

Preface

Topological insulators are crystalline solids with supposedly very special properties. If stumbling upon such a crystal, which is possible because topological insulators are known to occur naturally on earth [73], a curious investigator will discover that the electrons deep inside the material are locked and they do not flow under electric field excitations. The immediate conclusion will be that the crystal is an insulator. However, when examining the surface of the crystal, our fictitious character will discover that the surface electrons are free to move like in a metal. Perhaps the first reaction will be to assign this odd behavior to surface contaminants and other factors like that, and the natural course of action will be to cleave a new surface and see what happens. To one's surprise, no matter how careful the new surface is cleaved, the metallic character is still present. There are many untold details to the story, but, broadly speaking, this is what a topological insulator ought to be. As the story suggests, the special properties must be determined by the bulk characteristics of the material, but there must be a bulk-boundary correspondence principle which tells how these bulk characteristics determine the metallic character of the surface. We should specify here, at the beginning, that although the properties of the topological insulators are ultimately determined by the number, type, and arrangements of the atoms in the repeating cell of the crystal, the topology guaranteeing the metallic surface states is actually routed in the abstract space of electron ground states and has, for instance, nothing to do with the appearance and shape of the sample.

One may be reminded of the integer quantum Hall effect (IQHE) [117], where robust conducting channels occur along the edges of a specially prepared sample immersed in a relatively large magnetic field. In contradistinction, no magnetic fields were mentioned in the above story. The special properties of the topological insulators are intrinsic to the materials, which presumably will enable a broader range of applications. It was Haldane [80] who realized in 1988 that all the characteristics of the IQHE can occur naturally in materials with special unit cells and hopping matrices. The next milestone of the field occurred much later, in 2005, when Kane and Mele revealed that these special hopping matrices can be induced by the spin-orbit interaction [99, 100]. At the same time, they discovered a new

class of topological materials, the quantum spin-Hall insulators in two space dimensions which have topologically nontrivial time-reversal symmetric ground states. These developments gathered momentum with the theoretical prediction [26] and then the experimental confirmation [121] of the first quantum spin-Hall insulator, and then further with the theoretical prediction of new topological insulators in three space dimensions [70, 71, 141, 189] and their experimental realization [91]. The field of topological insulators is now fairly mature and there are several very good surveys [84, 86, 173, 174] and excellent monographs [25, 67, 150, 199], where the reader can also find extensive literature on the subject. We want to mention in particular the short survey by Ando [8], which includes a table of 34 topological materials that were synthesized and characterized in laboratories, together with a summary of the findings for each compound. Ando's analysis reveals that, while the patterns seen in the surface electronic band structure agree quite well with the theoretical predictions, the transport experiments indicate a weak bulk metallic character (i.e., large, but nevertheless finite resistivity at low temperatures) for all these materials (excepting the two-dimensional ones). Because of it, the transport characteristics of the surfaces were impossible to measure and the main conjecture about their metallic character is yet to be confirmed. The lack of insulating bulk character is usually attributed to the disorder in the samples, which is difficult to control for materials with such large and complex unit cells. A great deal of experimental effort was invested in overcoming this last hurdle, and one success has been recently reported for thin films [32]. On the theoretical front, these issues prompted the need for theoretical methods which can handle more realistic models of topological insulators, in particular, to incorporate the effects of disorder. On the fundamental level, a rigorous proof of the conjectures on topological insulators in such real-world conditions is highly desirable.

What are the main aims? The present monograph is a mathematically rigorous contribution to the theory of so-called complex classes of topological insulators, namely those classes which are not specified by symmetries invoking a real structure, such as time-reversal or particle-hole symmetries (see Chap. 2 for a concise description). The main objectives are to:

- Aim 1: Construct the observable algebras within an effective one-particle framework.
- Aim 2: Encode the nontrivial topology in bulk and boundary invariants which are robust against disorder and magnetic fields.
- Aim 3: Establish the equality between the bulk and the boundary invariants.
- Aim 4: Determine the range of the invariants using generalized Streda formulas which connect different invariants.
- Aim 5: Establish local index theorems for the so-called strong bulk and boundary invariants.
- Aim 6: Prove the defining property of topological insulators, i.e., the immunity of the boundary states against Anderson localization.
- Aim 7: Connect the invariants to response coefficients and other physical observables.

Which mathematical tools are used? The C^* -algebras describing the bulk systems are those introduced by Bellissard for the description of the quantum Hall effect and quasicrystals [17]. Algebras describing half-space models and their boundaries are the extensions of the bulk algebras introduced in [107, 197]. These algebras form a short exact sequence of C^* -algebras, which is central to the bulk-edge correspondence. In the mathematical literature, these algebras are respectively well known as (twisted) crossed product algebras [156, 223] and their Toeplitz extensions, as given by Pimsner and Voiculescu [160]. In a first step, the topological invariants are encoded in the K -theory of these algebras. Based on the Pimsner–Voiculescu six-term exact sequence [160] and on [60, 183, 185], these K -groups and their generators can be determined completely. In a second step, the K -theoretic content is extracted via pairings with the cyclic cohomology of the observables algebras, the latter being a key element of Connes’ non-commutative geometry [47]. At this step, numerical invariants are generated and, for bulk systems, these invariants extend those known in the physics literature [170, 190, 192]. It is then possible to prove duality results for the connecting maps of K -theory, such as the suspension map, Bott map, index map, exponential map, and their counterparts in cyclic cohomology [63, 107, 145, 159]. This allows to connect various invariants. In particular, the bulk invariants are equal to the boundary invariants as well as the Volovik–Essin–Gurarie invariants calculated in terms of the Green functions [64, 213]. Another technique used here is that of Fredholm modules for index calculations, as introduced by Atiyah [10] and further developed by Kasparov [101] and Connes [46]. This technique leads by rather elementary means to index theorems for the so-called strong invariants of topological insulators. Alternative mathematical approaches to the duality results behind the bulk-boundary correspondence were given in [79] and [30, 31]. To achieve Aim 4, we use another technical tool, namely the Ito derivative w.r.t. the magnetic field, as introduced by Rammal and Bellissard [176] and further elaborated in [198]. Resuming, this monograph shows how a variety of abstract mathematical tools, ranging from C^* -algebras and their K -theories to non-commutative geometry, can be put to work on very concrete problems coming from solid state physics, and help resolve issues which are presently addressed in the physics community.

What is new and what was known before? The real space versions of the bulk invariants in arbitrary dimensions already appeared in our prior works [139, 169, 171], where also the index theorems for these invariants were proved. These works paralleled the much earlier work of Bellissard on two-dimensional quantum Hall systems [17, 18, 20]. This approach to topological invariants allows to go beyond their definition based on Bloch theory, as it is usually done in the physics literature [172, 192]. The use of K -theory to connect with the invariants of Volovik [213] and Essin–Gurarie [64] is new. Also, the definitions of the boundary invariants for arbitrary dimensions are new, as are the index theorems for them. In the context of condensed matter physics, the connecting maps of K -theory were first put to work for integer quantum Hall systems, where they provided a structural framework for the proof of the equality between the bulk and edge Hall conductances, under quite

general assumptions [107, 109, 197]. This series of works was heavily inspired by Hatsugai's work [87] on edge states for the Harper model. Actually, these works only used the exponential connecting map which is also applied to higher even dimensions here. A key new element of the present work is the use of the index map for chiral systems (see Sects. 1.3 and 4.3.2), and actually for the much wider class of approximately chiral systems. The index map is the key to a sound definition of the boundary invariants and is also instrumental for the proof of the bulk-edge correspondence for chiral systems, from which the delocalized character of the boundary states follows (see Aim 6).

Another important new result is a generalized Streda formula and its corollaries on the ranges of the pairings of K -theory with cyclic cohomology. The classic Streda formula refers to the equality between the variation w.r.t. magnetic field of 0-cocycle pairings (particularly, the density of states) and 2-cocycle pairings (particularly, the Hall conductance) [176, 198, 204]. This equality will be generalized to cocycles of arbitrary dimensions and this will enable us to attach physical content to the abstractly defined topological invariants. As we shall see in Chap. 7, the generalized Streda formula has numerous physical applications and unifies other results obtained in the literature [172, 200]. Further new results in Chap. 7 concern the stroboscopic interpretation of the orbital polarization, the connection of orbital polarization to spectral flow of boundary states and the prediction of a quantum Hall effect in approximately chiral systems in dimension $d = 3$. Interestingly, the Hall conductance of these surface states is dictated by the bulk invariant.

What is left out? There is no attempt here to deal with systems having time-reversal symmetry, particle-hole symmetry or reflection symmetries. There is an exhaustive physical literature on such systems starting with [92, 172, 190], and a few more mathematical oriented works [11, 68, 76, 77, 85, 111, 162, 194, 207] which already proposed topological invariants for such systems. However, the bulk-boundary correspondence for these systems has only been established for very special situations [11, 76, 137, 138]. Based on [77, 194, 207], we expect that these symmetries can be accommodated in the framework developed here and that the bulk-boundary correspondence will follow for these systems, too, but this definitely requires further investigations. Even for the complex classes extensively treated here, K -theoretic techniques can supply further interesting results not included in the monograph. For example, in [56] it is shown that the Laughlin argument (piercing of a flux through a quantum Hall system and inducing an associated spectral flow) can be described by an exact sequence of C^* -algebras. This exact sequence is a mapping cone and is hence different from the exact sequence of the bulk-boundary correspondence. Nevertheless, the K -theory associated to that sequence links Hall conductance (i.e., Chern numbers) to a spectral flow and hence captures again the essence of Laughlin's argument. Implementing symmetries in this sequence allows to derive criteria for the existence of zero modes attached to flux tubes in dirty superconductors or Kramers bound states at defects in quantum spin-Hall systems [56]. Another example is boundary forces [103, 104, 110, 168]. It is actually the firm belief of the authors that other defects, e.g., as described in

[93, 188, 206], can also be described by adequate sequences of C^* -algebras and the associated K -theoretic sequences can be used to uncover new interesting topological effects. From this perspective, the bulk-boundary correspondence can be seen as one particular situation where these ideas can be implemented, albeit probably the most important one. To further support this belief, we included here the spectroscopic interpretation of the orbital polarization as a further example. Behind it is a natural exact sequence associated to the suspension construction in K -theory. Let us mention that the use of exact sequences to connect topological invariants in physics is not restricted to solid state systems, but has also been successfully implemented in scattering theory to prove Levinson's theorem [21, 105, 106].

Concerning the index theory, let us first point out that it has very recently been shown [30] how to obtain index theorems as stated in Chap. 6 by evaluating the general Connes–Moscovici local index formula [50] in a form proved in [34] under much broader assumptions. The argument is close to [7] and avoids using the intricate geometric identities discovered in [47, 169, 171] and presented in Sect. 6.4, but the price are other technicalities. We decided to stay with the more direct arguments which rely on the Calderon–Fedosov formula [33, 66] for the Fredholm index and the above-mentioned geometric identities. On another front, we did not attempt any (generalized) index theorems for the so-called weak topological invariants. Such results are possible [165], but one has to leave the realm of finitely summable Fredholm modules and work with semifinite spectral triples [37–39]. Actually, the latter framework was shown to be fruitful in much broader contexts, in some cases even for correlated quantum systems [35, 36, 152–154]. This brings the hope that the electron–electron interaction can be treated by these techniques. This is one of the big open issues in the field and is not dealt with in the present work. We also decided not to include any numerical evaluation of the invariants. This will be presented elsewhere. While completing the manuscript, we came across the following works [31, 137, 138] which open new directions and partially overlap with our presentation.

How is the monograph organized? Chapter 1 illustrates the key concepts on perhaps the simplest of all topological systems, a lattice model with chiral symmetry in space dimension $d = 1$. In this case, the bulk invariant is provided by the winding number of the so-called Fermi unitary operator and the edge effect consists in the emergence of zero-energy quantum states localized near the edge, called zero-edge modes. The space of zero-edge modes is invariant under the chiral symmetry, hence the zero modes have a specific chirality assigned to them. The bulk-boundary principle then asserts that the bulk invariant is equal to the number of zero-edge modes with positive chirality minus the number of zero-edge modes with negative chirality. As a result, if the bulk invariant is not zero, there will always be zero-edge modes and their number is necessarily larger or equal to the value of the bulk invariant. This statement, which is proved here using a K -theoretic approach, holds in the presence of disorder and regardless of how the lattice is terminated at the edge, provided the chiral symmetry is always present. Along the way, many of the concepts used later in the monograph are introduced. Actually the

key ideas on how to use the index map for the bulk-boundary correspondence in chiral systems is already exposed in Chap. 1.

Chapter 2 gives a brief overview of the classification table of topological insulators and superconductors [115, 190, 192], which is now accepted by the majority of the condensed matter physics community. The present work only deals with the first two rows of this table, the so-called unitary symmetry class A and the chiral unitary symmetry class AIII. They are also called the complex classes since they are classified by the complex K -theory while the remaining 8 classes are classified by real K -theory. The physics and the conjectures for the complex classes are presented in detail in Sects. 2.2 and 2.3. These sections also provide simple models in arbitrary dimensions where the bulk-boundary principle can be witnessed first-hand. The last section of Chap. 2 introduces the physical models which are studied in the remainder of the manuscript, together with technical conditions on these models.

Chapter 3 introduces the operator algebras for bulk, half-space, and boundary observables. Section 3.1 describes the disordered non-commutative torus which plays the role of bulk algebra. This C^* -algebra can be presented as a d -fold iterated crossed product (d is the dimension of the physical space) and it has a canonical representation on $\ell^2(\mathbb{Z}^d)$ which generates the bulk models discussed in Chap. 2. Section 3.2 then introduces the disordered non-commutative torus with a boundary. Here one of the unitary generators becomes a partial isometry which can be seen as introducing a defect. This algebra plays the role of the half-space algebra and it has a canonical representation on $\ell^2(\mathbb{Z}^{d-1} \times \mathbb{N})$ which generates the physical models on a half-space. The algebra of boundary observables is a prime ideal of the half-space algebra. The elements of this algebra generate the boundary conditions. The exact sequence between the bulk, half-space and boundary algebras is also discussed in this chapter. The last sections of the chapter present the non-commutative analysis tools for the observables algebras and the smooth sub-algebras where this calculus actually takes place.

Chapter 4 presents the K -theory of the observables algebras. It begins with a concise description of the basic principles of K -theory. The exact sequence of Chap. 3 is shown to be isomorphic to the Pimsner–Voiculescu exact sequence [160] and the latter is then used to compute the K -groups. In particular, the K -groups of the bulk algebra and of the non-commutative torus coincide. For the latter, the generators of the K -groups have been computed explicitly by Elliott [60] and Rieffel [183] and we reproduce them in Sect. 4.2.3. Section 4.3 computes various connecting maps between the K -groups of observables algebras. This section is central for the whole book.

Chapter 5 invokes the cyclic cohomology and its pairing with the K -theory to define the bulk and the boundary topological invariants in terms of the Chern characters paired with the appropriate elements of the K -groups. It is shown how to suspend these invariants and that this suspension does not alter the values of the invariants. The equality between the bulk and the boundary invariants is established using the duality between the pairings for bulk and boundary algebras. The range

of these pairings is calculated using a generalized Streda formula. Detailed proofs are provided for all of these central results.

Chapter 6 constructs finitely summable Fredholm modules canonically associated with the observables algebras. The pairings of the associated Connes–Chern characters with the K -groups are expressed as Fredholm indices. Section 6.3 establishes the equality between the Chern and Connes–Chern characters based on two remarkable geometric identities, which in turn provide the index formulas for the bulk and boundary invariants. The metallic character of the boundary states is established as a direct consequence of these index formulas.

Chapter 7 presents a series of corollaries which describe our physical predictions based on the mathematical statements from the previous chapters. The chapter starts with a brief introduction to the bulk and boundary transport coefficients of homogeneous disordered systems. These linear and nonlinear coefficients are then connected to the bulk and boundary topological invariants for systems of class A. Predictions about the quantized values and the robustness of these physically measurable properties are provided. Similar results are presented for the spontaneous electric polarization and the magneto-electric response coefficients. For chiral symmetric solid state systems, the physically relevant quantities are the spontaneous chiral electric polarization and its variations w.r.t. magnetic fields, which are shown to be of topological nature and connected to the bulk and boundary invariants constructed for systems from class AIII. Again several of these measurable quantities have quantized values. The chapter also includes a prediction and discussion of an IQHE at the surface of chiral or at least approximately chiral symmetric systems. The generalized Streda formula developed in Chap. 5 is an essential tool for the analysis in Chap. 7.

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