 7**  
**Lecture Notes:**  
**Topological Condensed Matter Physics**

Sebastian Huber and Titus Neupert

Department of Physics, ETH Zürich  
Department of Physics, University of Zürich

# Chapter 7

## The 10-fold way: Classification with respect to local symmetries

### Learning goals

- We know the three symmetries on which the table of topological insulators is based.
  - We know how, in principle, one can build the table.
  - We know how to derive the indices for each symmetry group.
  - We know how to make use of the table in real life.
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- C.-K. Chiu et al., *Rev. Mod. Phys.* **88**, 035005 (2016)

### 7.1 Motivation and definitions

In the chapters up to now we have seen a variety of systems that can be described with a topological quantum number. While the response to an electric field in the integer quantum Hall effect was described by the Chern number, we have seen how such topological indices also show up in simple one-, two- and three-dimensional toy-models. Moreover, these indices are not restricted to plain electron systems, but superconductors may show topological features as well. Some of these systems did not require any symmetries (the quantum Hall effect), see Chap. ??, while others either required local symmetries such as time reversal, see Chap. ??, or appear on Hilbert spaces that have some symmetries built in, cf. Chap. ??. The Nambu-space of superconductors being an example of the latter.

We now try to understand how one can rationalize the above observations in a bigger framework. Let us review which (topological) classification schemes we already encountered. The first example was the characterization of a spin-1/2 in a magnetic field in Sec. ??. There, we discussed the geometric phase as a function of a smooth change in parameters of a Hamiltonian. The mathematical structure behind that was a fibre bundle. A fiber bundle is an object which locally looks like  $M \times f$ , where  $M$  is some base manifold and  $f$  the “fibre”. For our case of the geometric phase, the base manifold was  $S^2$  describing the parameter space of the ground state projector  $|\psi_0\rangle\langle\psi_0|$ . The fiber  $f = U(1)$  was the phase of the ground state  $|\psi_0\rangle$  that dropped out when we considered the projector. We have seen that one can classify such fibre bundles via a *Chern* number  $C^{(1)}$ . For the example of a spin-1/2 in a magnetic field, the Chern number took the value  $C^{(1)} = -2\pi$ . For the quantum Hall effect, we identified the fibre bundle with what looks locally like  $\mathbb{T}^2 \times U(1)$  where  $\mathbb{T}^2$  is the torus defined by the Aharonov-Bohm fluxes through the openings of the (real space!) torus. We argued that also in this case the fibre bundle is characterized by the Chern number which can take any value in  $2\pi\nu$  with  $\nu \in \mathbb{Z}$  [1, 2].

We also considered special cases where the Aharonov-Bohm fluxes could be replaced by lattice momenta  $(k_x, k_y)$ . Moreover, in the simple case of a two-band Chern insulator the Chern number was shown to be equivalent to the Skyrmion number which characterizes mappings  $\mathbb{T}^2 \rightarrow S^2$  instead of fibre bundles. In general, we can hope to find the classification of mappings  $\mathbb{T}^d \rightarrow M$ , where  $\mathbb{T}^d$  is the  $d$ -dimensional Brillouin zone and  $M$  is some target manifold.

Attempting a topological classification of free fermion systems really means to define equivalence classes of first quantized Hamiltonians. Not so surprisingly, such equivalence classes depend strongly on the presence of symmetries: If we allow for arbitrary deformations of Hamiltonians (of course without the closing of the gap above the ground state!), we might be able to deform two Hamiltonians into each other that are distinct if we restrict the possible interpolation path by requiring symmetries.

A simple example of such a symmetry constraint we encountered in Chap. ???: Consider the restricted one-dimensional two-band system

$$H = \sum_i d_i(k) \sigma_i \quad \text{with} \quad \{H, \sigma_z\} = 0. \quad (7.1.1)$$

This symmetry requirement is identical with the demand that there is no  $z$ -component of the  $d$ -vector as we have observed for the SSH model. In other words, the normalized  $d$ -vector lives on  $S^1$ . Thanks to this restriction, or symmetry, each Hamiltonian in this class defines a mapping

$$S^1 \rightarrow S^1 \quad (7.1.2)$$

which is characterized by the winding number  $W^{(0)}$ . In the absence of the symmetry  $\{H, \sigma_z\} = 0$ , the  $d$ -vector could point anywhere on  $S^2$ . Mappings

$$S^1 \rightarrow S^2 \quad (7.1.3)$$

are all trivial, however, as any closed one-dimensional path defined by the image of  $S^1$  is smoothly contractible to a point. Hence, we cannot define a winding number in this case.

We can now attempt to use arbitrary symmetries for our classification task. In the present chapter we focus on three important local symmetries that we want to introduce carefully in the following. After their introduction we are in the position to outline our classification goals more precisely.

### 7.1.1 Anti-unitary symmetries

When we discuss symmetry constraints on possible equivalence relations between Hamiltonians we want to consider anti-unitary symmetries such as time reversal invariance with  $\mathcal{T}i\mathcal{T}^{-1} = -i$ . Simple local unitary symmetries  $S$  that commute with the Hamiltonian  $[H, S] = 0$  are not of interest for us in this chapter for the following reason: We could simply go to combined eigenstates of both the symmetry  $S$  and the Hamiltonian. We want to assume that we only deal with such block-diagonal Hamiltonians from the outset. If we deal with anti-unitary symmetries, we do not have the eigenstates at hand and we cannot use this program of decomposing  $H$  into symmetric sub-blocks. The same holds for unitary symmetries  $S$  that anti-commute with the Hamiltonian, i.e.,  $\{H, S\} = 0$ . We will see how such ‘‘symmetries’’ help us to classify topological insulators.

In the following, we use a first quantized language where we write the single particle Hamiltonian as

$$H = \sum_{AB} \psi_A^\dagger \mathcal{H}_{AB} \psi_B, \quad (7.1.4)$$

where  $A, B$  run over all relevant quantum numbers. The object of interest is the matrix  $\mathcal{H}_{AB}$ . In case we deal with superconducting problems the corresponding matrix is constructed from

the Nambu spinor

$$H = \sum_{AB} \begin{pmatrix} \psi_A^\dagger & \psi_{\bar{A}} \end{pmatrix} \mathcal{H}_{AB} \begin{pmatrix} \psi_B \\ \psi_{\bar{B}}^\dagger \end{pmatrix}. \quad (7.1.5)$$

Here  $A$  and  $\bar{A}$  correspond to the paired quantum numbers: For example for an  $s$ -wave superconductor  $A = (\mathbf{k}, \uparrow)$  and  $\bar{A} = (-\mathbf{k}, \downarrow)$ .

### Time reversal

Let us now start with the anti-unitary time reversal symmetry

$$\mathcal{T}: \quad U_{\mathcal{T}}^\dagger \mathcal{H}^* U_{\mathcal{T}} = \mathcal{H}, \quad \text{with} \quad U_{\mathcal{T}}^\dagger U_{\mathcal{T}} = \mathbb{1}, \quad (7.1.6)$$

for some unitary rotation  $U_{\mathcal{T}}$ . Using the second quantized language we find for these matrices

$$\mathcal{T} \psi_A \mathcal{T}^{-1} = \sum_B [U_{\mathcal{T}}]_{AB} \psi_B. \quad (7.1.7)$$

Applying this identity twice, and making use of the fact that  $\mathcal{T}$  is anti-unitary, we find

$$\mathcal{T}^2 \psi_A \mathcal{T}^{-2} = \sum_B [U_{\mathcal{T}}^* U_{\mathcal{T}}]_{AB} \psi_B = \pm \psi_A, \quad \text{i.e.,} \quad U_{\mathcal{T}}^* U_{\mathcal{T}} = \pm \mathbb{1}. \quad (7.1.8)$$

Here we used that  $\mathcal{T}^2 = -\mathbb{1}$  or  $\mathcal{T}^2 = \mathbb{1}$ , depending on whether we deal with systems of half-integer spins or not. The last equation can also be written as

$$U_{\mathcal{T}} = \pm U_{\mathcal{T}}^\top. \quad (7.1.9)$$

### Charge conjugation

The next (anti-) symmetry we consider is the charge-conjugation, or particle-hole symmetry

$$\mathcal{P}: \quad U_{\mathcal{P}}^\dagger \mathcal{H}^* U_{\mathcal{P}} = -\mathcal{H} \quad \text{with} \quad U_{\mathcal{P}}^\dagger U_{\mathcal{P}} = \mathbb{1}. \quad (7.1.10)$$

Where again we find  $U_{\mathcal{P}}$  via

$$\mathcal{P} \psi_A \mathcal{P}^{-1} = \sum_B [U_{\mathcal{P}}^*]_{AB} \psi_B^\dagger. \quad (7.1.11)$$

And also in this case we can either have

$$U_{\mathcal{P}} = \pm U_{\mathcal{P}}^\top, \quad (7.1.12)$$

depending on whether  $\mathcal{P}^2 = \pm \mathbb{1}$ . As this particle hole symmetry is slightly less standard than the time reversal symmetry, we give two concrete examples. First, the Hamiltonian of an  $s$ -wave superconductor can be written as

$$H = \sum_k \begin{pmatrix} c_{k\uparrow} & c_{k\downarrow} & c_{-k\uparrow}^\dagger & c_{-k\downarrow}^\dagger \end{pmatrix}^\dagger \underbrace{\begin{pmatrix} \xi(k) & 0 & 0 & \Delta_s \\ 0 & \xi(k) & -\Delta_s & 0 \\ 0 & -\Delta_s^* & -\xi(k) & 0 \\ \Delta_s^* & 0 & 0 & -\xi(k) \end{pmatrix}}_{\mathcal{H}_s} \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \\ c_{-k\uparrow}^\dagger \\ c_{-k\downarrow}^\dagger \end{pmatrix}. \quad (7.1.13)$$

This Hamiltonian has the anti-symmetry

$$U_{\mathcal{P}}^\dagger \mathcal{H}_s^* U_{\mathcal{P}} = -\mathcal{H}_s \quad \text{with} \quad U_{\mathcal{P}} = i\sigma_y \otimes \mathbb{1} \quad \text{and hence} \quad U_{\mathcal{P}} = -U_{\mathcal{P}}^\top. \quad (7.1.14)$$

On the other hand, a triplet superconductor can be of the form

$$H = \sum_k \left( c_{k\uparrow} \quad c_{k\downarrow} \quad c_{-k\uparrow}^\dagger \quad c_{-k,\downarrow}^\dagger \right)^\dagger \underbrace{\begin{pmatrix} \xi(k) & 0 & 0 & \Delta_t \\ 0 & \xi(k) & \Delta_t & 0 \\ 0 & \Delta_t^* & -\xi(k) & 0 \\ \Delta_t^* & 0 & 0 & -\xi(k) \end{pmatrix}}_{\mathcal{H}_t} \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \\ c_{-k\uparrow}^\dagger \\ c_{-k,\downarrow}^\dagger \end{pmatrix}. \quad (7.1.15)$$

Now the Hamiltonian has the anti-symmetry

$$U_{\mathcal{P}}^\dagger \mathcal{H}_t^* U_{\mathcal{P}} = -\mathcal{H}_t \quad \text{with} \quad U_{\mathcal{P}} = \sigma_x \otimes \mathbb{1} \quad \text{and hence} \quad U_{\mathcal{P}} = U_{\mathcal{P}}^T. \quad (7.1.16)$$

Note, that all Bogoliubov-de Gennes (BdG) Hamiltonians of mean-field superconductors have a  $\mathcal{P}$ -type symmetry built in by construction (via the Nambu formalism).

### Chiral symmetry

One more option is for the Hamiltonian to possess the following anti-symmetry

$$\mathcal{C} : \quad U_{\mathcal{C}}^\dagger \mathcal{H} U_{\mathcal{C}} = -\mathcal{H} \quad \text{with} \quad U_{\mathcal{C}}^\dagger U_{\mathcal{C}} = \mathbb{1}. \quad \text{and} \quad U_{\mathcal{C}}^2 = \mathbb{1}. \quad (7.1.17)$$

This symmetry is called chiral or *sub-lattice* symmetry as it often occurs on bipartite lattice models. Note, that whenever the system has a chiral symmetry and either a particle-hole or time-reversal, it actually possesses all three of them (show!).

## 7.2 The periodic table

Let us now classify all possible symmetry classes according to the above three ‘‘symmetries’’. For the time-reversal and particle-hole symmetry we have three options. Either there is no symmetry, one that squares to  $\mathbb{1}$ , or one that squares to  $-\mathbb{1}$ . We denote these cases with 0, 1,  $-1$ . Together, there are  $3 \times 3 = 9$  different options. Turning around the argument above that a  $\mathcal{P}$  ( $\mathcal{T}$ ) together with a  $\mathcal{C}$  type symmetry implies a  $\mathcal{T}$  ( $\mathcal{P}$ ) symmetry, we see that  $\mathcal{C} = \mathcal{P} \circ \mathcal{T}$ . Therefore, for all cases where either  $\mathcal{T}$  or  $\mathcal{P}$  are present the presence or absence of  $\mathcal{C}$  is fixed. Only if both particle-hole and time-reversal symmetry are absent,  $\mathcal{C}$  can be either present (1) or absent (0). This yields in total 10 different symmetry classes in Tab. 7.1. We would now like to achieve the following goals with respect to Tab. 7.1:

1. We know of three ways to construct this table. This amounts to understand the columns ‘‘target spaces’’. One can do this for systems only respecting the symmetries  $\mathcal{T}$ ,  $\mathcal{P}$ ,  $\mathcal{C}$ , i.e., for system with spatial disorder, or for Bloch Hamiltonians in lattice systems. We expose the latter in some detail, for the rest we refer to [3–5].
2. We would like to know how one can derive explicit formulas for indices characterizing the various entries in Tab. 7.1. We cover some of these derivations, for the rest we refer to [6].

Let us start with a quick summary of how to construct the table, not making use of translation symmetry.

### 7.2.1 Random matrices and non-linear sigma models

For now, we do not impose any further symmetries on the Hamiltonian, such as invariance under translations (a unitary symmetry). Hence, we should think of the Hamiltonian as a *random matrix subject to the symmetry constraint* of a given class. In a seminal work, Altland and Zirnbauer [4] established a one-to-one correspondence between the symmetry classes of

label	symmetry			target space			spatial dimension $d$							
	$\mathcal{T}$	$\mathcal{P}$	$\mathcal{C}$	$X_{\text{evol}}$	$X_{\sigma}$	$X_{\mathcal{Q}}$	1	2	3	4	5	6	7	8
the complex cases:														
A	0	0	0	$C_1$	$C_0$	$C_0$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AIII	0	0	1	$C_0$	$C_1$	$C_1$	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
the real cases:														
AI	1	0	0	$R_7$	$R_4$	$R_0$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
BDI	1	1	1	$R_0$	$R_3$	$R_1$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
D	0	1	0	$R_1$	$R_2$	$R_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
DIII	-1	1	1	$R_2$	$R_1$	$R_3$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0
AII	-1	0	0	$R_3$	$R_0$	$R_4$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$
CII	-1	-1	1	$R_4$	$R_7$	$R_5$	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
C	0	-1	0	$R_5$	$R_6$	$R_6$	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
CI	1	-1	1	$R_6$	$R_5$	$R_7$	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0

Table 7.1: Periodic table of topological insulators and superconductors.  $\mathbb{Z}_2$  and  $\mathbb{Z}$  denote binary and integer topological indices, respectively.  $2\mathbb{Z}$  denotes an even integer. The symmetries  $\mathcal{T}$ ,  $\mathcal{P}$  and  $\mathcal{C} = \mathcal{T} \circ \mathcal{P}$  are explained in the text. A zero denotes the absence of the symmetry and for  $\mathcal{T}$  and  $\mathcal{P}$ , the  $\pm 1$  indicates if these symmetries square to  $\pm 1$ . The target spaces are listed in Tab. 7.2

$C_0$	$C_1$	$R_0$	$R_1$	$R_2$	$R_3$	$R_4$	$R_5$	$R_6$	$R_7$
$\frac{U(n+m)}{U(n) \times U(m)}$	$U(n)$	$\frac{O(n+m)}{O(n) \times O(m)}$	$O(n)$	$\frac{O(2n)}{U(n)}$	$\frac{U(2n)}{Sp(n)}$	$\frac{Sp(n+m)}{Sp(n) \times Sp(m)}$	$Sp(n)$	$\frac{Sp(2n)}{U(n)}$	$\frac{U(n)}{O(n)}$

Table 7.2: List of target spaces used for the definition of the 10-fold way.

Hamiltonians and a classification of symmetric spaces in differential geometry that was obtained by Cartan (see Tab. 7.1 and Tab. 7.2).

Their work is an extension of a classification that goes back to Wigner and Dyson and relied on time-reversal symmetry alone. There are two complex classes which possess no anti-unitary symmetry and eight real classes with at least one anti-unitary symmetry. The nomenclature complex and real corresponds to the fact that the anti-unitary symmetries impose reality constraints for the elements of the latter classes, while the former can be represented by complex matrices.

The column  $X_{\text{evol}}$  of Tab. 7.1 lists the symmetric spaces  $X_{\text{evol}}$  to which the time-evolution operators  $\exp(-itH)$  of each class belong. While the columns noting the symmetries and the target spaces of Tab. 7.1 provide an exhaustive classification of noninteracting fermionic Hamiltonians into symmetry classes, it does as such not provide physical information. The physical manifestation of this classification lies in the correspondence between the topological sector of a bulk Hamiltonian and protected gapless modes at the boundary of the system.

Establishing this connection is the main result of Schnyder *et al.* [5]. It is achieved by studying the problem of Anderson localization of non-interacting electrons that are subject to static disorder potentials on the  $(d-1)$ -dimensional boundary of the system. For every given symmetry class and every dimension of space, they pose the following question: How many fermionic modes can exist on the boundary that are inert to Anderson localization? It is answered in

a long wavelength-approximation by studying non-linear sigma-model field theories. While we do not want to enter the discussion of non-linear sigma models here, we note that the result is determined by two ingredients, (i) the dimension  $d - 1$  of the boundary and (ii) the target space  $X_\sigma$  in which the dynamical field of the nonlinear sigma model lives. Remarkably, these target spaces are a permutation of the spaces  $X_{\text{evol}}$  of the time-evolution operator.<sup>1</sup>

### 7.2.2 Flatband Hamiltonians

Let us now move to understanding the target spaces  $X_Q$  in a bit more detail. In other words, we now consider on top of the local symmetries also translation symmetry. In particular, we want to exemplify how the symmetric spaces that are listed under  $X_Q$  in Tab. 7.1 arise in a physical context from symmetry constraints.

#### Class A

Let us start with the most generic case of class A, in which no symmetry constraints are imposed on the single-particle Hamiltonian. We consider a Hamiltonian  $H$  with the full translational invariance of continuous configuration space with periodic boundary conditions imposed. In second quantization, it has the Bloch representation

$$H = \int d^d \mathbf{k} \psi_\alpha^\dagger(\mathbf{k}) \mathcal{H}_{\alpha, \alpha'}(\mathbf{k}) \psi_{\alpha'}(\mathbf{k}), \quad (7.2.1)$$

where  $\psi_\alpha^\dagger(\mathbf{k})$  creates a fermion of flavor  $\alpha = 1, \dots, N$  at momentum  $\mathbf{k}$  in the Brillouin zone (BZ) and the summation over  $\alpha$  and  $\alpha'$  is implicit. The flavor index may represent orbital, spin, or sublattice degrees of freedom. Energy bands are obtained by diagonalizing the  $N \times N$  matrix  $\mathcal{H}(\mathbf{k})$  at every momentum  $\mathbf{k} \in \text{BZ}$  with the aid of a unitary transformation  $U(\mathbf{k})$

$$U^\dagger(\mathbf{k}) \mathcal{H}(\mathbf{k}) U(\mathbf{k}) = \text{diag} [\varepsilon_{m+n}(\mathbf{k}), \dots, \varepsilon_{n+1}(\mathbf{k}), \varepsilon_n(\mathbf{k}), \dots, \varepsilon_1(\mathbf{k})], \quad (7.2.2)$$

where the energies are arranged in descending order on the righthand side and  $n, m \in \mathbb{Z}$  such that  $n + m = N$ . So as to start from an insulating fermi-sea ground state, we assume that there exists an energy gap between the bands  $n$  and  $n + 1$  and that the chemical potential  $\mu$  lies in this gap

$$\varepsilon_n(\mathbf{k}) < \mu < \varepsilon_{n+1}(\mathbf{k}), \quad \forall \mathbf{k} \in \text{BZ}. \quad (7.2.3)$$

The presence of the gap allows us to adiabatically deform the Bloch Hamiltonian  $\mathcal{H}(\mathbf{k})$  to the flatband Hamiltonian

$$\mathcal{Q}(\mathbf{k}) := U(\mathbf{k}) \begin{pmatrix} \mathbb{1}_m & 0 \\ 0 & -\mathbb{1}_n \end{pmatrix} U^\dagger(\mathbf{k}) \quad (7.2.4)$$

that assigns the energy  $-1$  and  $+1$  to all states in the bands below and above the gap, respectively. This deformation preserves the eigenstates, but removes the non-universal information about energy bands from the Hamiltonian. In other words, the degenerate eigenspaces of the eigenvalues  $\pm 1$  of  $\mathcal{Q}(\mathbf{k})$  reflect the partitioning of the single-particle Hilbert space introduced by the spectral gap in the spectrum of  $\mathcal{H}(\mathbf{k})$ . The degeneracy of its eigenspaces equips  $\mathcal{Q}(\mathbf{k})$  with

<sup>1</sup>The result is that the number of boundary modes that are topologically protected against symmetry-preserving disorder at the  $(d - 1)$ -dimensional boundary belong to the homotopy group  $\pi_{d-1}(X_\sigma)$ , if  $\pi_{d-1}(X_\sigma) = \mathbb{Z}_2$  (in which case a so-called  $\mathbb{Z}_2$  term can be added to the nonlinear sigma model to prevent localization) and to the homotopy group  $\pi_d(X_\sigma)$ , if  $\pi_d(X_\sigma) = \mathbb{Z}$  (in which case a so-called Wess-Zumino-Witten term can be added to the nonlinear sigma model to prevent localization, for a given class  $X_\sigma$  and a given dimension  $d$  of space.

The homotopy group is a topological characterization of the symmetric space. Loosely speaking,  $\pi_d(X)$ ,  $d = 1, 2, \dots$ , of a symmetric space  $X$  is formed by homotopic equivalence classes of maps from the  $d$ -dimensional sphere to the symmetric space. Two such maps are homotopic if there exists a continuous function that deforms one map into the other. The homotopy groups for  $d = 1, \dots, 8$  are listed in Tab. 7.1.

an extra  $U(n) \times U(m)$  gauge symmetry: While the  $(n+m) \times (n+m)$  matrix  $U(\mathbf{k})$  of Bloch eigenvectors that diagonalizes  $\mathcal{Q}(\mathbf{k})$  is an element of  $U(n+m)$  for every  $\mathbf{k} \in \text{BZ}$ , we are free to change the basis for its lower and upper bands by a  $U(n)$  and  $U(m)$  transformation, respectively. Hence  $\mathcal{Q}(\mathbf{k})$  is an element of the symmetric space  $C_0$  defining a map

$$\mathcal{Q}: \text{BZ} \rightarrow C_0 = \frac{U(n+m)}{U(n) \times U(m)}. \quad (7.2.5)$$

The group of topologically distinct maps  $\mathcal{Q}$ , or, equivalently, the number of topologically distinct Hamiltonians  $\mathcal{H}$ , is given by the homotopy group

$$\pi_d(C_0) \quad (7.2.6)$$

for any dimension  $d$  of the BZ. For example, in  $d=2$  we have  $\pi_2(C_0) = \mathbb{Z}$ . A physical example of a family of Hamiltonians that exhausts the topological sectors of this group is found in the quantum Hall effect (QHE). The incompressible ground state with  $r \in \mathbb{N}$  filled Landau levels is topologically distinct from the ground state with  $\mathbb{N} \ni r' \neq r$  filled Landau levels. Two different patches of space with  $r$  and  $r'$  filled Landau levels have  $|r - r'|$  gapless edge modes running at their interface, reflecting the bulk-boundary correspondence of the topological phases. In contrast,  $\pi_3(C_0) = 0$  renders all noninteracting fermionic Hamiltonians in three dimensional space (3D) topologically equivalent to the vacuum, if no further symmetries are imposed.

### Class AIII

As a second example, let us discuss a Hamiltonian that has only chiral symmetry and hence belongs to the symmetry class AIII. As above, we assume translational invariance and work directly with the Bloch Hamiltonian  $\mathcal{H}(\mathbf{k})$  for  $\mathbf{k} \in \text{BZ}$ . The chiral symmetry implies a spectral symmetry of  $\mathcal{H}(\mathbf{k})$ . If gapped,  $\mathcal{H}(\mathbf{k})$  must have an even number of bands  $N = 2n$ ,  $n \in \mathbb{Z}$ . When represented in the eigenbasis of the chiral symmetry operator  $U_C$ , the spectrally flattened Hamiltonian  $\mathcal{Q}(\mathbf{k})$  and the chiral symmetry operator have the representations

$$\mathcal{Q}(\mathbf{k}) = \begin{pmatrix} 0 & q(\mathbf{k}) \\ q^\dagger(\mathbf{k}) & 0 \end{pmatrix}, \quad U_C = \begin{pmatrix} \mathbb{1}_n & 0 \\ 0 & -\mathbb{1}_n \end{pmatrix}, \quad (7.2.7a)$$

respectively. From  $\mathcal{Q}(\mathbf{k})^2 = 1$ , one concludes that  $q(\mathbf{k})$  can be an arbitrary unitary matrix. We are thus led to consider the homotopy group  $\pi_d(C_1)$  of the mapping

$$q: \text{BZ} \rightarrow C_1 = U(n). \quad (7.2.7b)$$

For example, in  $d=3$  spatial dimensions  $\pi_3(C_1) = \mathbb{Z}$ .

With these examples, we have discussed the two complex classes A and AIII. In the real classes, which have at least one antiunitary symmetry, it is harder to obtain the constraints on the spectrally flattened Hamiltonian  $\mathcal{Q}(\mathbf{k})$ . Further, if TRS and PHS are constraining the system, the space of  $\mathcal{Q}(\mathbf{k})$ ,  $X_{\mathcal{Q}}$ , and the target space of the nonlinear sigma model,  $X_{\sigma}$ , do not agree anymore with one another (see Tab. 7.1). The origin for this complication is that the antiunitary symmetry relates  $\mathcal{Q}(\mathbf{k})$  and  $\mathcal{Q}(-\mathbf{k})$  rather than acting locally in momentum space.

One last comment is in order: The homotopy groups of symmetric spaces, as arranged in Tab. 7.1 follow a regular periodic pattern as pointed out by Kitaev, the so-called Bott periodicity. That is, the table is periodic under a shift in  $d$  with period two and eight for the complex and real cases, respectively. More precisely,  $\pi_d(R_q)$ , with  $q$  understood modulo 8, depends only on  $q+d$

$$\pi_d(R_q) = \pi_{d-p}(R_{q+p}), \quad p \in \mathbb{Z}. \quad (7.2.8)$$



### 7.2.3 $\mathbb{Z}$ topological invariants

As mentioned in the last section, for situations other than class A and AIII with relatively simple target spaces, it becomes difficult to work directly with the flat band Hamiltonians  $\mathcal{Q}(\mathbf{k})$ . Therefore, we want to shift gears and approach the complete classification in a way more directly related to differential geometry. To this end, let us quickly remind ourselves of the Gauss-Bonnet theorem for Riemannian manifolds before we extend it to our case of Bloch bands. For convenience, we restrict ourselves to translation invariant systems. All results can be extended to weakly disordered systems, however [3].

In physics, topological attributes refer to *global* properties of physical system that is made out of *local* degrees of freedom and might only have local, i.e., short-ranged, correlations. This parallels the distinction between topology and geometry in mathematics, where the former refers to global structure, while the latter refers to local structure of objects. In differential geometry, a bridge between topology and geometry is given by the Gauss-Bonnet theorem. It states that for compact 2D Riemannian manifolds  $M$  without boundary, the integral over the Gaussian curvature  $F(\mathbf{x})$  of the manifold is (i) integer and (ii) a topological invariant

$$2(1 - g) = \frac{1}{2\pi} \int_M d^2\mathbf{x} F(\mathbf{x}). \quad (7.2.9)$$

Here,  $g$  is the genus of  $M$ , e.g.,  $g = 0$  for a 2D sphere and  $g = 1$  for a 2D torus. The Gaussian curvature  $F(\mathbf{x})$  can be defined as follows. Attach to every point on  $M$  the tangential plane, a two-dimensional vector space (The collection of these tangential spaces is called a vector bundle.). Take some vector from the tangential plane at a given point on  $M$  and parallel transport it around a closed loop on  $M$ . The angle mismatch of the vector before and after the transport is proportional to the Gaussian curvature enclosed in the loop.

In the physical systems that we want to describe, the manifold  $M$  is the BZ and the analogue of the tangential plane on  $M$  is a space spanned by the Bloch states at a given momentum  $\mathbf{k} \in \text{BZ}$ . Let us state this fact more precisely. We have seen in Sec. 7.2.2 that the Bloch Hamiltonian defines a mapping from the BZ to some symmetric space. The single-particle Hilbert space  $\mathfrak{H}_0$  is the  $N$ -dimensional projective space over the complex numbers at every momentum  $\mathbf{k} \in \text{BZ}$ . The Bloch states of the  $n < N$  filled bands span at every momentum  $\mathbf{k} \in \text{BZ}$  an  $n$ -dimensional space  $\mathfrak{h}_{\mathbf{k}}$  that is a subspace of  $\mathfrak{H}_0$ . In mathematical terms, the  $\mathfrak{h}_{\mathbf{k}}$  as a set form a vector bundle over the BZ. In contrast to the example from differential geometry above, the ‘‘tangent space’’  $\mathfrak{h}_{\mathbf{k}}$  is not a Riemannian metric space and can thus no longer be embedded in the same space as the manifold  $M$  itself. At the same time, the Gaussian curvature is generalized to a curvature form, that is called Berry curvature  $F$  in physics. In our case, it is given by an  $n \times n$  matrix of differential forms that is defined via the Berry connection  $A$  as

$$F := \mathcal{F}_{ij}(\mathbf{k}) dk_i \wedge dk_j \quad (7.2.10a)$$

$$\mathcal{F}_{ij}(\mathbf{k}) := \partial_i \mathcal{A}_j(\mathbf{k}) - \partial_j \mathcal{A}_i(\mathbf{k}) - i[\mathcal{A}_i(\mathbf{k}), \mathcal{A}_j(\mathbf{k})], \quad i, j = 1, \dots, d, \quad (7.2.10b)$$

$$A := \mathcal{A}_i(\mathbf{k}) dk_i, \quad (7.2.10c)$$

$$\mathcal{A}_i^{(ab)}(\mathbf{k}) := i \sum_{\alpha=1}^N U_{\alpha\alpha}^\dagger(\mathbf{k}) \partial_i U_{\alpha b}(\mathbf{k}), \quad a, b = 1, \dots, n, \quad i = 1, \dots, d. \quad (7.2.10d)$$

The unitary transformation  $U(\mathbf{k})$  that diagonalizes the Hamiltonian was defined in Eq. (7.2.2), both  $\mathcal{A}_i(\mathbf{k})$  and  $\mathcal{F}_{ij}(\mathbf{k})$  are  $n \times n$  matrices, we write  $\partial_i \equiv \partial/\partial k_i$  and the sum over repeated spatial coordinate components  $i, j$  is implicit.

Under a local  $U(n)$  gauge transformation in momentum space that acts on the states of the lower bands and is parametrized by the  $n \times n$  matrix  $G(\mathbf{k})$

$$U_{\alpha a}(\mathbf{k}) \longrightarrow U_{\alpha b}(\mathbf{k}) G_{ba}(\mathbf{k}), \quad \alpha = 1, \dots, N, \quad a = 1, \dots, n, \quad (7.2.11a)$$

the Berry connection  $A$  changes as

$$A \longrightarrow G^\dagger A G + iG^\dagger dG, \quad (7.2.11b)$$

while the Berry curvature  $F$  changes covariantly

$$F \longrightarrow G^\dagger F G, \quad (7.2.11c)$$

leaving its trace invariant.

For the spatial dimension  $d = 2$ , the generalization of the Gauss-Bonnet theorem (7.2.9) in algebraic topology was found by Chern to be

$$\begin{aligned} 2C^{(1)} &:= \frac{1}{2\pi} \int_{\text{BZ}} \text{tr} F \\ &= 2 \frac{1}{2\pi} \int_{\text{BZ}} d^2 \mathbf{k} \text{tr} \mathcal{F}_{12}. \end{aligned} \quad (7.2.12)$$

This defines a gauge-invariant quantity, the first Chern number  $C^{(1)}$ . Remarkably,  $C^{(1)}$  can only take integer values: It counts the number of vortices of the vector field  $\text{tr} [\mathcal{A}(\mathbf{k})]$  in the BZ.

### Without chiral symmetry

In order to obtain a topological invariant for any even dimension  $d = 2s$  of space, we can use the  $s$ -th power of the Berry field  $F$  to build a gauge invariant  $d$ -form that can be integrated over the BZ to obtain scalar (0-form). Upon taking the trace, this scalar is invariant under the gauge transformation (7.2.11a) and defines the  $s$ -th Chern number

$$2C^{(s)} := \frac{1}{s!} \left( \frac{1}{2\pi} \right)^s \int_{\text{BZ}} \text{tr} [F^s], \quad (7.2.13)$$

where  $F^s = F \wedge \cdots \wedge F$ . As with the case  $s = 1$  that we have exemplified above,  $C^{(s)}$  is integer for any  $s = 1, 2, \dots$ . This can be understood as follows. Locally in the BZ, for any  $s = 1, 2, \dots$ , the integrand of Eq. (7.2.13) can be written as differential of a  $(d - 1)$  differential form, the so-called Chern-Simons form  $Q^{(s)}$ ,

$$\text{tr} [F^s] = \text{tr} [dQ^{(s)}]. \quad (7.2.14)$$

The lowest order Chern-Simons forms are given by

$$Q^{(1)} := A, \quad (7.2.15a)$$

$$Q^{(2)} := A \wedge dA - \frac{2i}{3} A \wedge A \wedge A, \quad (7.2.15b)$$

$$Q^{(3)} := dA \wedge dA \wedge A - \frac{3i}{2} dA \wedge A \wedge A \wedge A - \frac{3}{5} A \wedge A \wedge A \wedge A \wedge A. \quad (7.2.15c)$$

Unlike  $F$ ,  $Q^{(s)}$  depends on the gauge choice. If the Chern number is non-vanishing, there is an obstruction to define  $Q^{(s)}$  globally over the BZ, i.e., to define a globally smooth gauge. (Otherwise, the Chern number would vanish due to Stoke's theorem.) The dual form to  $Q^{(s)}$  can be regarded as a  $d$ -dimensional vector field on the BZ. The Chern number  $C^{(s)}$  simply counts the number of point-like singularities in this vector field on the BZ in a given gauge and is hence integer.

From inspection of Tab. 7.1 we see that symmetry classes without chiral symmetry may have integer topological invariants  $\mathbb{Z}$  only when the dimension  $d$  of space is even. In fact, all the integer invariants of these classes are given by the Chern number  $C^{(s)}$  of the respective dimension. However, not for every even dimension does every symmetry class have a  $\mathbb{Z}$  homotopy group. This is in one-to-one correspondence to the vanishing of the Chern numbers under some symmetry constraints, as we will now explain.

**Class A** The Chern numbers are the topological invariants that characterize a Hamiltonian without symmetry constraints in symmetry class A for *every* even dimension  $d = 2s$ .

**Classes AI and AII** If TRS but no PHS is present, as it is the case for classes AI and AII, both the Berry connection and the Berry field satisfy

$$\mathcal{A}_i(\mathbf{k}) = +\mathcal{A}_i^\top(-\mathbf{k}), \quad i = 1, \dots, d, \quad (7.2.16a)$$

$$\mathcal{F}_{ij}(\mathbf{k}) = -\mathcal{F}_{ij}^\top(-\mathbf{k}), \quad i, j = 1, \dots, d. \quad (7.2.16b)$$

As a consequence, if  $s$  is odd, the integrand in Eq. (7.2.13) is an odd function of momentum and the Chern number vanishes. In contrast, if  $s = 2s'$ ,  $s' \in \mathbb{Z}$ , such that  $d = 4s'$ , there is no reason for  $\mathcal{C}^{(2s')}$  to vanish. Indeed  $\mathcal{C}^{(2s')}$  is the integer topological invariant for classes AI and AII *whenever*  $d = 4s'$ .

**Classes C and D\*** Let us now consider the symmetry classes with PHS but no TRS. If PHS is present, as it is the case for classes C and D, the spectrum of the Hamiltonian is symmetric about the Fermi energy, supporting as many bands below it as above it. The Berry field of the lower bands  $\mathcal{F}$  is related to the Berry field of the upper bands  $\tilde{\mathcal{F}}$

$$\mathcal{F}_{ij}(\mathbf{k}) = -\tilde{\mathcal{F}}_{ij}^\top(-\mathbf{k}), \quad i, j = 1, \dots, d. \quad (7.2.17)$$

It follows that the Chern number of the lower bands  $\mathcal{C}^{(s)}$  and the Chern number of the upper bands  $\tilde{\mathcal{C}}^{(s)}$  [given by Eq. (7.2.13) with  $\mathcal{F}_{ij}$  replaced by  $\tilde{\mathcal{F}}_{ij}$ ] are related by

$$\mathcal{C}^{(s)} = (-1)^s \tilde{\mathcal{C}}^{(s)}. \quad (7.2.18)$$

Further, the topological sector of the full system must be trivial

$$\mathcal{C}^{(s)} + \tilde{\mathcal{C}}^{(s)} = 0. \quad (7.2.19)$$

We conclude from Eqs. (7.2.18) and (7.2.19) that whenever  $s$  is even, the Chern number  $\mathcal{C}^{(s)}$  vanishes. In contrast, if  $s = 2s' + 1$ ,  $s' \in \mathbb{Z}$ , such that  $d = 4s' + 2$  there is no reason for  $\mathcal{C}^{(2s'+1)}$  to vanish. Indeed  $\mathcal{C}^{(2s'+1)}$  is the integer topological invariant for classes C and D *whenever*  $d = 4s' + 2$ .

### With chiral symmetry

In systems with chiral symmetry the energy spectrum is symmetric about the Fermi energy, and there exists a *unitary* transformation  $U_C$  that maps states from the lower bands to the upper bands. As a consequence, the Berry field of the lower bands  $\mathcal{F}$  is related to the Berry field of the upper bands  $\tilde{\mathcal{F}}$

$$\mathcal{F}_{ij}(\mathbf{k}) = \tilde{\mathcal{F}}_{ij}(\mathbf{k}), \quad i, j = 1, \dots, d. \quad (7.2.20)$$

It follows that the Chern number of the lower bands  $\mathcal{C}^{(s)}$  and the Chern number of the upper bands  $\tilde{\mathcal{C}}^{(s)}$  are equal

$$\mathcal{C}^{(s)} = \tilde{\mathcal{C}}^{(s)}. \quad (7.2.21)$$

This is at odds with the fact that the topological sector of the full system must be trivial [see Eq. (7.2.19)]. We conclude that the Chern numbers of any system with chiral symmetry vanish

$$\mathcal{C}^{(s)} = 0. \quad (7.2.22)$$

However, the chiral symmetry allows us to define an alternative topological characterization. To see how it arises as a natural extension of the above, we consider a different representation of

the Chern numbers  $C^{(s)}$ . In terms of the flatband projector Hamiltonian  $\mathcal{Q}(\mathbf{k})$  that was defined in Eq. (7.2.4), we can write

$$C^{(s)} \propto \varepsilon_{i_1 \dots i_d} \int_{\text{BZ}} d^d \mathbf{k} \operatorname{tr} \left[ \mathcal{Q}(\mathbf{k}) \partial_{i_1} \mathcal{Q}(\mathbf{k}) \cdots \partial_{i_d} \mathcal{Q}(\mathbf{k}) \right], \quad d = 2s. \quad (7.2.23)$$

The form of Eq. (7.2.23) allows to interpret  $C^{(s)}$  as the *winding number* of the unitary transformation  $\mathcal{Q}(\mathbf{k})$  over the compact  $\text{BZ}^2$ . One verifies that  $C^{(s)} = 0$  for symmetry classes with chiral symmetry by inserting  $U_C U_C^\dagger$  at some point in the expression and anticommuting  $U_C$  with all  $\mathcal{Q}$ , using the cyclicity of the trace. After  $2s + 1$  anticommutations, we are back to the original expression up to an overall minus sign and found  $C^{(s)} = -C^{(s)}$  implying Eq. (7.2.22).

In odd dimensions of space, we can define a topological invariant by modifying Eq. (7.2.23) and using the chiral operator  $U_C$

$$\begin{aligned} W^{(s)} &:= \frac{(-1)^s s!}{2(2s+1)!} \left( \frac{i}{2\pi} \right)^{s+1} \varepsilon_{i_1 \dots i_d} \int_{\text{BZ}} d^d \mathbf{k} \operatorname{tr} \left[ U_C \mathcal{Q}(\mathbf{k}) \partial_{i_1} \mathcal{Q}(\mathbf{k}) \cdots \partial_{i_d} \mathcal{Q}(\mathbf{k}) \right] \\ &= \frac{(-1)^s s!}{(2s+1)!} \left( \frac{i}{2\pi} \right)^{s+1} \varepsilon_{i_1 \dots i_d} \int_{\text{BZ}} d^d \mathbf{k} \operatorname{tr} \left[ q(\mathbf{k}) \partial_{i_1} q^\dagger(\mathbf{k}) \partial_{i_2} q(\mathbf{k}) \cdots \partial_{i_d} q^\dagger(\mathbf{k}) \right], \quad d = 2s + 1. \end{aligned} \quad (7.2.31)$$

By anticommuting the chiral operator  $U_C$  once with all matrices  $\mathcal{Q}$  and using the cyclicity of the trace, one finds that the expression for  $W^{(s)}$  vanishes for even dimensions. The second line

<sup>2</sup>Let us illustrate for the first Chern number the equivalence of the characterizations in terms of the Berry curvature and the flatband Hamiltonian  $\mathcal{Q}(\mathbf{k})$ . The Berry connection is  $\mathcal{A}_i^{(\alpha\beta)}(\mathbf{k}) = i \langle \alpha | \partial_i | \beta \rangle$ , where  $|\alpha\rangle$  and  $|\beta\rangle$  are occupied bands. The Berry curvature can then be written as:

$$\mathcal{F}_{ij}^{(\alpha\beta)} = i (\langle \partial_i \alpha | \partial_j \beta \rangle - \langle \partial_j \alpha | \partial_i \beta \rangle) - i \sum_{\gamma=1}^n (\langle \partial_i \alpha | \gamma \rangle \langle \gamma | \partial_j \beta \rangle - \langle \partial_j \alpha | \gamma \rangle \langle \gamma | \partial_i \beta \rangle). \quad (7.2.24)$$

We can insert the identity resolution  $\sum_{\gamma=1}^N |\gamma\rangle \langle \gamma|$  in the first two terms such that only the sum over un-occupied bands survives:

$$\mathcal{F}_{ij}^{(\alpha\beta)} = i \sum_{\gamma=n+1}^N (\langle \partial_i \alpha | \gamma \rangle \langle \gamma | \partial_j \beta \rangle - \langle \partial_j \alpha | \gamma \rangle \langle \gamma | \partial_i \beta \rangle) \quad (7.2.25)$$

and

$$\mathcal{F}_{ij} = \sum_{\alpha, \beta=1}^n |\alpha\rangle F_{ij}^{(\alpha\beta)} \langle \beta| = i \varepsilon_{ij} (\partial_i P_-) P_+ (\partial_j P_-), \quad (7.2.26)$$

where we introduced the projectors on the occupied bands  $P_- = \sum_{\gamma=1}^n |\gamma\rangle \langle \gamma|$  and on the unoccupied ones  $P_+ = \sum_{\gamma=n+1}^N |\gamma\rangle \langle \gamma|$ . Note that we have  $\mathcal{Q} = P_+ - P_-$  and  $P_-^2 = P_-$ ,  $P_+^2 = P_+$ . Since  $P_-^2 = P_-$ , we have:

$$\partial_i P_- = \partial_i P_-^2 = P_- \partial_i P_- + (\partial_i P_-) P_-, \quad (7.2.27)$$

from which follows:

$$\partial_i P_- (\mathbb{1} - P_-) = (\partial_i P_-) P_+ = P_- \partial_i P_-. \quad (7.2.28)$$

We can then write

$$\operatorname{tr} [\mathcal{F}_{ij}] = i \varepsilon_{ij} \operatorname{tr} [P_- \partial_i P_- \partial_j P_-]. \quad (7.2.29)$$

Here, we managed to express the trace of the Berry curvature in terms of the projector unto the occupied bands. Let us now see how we can reach a final expression in terms of the flatband Hamiltonian  $\mathcal{Q}$ . We first notice how  $\mathcal{Q} = \mathbb{1} - 2P_-$ , hence all derivative operators satisfy  $\partial_i \mathcal{Q} = -2\partial_i P_-$ . We then have

$$\varepsilon_{ij} \operatorname{tr} [\mathcal{Q} \partial_i \mathcal{Q} \partial_j \mathcal{Q}] = \varepsilon_{ij} \operatorname{tr} [4(\mathbb{1} - 2P_-) \partial_i P_- \partial_j P_-] = -8 \varepsilon_{ij} \operatorname{tr} [P_- \partial_i P_- \partial_j P_-], \quad (7.2.30)$$

where the terms with  $\mathbb{1}$  vanishes because of the cyclicity of the trace and the antisymmetric tensor  $\varepsilon_{ij}$ . We hence succeeded in expressing the first Chern number in terms of the flatband Hamiltonian  $\mathcal{Q}$ . Similar calculations prove the validity of Eq. (7.2.23) for higher Chern numbers.

of Eq. (7.2.31) allows to interpret  $W^{(s)}$  as the *winding number* of the unitary off-diagonal part of the chiral Hamiltonian  $q(\mathbf{k})$  that was defined in Eq. (7.2.7a).

**Class AIII** The chiral winding numbers defined in Eq. (7.2.31) are the topological invariants that characterize a Hamiltonian without symmetry constraints other than chiral symmetry in symmetry class AIII for *every* odd dimension  $d = 2s + 1$ .

**Classes BDI and CII\*** If both TRS and PHS are present and  $\mathcal{P}^2 = \mathcal{T}^2$  as it is the case for classes BDI and CII, the flatband Hamiltonian  $\mathcal{Q}$  that enters Eq. (7.2.31) satisfies

$$U_{\mathcal{P}}\mathcal{Q}(\mathbf{k})U_{\mathcal{P}}^{-1} = -\mathcal{Q}^{\top}(-\mathbf{k}), \quad (7.2.32a)$$

$$U_{\mathcal{T}}\mathcal{Q}(\mathbf{k})U_{\mathcal{T}}^{-1} = +\mathcal{Q}^{\top}(-\mathbf{k}). \quad (7.2.32b)$$

Furthermore,

$$U_{\mathcal{T}} = \pm U_{\mathcal{T}}^{\top}, \quad U_{\mathcal{T}}^{-1} = \pm (U_{\mathcal{T}}^{-1})^{\top}, \quad (7.2.33)$$

with the sign given by  $\mathcal{T}^2$ . The same relations hold for  $U_{\mathcal{P}}$ . As a consequence, the chiral operator  $U_{\mathcal{C}} = U_{\mathcal{T}}(U_{\mathcal{P}}^{-1})^{\top}$  transforms as

$$U_{\mathcal{T}}^{-1}U_{\mathcal{C}}U_{\mathcal{T}} = (\mathcal{P}^2\mathcal{T}^2)U_{\mathcal{C}}^{\top}. \quad (7.2.34)$$

Using the time-reversal symmetry of  $\mathcal{Q}$  in Eq. (7.2.31) yields, for  $d$  odd,

$$\begin{aligned} W^{(s)} &= \frac{(-1)^s s!}{2(2s+1)!} \left(\frac{i}{2\pi}\right)^{s+1} \varepsilon_{i_1 \dots i_d} \int_{\text{BZ}} d^d \mathbf{k} \operatorname{tr} \left[ U_{\mathcal{T}}^{-1} U_{\mathcal{C}} U_{\mathcal{T}} \mathcal{Q}^{\top}(-\mathbf{k}) \partial_{i_1} \mathcal{Q}^{\top}(-\mathbf{k}) \dots \partial_{i_d} \mathcal{Q}^{\top}(-\mathbf{k}) \right] \\ &= \frac{(-1)^s s!}{2(2s+1)!} \left(\frac{i}{2\pi}\right)^{s+1} \varepsilon_{i_1 \dots i_d} \int_{\text{BZ}} d^d \mathbf{k} \operatorname{tr} \left[ (\mathcal{P}^2 \mathcal{T}^2) U_{\mathcal{C}} \mathcal{Q}(\mathbf{k}) \partial_{i_d} \mathcal{Q}(\mathbf{k}) \dots \partial_{i_1} \mathcal{Q}(\mathbf{k}) \right] \\ &= (-1)^s W^{(s)}, \quad d = 2s + 1, \end{aligned} \quad (7.2.35)$$

where we used that  $\mathcal{Q}$  anticommutes with  $U_{\mathcal{C}}$ . If  $s$  is odd, as is the case for  $d = 3$ ,  $W^{(s)}$  is bound to vanish for the classes BDI and CII. In contrast, if  $s = 2s'$ ,  $s' \in \mathbb{Z}$ , such that  $d = 4s' + 1$ , there is no reason for  $W^{(s)}$  to vanish. Indeed,  $W^{(s)}$  is the integer topological invariant for classes BDI and CII *whenever*  $d = 4s' + 1$ .

**Classes CI and DIII\*** If both TRS and PHS are present and  $\mathcal{P}^2 = -\mathcal{T}^2$  as it is the case for classes CI and DIII, the manipulations of Eq. (7.2.35) still apply, except for the last equality. As  $\mathcal{P}^2 \mathcal{T}^2 = -1$ , it now reads

$$W^{(s)} = (-1)^{s+1} W^{(s)}, \quad d = 2s + 1. \quad (7.2.36)$$

We conclude that  $W^{(s)}$  is the integer topological invariant for classes CI and DIII *whenever*  $d = 4s' + 3$ , while it vanishes otherwise.

In summary, we have now given explicit formulas for the topological invariants for all entries  $\mathbb{Z}$  in Tab. 7.1.

### 7.2.4 Dimensional reduction: $\mathbb{Z}_2$ topological invariants

In this section, we will discuss explicit formulas for all entries  $\mathbb{Z}_2$  in Tab. 7.1. By inspection of Tab. 7.1, we notice that  $\mathbb{Z}_2$  always appears one or two dimensions lower than an entry  $\mathbb{Z}$ . We will see that the system with  $\mathbb{Z}$  is in a sense a parent system from which the lower dimensional  $\mathbb{Z}_2$  topological insulators and superconductors, the first and second descendants, can be deduced. First, we will review these dimensional reduction arguments for the real symmetry classes with chiral symmetry. In contrast, for the real symmetry classes without chiral symmetry, we are going to derive more accessible formulas for the topological invariants that do not rely on dimensional reduction.

#### With chiral symmetry

**First descendants** For the real classes with chiral symmetry (classes BDI, CI, CII, DIII), we will sketch the so-called dimensional reduction procedure. As an underlying invariant, we will use the winding number  $W^{(s)}[q]$  defined for the off-diagonal projector  $q$  in  $(2s + 1)$ -dimensional space in Eq. (7.2.31). In  $d = 2s$  dimensions, we can define a relative index between two systems described by the projectors  $q_1(\mathbf{k})$  and  $q_2(\mathbf{k})$  by constructing an interpolation  $q(\mathbf{k}, t)$  that depends on the parameter  $t \in [0, \pi]$  such that

$$q(\mathbf{k}, t = 0) = q_1(\mathbf{k}), \quad q(\mathbf{k}, t = \pi) = q_2(\mathbf{k}). \quad (7.2.37)$$

This interpolation is extended for parameter values  $t \in [-\pi, 0]$  by demanding that the flatband Hamiltonian  $\mathcal{Q}(\mathbf{k}, t)$  associated with  $q(\mathbf{k}, t)$  satisfies the symmetry constraints of the symmetry class that  $q_1(\mathbf{k})$  and  $q_2(\mathbf{k})$  belong to in the  $(2s + 1)$ -dimensional space spanned by  $\mathbf{k}$  and  $t$ . Then, the winding number  $W^{(s)}[q]$  is well defined. We can now show that the parity of this winding number is independent of the parametrization  $q(\mathbf{k}, t)$ . To see this, consider a second parametrization  $q'(\mathbf{k}, t)$  that also satisfies Eq. (7.2.37) and the symmetry constraints of the respective class. Define further the two "twisted" interpolations

$$\tilde{q}(\mathbf{k}, t) := \begin{cases} q(\mathbf{k}, -t) & t \in [-\pi, 0] \\ q'(\mathbf{k}, t) & t \in (0, \pi] \end{cases}, \quad \tilde{q}'(\mathbf{k}, t) := \begin{cases} q'(\mathbf{k}, t) & t \in [-\pi, 0] \\ q(\mathbf{k}, -t) & t \in (0, \pi] \end{cases}. \quad (7.2.38)$$

From this definition of  $\tilde{q}(\mathbf{k}, t)$  and  $\tilde{q}'(\mathbf{k}, t)$  follows the equality

$$W^{(s)}[q] - W^{(s)}[q'] = W^{(s)}[\tilde{q}] + W^{(s)}[\tilde{q}']. \quad (7.2.39)$$

Further, with the help of TRS, following the steps in Eq. (7.2.35), one can show that  $W^{(s)}[\tilde{q}] = W^{(s)}[\tilde{q}']$ . Hence, the winding numbers of any two symmetry-respecting interpolations between  $q_1(\mathbf{k})$  and  $q_2(\mathbf{k})$  share the same parity. We can use this parity to define two equivalence classes of Hamiltonians  $q(\mathbf{k})$  in each of the symmetry classes BDI, CI, CII, and DIII. We are thus lead to define the parity

$$\nu_1[q_1, q_2] := (-1)^{W^{(s)}[q]} \in \{1, -1\}, \quad (7.2.40)$$

with  $q$  being any symmetry-respecting interpolation between  $q_1$  and  $q_2$ . The winding number  $W^{(s)}$  of an interpolation between any two trivial Hamiltonians (Hamiltonians without  $\mathbf{k}$ -dependence) vanishes. Thus, the parity of a given off-diagonal projector  $q_1(\mathbf{k})$  with any trivial reference off-diagonal projector  $q_0$

$$\nu_1[q_1, q_0] \equiv \nu_1[q_1] \quad (7.2.41)$$

constitutes the  $\mathbb{Z}_2$  invariant for  $q_1(\mathbf{k})$ , with  $\nu_1 = +1$  being the topologically trivial class.

**Second descendants\*** We continue to derive the  $\mathbb{Z}_2$  classification of the second descendants for the symmetry classes BDI, CI, CII, and DIII. To this end, consider a pair of off-diagonal projectors  $q_a(\mathbf{k})$  and  $q_b(\mathbf{k})$  that belong to the same symmetry class and are defined in a  $(d = 2s - 1)$ -dimensional BZ. We define two interpolations  $q_1(\mathbf{k}, r)$  and  $q_2(\mathbf{k}, r)$  that are parametrized by  $r \in [0, \pi]$  such that

$$q_i(\mathbf{k}, r = 0) = q_a(\mathbf{k}), \quad q_i(\mathbf{k}, r = \pi) = q_b(\mathbf{k}), \quad i = 1, 2. \quad (7.2.42)$$

Again, these interpolations are extended for parameter values  $t \in [-\pi, 0]$  by demanding that the flatband Hamiltonians  $\mathcal{Q}_i(\mathbf{k}, r)$  associated with  $q_i(\mathbf{k}, r)$ ,  $i = 1, 2$ , satisfy – in the  $2s$ -dimensional space spanned by  $\mathbf{k}$  and  $r$  – the symmetry constraints of the symmetry class that  $q_a(\mathbf{k})$  and  $q_b(\mathbf{k})$  belong to. Then, the parities  $\nu_1[q_1]$  and  $\nu_1[q_2]$  are well defined via Eq. (7.2.41). The crucial point is that one can now show  $\nu_1[q_1] = \nu_1[q_2]$ , that is,  $\nu_1[q]$  is independent of the interpolation (7.2.42) and depends only on the endpoints  $q_a(\mathbf{k})$  and  $q_b(\mathbf{k})$ . To see this, consider an interpolation  $q(\mathbf{k}, r, t)$  between the interpolations, parametrized by  $t \in [0, \pi]$  such that

$$q(\mathbf{k}, r, t = 0) = q_1(\mathbf{k}, r), \quad q(\mathbf{k}, r, t = \pi) = q_2(\mathbf{k}, r), \quad r \in [-\pi, \pi]. \quad (7.2.43)$$

As before,  $q(\mathbf{k}, r, t)$  is extended to the interval  $t \in [-\pi, 0]$  such that it satisfies the symmetry constraints of the respective class. We have shown in Eq. (7.2.39) that the parity  $\nu_1[q_1, q_2]$ , computed using Eq. (7.2.40), is independent of the particular choice of interpolation (7.2.37). It follows from Eq. (7.2.37) that

$$q(\mathbf{k}, r = 0, t) = q_a(\mathbf{k}), \quad q(\mathbf{k}, r = \pi, t) = q_b(\mathbf{k}), \quad t \in [-\pi, \pi], \quad (7.2.44)$$

which is independent of  $t$ . We might thus as well think of  $\nu_1[q_1, q_2]$  that is computed using Eq. (7.2.40) as a relative parity of the second descendants

$$\nu_2[q_a, q_b] := (-1)^{W^{(s)}[q]} \in \{1, -1\}, \quad (7.2.45)$$

if  $q(\mathbf{k}, r, t)$  satisfies Eq. (7.2.44) and the respective symmetry constraints. This constitutes the  $\mathbb{Z}_2$  index of the second descendants.

### Without chiral symmetry\*

For real symmetry classes without chiral symmetry, i.e., classes AI, AII, C, and D, the  $\mathbb{Z}_2$  invariant is related to the Chern number in one or two dimensions higher. Thus, one could apply the exactly same arguments that lead to Eqs. (7.2.40) and (7.2.45), if one replaces the winding number  $W^{(s)}$  by the Chern number  $C^{(s)}$  of the Hamiltonian. However, to arrive at more explicit formulas for the  $\mathbb{Z}_2$  invariants, we will depart from this strategy.

**First descendants** We consider in  $(d = 2s - 1)$ -dimensional space the flatband Hamiltonian  $\mathcal{Q}(\mathbf{k})$  that we want to study and a reference flatband Hamiltonian  $\mathcal{Q}_0$  that belongs to the same symmetry class as  $\mathcal{Q}(\mathbf{k})$ , but has no momentum dependence. Instead of constructing an interpolation between these two systems on the level of the Hamiltonians, as was done in the case of the chiral class, let us propose an explicit interpolation between the Berry connection  $A$  associated with  $\mathcal{Q}(\mathbf{k})$  and the vanishing Berry connection of  $\mathcal{Q}_0$ . The interpolating Berry connection  $\tilde{A}$  depends on the extra parameter  $t \in [-\pi, \pi]$  and reads

$$\tilde{A} := \frac{|t|}{\pi} A, \quad (7.2.46a)$$

with

$$\begin{aligned} \tilde{F} &:= d\tilde{A} - i\tilde{A} \wedge \tilde{A} \\ &= \frac{t}{|t|\pi} A \wedge dt + \frac{|t|}{\pi} dA - i\frac{t^2}{\pi^2} A \wedge A \end{aligned} \quad (7.2.46b)$$

being the corresponding curvature form defined for  $t \neq 0$ . Since  $\tilde{F}$  is a curvature form on a  $2s$ -dimensional torus parametrized by  $\mathbf{k}$  and  $t$ , it can be associated to a Chern number  $\tilde{C}^{(s)}$ . Using the fact that  $\tilde{F}(\mathbf{k}, t) = \tilde{F}(\mathbf{k}, -t)$ , we can reduce the  $t$  integration from the interval  $[-\pi, \pi]$  to the interval  $[0, \pi]$  by multiplication with a factor of 2

$$\tilde{C}^{(s)} = 2 \times \frac{1}{2s!} (12\pi)^s \int_{\text{BZ} \times [0, \pi]} \text{tr} [\tilde{F}^s]. \quad (7.2.47a)$$

Upon explicitly performing the  $t$ -integration using the form of  $\tilde{F}$  in Eq. (7.2.46b), we find that the Chern number is given as an integral of the  $(d = 2s - 1)$ -forms  $Q^{(s)}$  defined in Eq. (7.2.15c) over the BZ

$$\tilde{C}^{(s)} = 2 \times \frac{1}{s!} \left( \frac{1}{2\pi} \right)^s \int_{\text{BZ}} \text{tr} [Q^{(s)}]. \quad (7.2.47b)$$

We have thus obtained a form of  $\tilde{C}^{(s)}$  that is expressed in terms of  $Q(\mathbf{k})$  in the  $(2s-1)$ -dimensional BZ alone. As the Chern-number  $\tilde{C}^{(s)}$  may only take integer values, the  $(2s - 1)$ -dimensional polarization

$$\mathbf{P}^{(2s-1)} := \frac{1}{s!} \left( \frac{1}{2\pi} \right)^s \int_{\text{BZ}} \text{tr} [Q^{(s)}], \quad (7.2.48)$$

may only take half-integer values. This is a consequence of the symmetry constraints. For systems in symmetry class A,  $\mathbf{P}^{(2s-1)}$  is still well defined, but loses its relation to a Chern number in one dimension higher and thus does not need to be quantized. One might wonder whether we have now obtained a  $\mathbb{Z}$  classification in terms of  $\mathbf{P}^{(2s-1)}$ , instead of the  $\mathbb{Z}_2$  classification we were aiming at. That this is not the case can be deduced from carefully considering the effect of gauge transformations. The physical gauge transformations to be considered are those affecting the Berry connection  $A$  as given by Eq. (7.2.11a). However, these transformations do not take the form of a gauge transformation for the one-form  $\tilde{A}$  in the auxiliary space  $\text{BZ} \times [-\pi, \pi]$ . As a consequence, neither transforms  $\tilde{F}$  gauge covariantly nor is  $\tilde{C}^{(s)}$  invariant under the physical gauge transformations (7.2.11a) on  $A$ . More precisely, the polarization  $\mathbf{P}^{(2s-1)}$  changes under such a gauge transformation (7.2.11a) by

$$\mathbf{P}^{(2s-1)} \longrightarrow \mathbf{P}^{(2s-1)} + \frac{1}{s!} \left( \frac{i}{2\pi} \right)^s \int_{\text{BZ}} \text{tr} [(G^\dagger dG)^{2s-1}]. \quad (7.2.49)$$

The additive change is the winding number  $W^{(s-1)}$  of the gauge transformation  $G$  over the BZ. As this winding number takes only integer values, the non-integer part of  $\mathbf{P}^{(2s-1)}$  is a well-defined quantity, i.e., gauge invariant. Gauge transformations with non-vanishing winding number are referred to as large gauge transformations. This defines two equivalence classes of systems in each of the symmetry classes AI, AII, C, and D, distinguished by the parity

$$\nu_1 := (-1)^{2\mathbf{P}^{(2s-1)}} \in \{1, -1\}. \quad (7.2.50)$$

Between any two systems with different  $\nu_1$ , there exists no smooth interpolation that respects the symmetry. Any vacuum with  $A = 0$  has  $\nu_1 = +1$ , rendering this class topologically trivial. We have thus obtained the desired  $\mathbb{Z}_2$  classification in terms of the parity index  $\nu_1$  for the entries  $\mathbb{Z}_2$  to the immediate left of  $\mathbb{Z}$  in classes AI, AII, C, and D shown in Tab. 7.1.



**Second descendants** To directly obtain a convenient form of the topological invariant of the second descendant, we shall construct its index  $\nu_2$  from gauge obstruction arguments generalizing the derivation by Fu and Kane.

The TRS and PHS constraints in the symmetry classes AI, AII, C, and D relate the wave function *including the gauge choice* at points  $\mathbf{k}$  and  $-\mathbf{k}$  in the ( $d = 2s$ )-dimensional BZ. Effectively, the system thus only depends on degrees of freedom on one half of momentum space, the effective BZ (EBZ). Without loss of generality, we can define the EBZ as

$$\text{EBZ} := \{\mathbf{k} \in \text{BZ} : k_1 \in [0, \pi]\}. \quad (7.2.51)$$

We want to find a topological characterization of the flatband Hamiltonian on the EBZ. In contrast to the BZ, the EBZ is a manifold with boundary, namely a  $d$ -dimensional torus cut open in one direction (a cylinder in  $d = 2$ ). Consider a situation where the EBZ is divided into two regions  $V_1$  and  $V_2$ , each of which is not necessarily simply connected. Suppose that  $V_1$  and  $V_2$  overlap only at their interface

$$\text{EBZ} = V_1 \cup V_2, \quad \partial V_1 \setminus \partial \text{EBZ} = \partial V_2 \setminus \partial \text{EBZ}. \quad (7.2.52)$$

Further, suppose that there exists a smooth gauge on each of  $V_1$  and  $V_2$ , with  $A_1$  and  $A_2$  being the respective Berry connections. The two gauges are related by a gauge transformation  $G$  of the form (7.2.11a) that is defined on the closed surface  $\partial V_1$ . We can thus consider its winding number around  $\partial V_1$

$$D^{(s)} := \frac{1}{s!} \left( \frac{i}{2\pi} \right)^s \int_{\partial V_1} \text{tr} \left[ (G^\dagger dG)^{2s-1} \right] \quad (7.2.53)$$

which is bound to be integer for a closes surface. As we have seen in Eq. (7.2.49), the integrand of the winding number is the difference between the Chern-Simons forms  $Q_1^{(s)}$  and  $Q_2^{(s)}$  in the two gauges  $A_1$  and  $A_2$ , respectively

$$\begin{aligned} D^{(s)} &= \frac{1}{s!} \left( \frac{1}{2\pi} \right)^s \int_{\partial V_1} \text{tr} \left[ Q_1^{(s)} - Q_2^{(s)} \right] \\ &= \frac{1}{s!} \left( \frac{1}{2\pi} \right)^s \int_{\partial V_1} \text{tr} \left[ Q_1^{(s)} \right] + \int_{\partial V_2} \text{tr} \left[ Q_2^{(s)} \right] - \int_{\partial \text{EBZ}} \text{tr} \left[ Q_2^{(s)} \right] \end{aligned} \quad (7.2.54a)$$

To obtain the second line in Eq. (7.2.54a), we used that in view of the opposite orientation of the overlap region of  $\partial V_1$  and  $\partial V_2$

$$\int_{\partial \text{EBZ}} = \int_{\partial V_1} + \int_{\partial V_2}. \quad (7.2.54b)$$

As  $Q_i^{(s)}$  is defined smoothly in  $V_i$ ,  $i = 1, 2$ , we can use Stokes' theorem to relate it to the Berry curvature via Eq. (7.2.14)

$$D^{(s)} = \frac{1}{s!} \left( \frac{1}{2\pi} \right)^s \left( \int_{\text{EBZ}} \text{tr} [F^s] - \int_{\partial \text{EBZ}} \text{tr} \left[ Q_2^{(s)} \right] \right). \quad (7.2.55)$$

If any gauge transformation was allowed to be applied to  $A_2$ , Eq. (7.2.55) would be meaningless, since the second term would change  $D^{(s)}$  by the winding number of the gauge transformation, an integer. However, for the symmetry classes under consideration, either PHS or TRS restricts the allowed gauge transformations. It turns out that the allowed gauge transformations have even

winding number on  $\partial\text{EBZ}$ . Thus, the parity of  $D^{(s)}$  is a gauge invariant quantity that allows to define the  $\mathbb{Z}_2$  index for the second descendants

$$\nu_2 := (-1)^{D^{(s)}} \in \{1, -1\}. \quad (7.2.56)$$

in symmetry classes AI, AII, C, and D. There is a plethora of different but equivalent formulas for this  $\mathbb{Z}_2$  index. For example, the original formulation for class AII in  $d = 2$  by Kane and Mele employs the antisymmetric overlap matrix  $U^\dagger(\mathbf{k})U_{\mathcal{T}}U^*(\mathbf{k})$  to establish the formula

$$D^{(1)} = \frac{i}{2\pi} \int_{\partial\text{EBZ}} d \log \left\{ \text{Pf} \left[ U^\dagger(\mathbf{k})U_{\mathcal{T}}U^*(\mathbf{k}) \right] + i\delta \right\}, \quad (7.2.57)$$

where Pf denotes the Pfaffian of a matrix and  $\delta > 0$  is a regulator. If the system obeys inversion symmetry, Eq. (7.2.57) reduces to a finite product of parity eigenvalues at inversion-symmetric momenta in the BZ. In this form, the index can be computed numerically very efficiently.

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