

Chapter 2

Electron Dynamics: Concrete Physical Models

Abstract This Chapter introduces and characterizes the so called lattice models, which integrate naturally in the general framework for homogeneous materials introduced in Chap. 1. It also fixes the notations and the conventions used throughout. A model of disorder is introduced and the various regimes of disorder are discussed. The Chapter concludes with the introduction and characterization of the topological invariants corresponding to the phases classified by \mathbb{Z} and $2\mathbb{Z}$ in Table 1.1.

2.1 Notations and Conventions

From now on, our exposition deals exclusively with discrete lattice models. These models give accurate representations of the low-energy excitations which are responsible for the physics observed in the typical experiments performed on solid state phases, such as the transport measurements. Given a concrete material, accurate lattice models can be generated from first principles [17, 20, 28, 29]. One such technique is based on projecting the continuum models on a discrete, periodic and localized partial basis set which accurately represents the spectral subspace in a finite energy window around the Fermi level. Benchmarks of this method can be found in [18]. The models can be also generated empirically by fitting the available experimental data. One relevant example of this type is the lattice model of the HgTe quantum wells [9, 15], the prototypical topological insulator from class AII in dimension two.

The Hilbert spaces of the lattice models take the generic form $\mathcal{H} = \mathbb{C}^N \otimes \ell^2(\mathbb{Z}^d)$, where d is the dimension of the physical space and \mathbb{C}^N is often referred to as the fiber. As before, the algebra of bounded linear operator over \mathcal{H} will be denoted by $\mathbb{B}(\mathcal{H})$. Let us specify from the beginning that \mathbb{Z}^d does not represent the position of the atoms but it rather labels the primitive cells. The dimension d needs to be understood accordingly, e.g. $d = 1$ for a molecular chain, $d = 2$ for graphene and $d = 3$ for an ordinary crystal. This dimension can be higher than three, since one can add virtual dimensions by varying the parameters of the models [23]. The primitive cells of topological insulators contain many atoms, in many cases 10 or even more, hence they are quite complex. The dimension N of the fiber represents the number of molecular orbitals per primitive cell included in the model. The larger this number

the more precise the model is. Due to the complex primitive cell of the topological materials, this number can be quite large in the first principle calculations (within the hundreds!). This is to be contrasted with the simple analytic models used by theoretical physicists, which quite often assume $N = 2$.

Throughout, we denote the space of $N \times N$ matrices with complex entries by $M_N(\mathbb{C})$. Also, tr will denote the normalized trace of matrices, such as those from $M_N(\mathbb{C})$, or more general the standard normalized traces over finite dimensional Hilbert spaces. The semi-finite traces over infinite Hilbert spaces, such as $\ell^2(\mathbb{Z}^d)$ or $\mathbb{C}^N \otimes \ell^2(\mathbb{Z}^d)$, will be denoted as usual by Tr . We will adopt the Dirac notation $|\alpha, x\rangle$ for the standard basis of $\mathbb{C}^N \otimes \ell^2(\mathbb{Z}^d)$ and, throughout, X will denote the position operator on $\ell^2(\mathbb{Z}^d)$, $X|x\rangle = x|x\rangle$. For an operator T on $\mathbb{C}^N \otimes \ell^2(\mathbb{Z}^d)$, the notation $\langle x|T|y\rangle$ stands for the $N \times N$ matrix with entries $\langle \alpha, x|T|\beta, y\rangle$, $\alpha, \beta = 1, \dots, N$. Another set of useful operators on $\ell^2(\mathbb{Z}^d)$ are the shift operators $S_j|x\rangle = |x + e_j\rangle$, where e_j , $j = 1, \dots, d$, are the generators of \mathbb{Z}^d . The following notation:

$$S_y = S_1^{y_1} \dots, S_d^{y_d}, \quad S_y|x\rangle = |x + y\rangle, \quad y \in \mathbb{Z}^d, \quad (2.1)$$

will be adopted throughout. Lastly, if V is a finite subset of \mathbb{Z}^d , then we can consider the associated finite-dimensional Hilbert space $\mathbb{C}^N \otimes \ell^2(V)$ and we denote the corresponding normalized trace by tr_V , and the partial isometry from $\mathbb{C}^N \otimes \ell^2(\mathbb{Z}^d)$ to $\mathbb{C}^N \otimes \ell^2(V)$ by $\Pi_V = 1 \otimes \sum_{x \in V} |x\rangle\langle x|$.

Another convention we adopt throughout concerns the notation for the norms. While, the norms on different algebras will be defined explicitly, to simplify the notation, we will use most of the time the same symbol $\|\cdot\|$ for all of them. There should be no confusion in the calculations, because in all such instances the algebras can be easily identified. For example, the norm appearing in $\|\langle x|T|y\rangle\|$ is the one on $M_N(\mathbb{C})$.

2.2 Physical Models

In the periodic or translational invariant case, the most general Hamiltonian that can be defined on a lattice takes the form:

$$H : \mathbb{C}^N \otimes \ell^2(\mathbb{Z}^d) \rightarrow \mathbb{C}^N \otimes \ell^2(\mathbb{Z}^d), \quad H = \sum_{y \in \mathbb{Z}^d} w_y \otimes S_y, \quad (2.2)$$

where the hopping matrices $w_y \in M_N(\mathbb{C})$ satisfy the basic constraint $w_y^* = w_{-y}$ ensuring that H is self-adjoint. When symmetries are present, the hopping matrices acquire additional structure. In particular, when the chiral symmetry is present and the dimension of the fiber is even, the hopping matrices have the structure:

$$w_y = \begin{pmatrix} 0 & g_y \\ g_y^* & 0 \end{pmatrix}, \quad (2.3)$$

which manifests in the chiral symmetry of the Hamiltonian [27]:

$$S H S^* = -H, \quad S = \begin{pmatrix} I_N & 0 \\ 0 & -I_N \end{pmatrix}. \quad (2.4)$$

By examining the classification Table 1.1, we can see that the chiral symmetry is present for all phases classified by \mathbb{Z} or $2\mathbb{Z}$ in odd dimensions.

As it is well known, the energy spectrum of the translational invariant Hamiltonians is continuous and, since we want to deal only with insulators, the only way to accommodate that is to assume a gap in the energy spectrum and that the Fermi level ε_F is somehow pinned inside this spectral gap. In the independent electron approximation, assumed throughout, the ground state of the Hamiltonian is encoded in the Fermi projection, that is, the spectral projection onto the energy spectrum below the Fermi level ε_F :

$$P_F = \chi(H \leq \varepsilon_F) \in \mathbb{B}(\mathcal{H}), \quad (2.5)$$

where χ stands for the indicator function. For all topological phases in even dimensions that are classified by \mathbb{Z} or $2\mathbb{Z}$ in Table 1.1, the topology is encoded in P_F . When the chiral symmetry is present, the Fermi projection has a particular structure:

$$P_F = \frac{1}{2} \begin{pmatrix} 1 & -U_F^* \\ -U_F & 1 \end{pmatrix}, \quad U_F^* U_F = U_F U_F^* = I, \quad (2.6)$$

and the topology is encoded in the unitary operator U_F rather than P_F itself. We refer to U_F as the unitary Fermi operator. The strong topological invariants for the phases classified by \mathbb{Z} or $2\mathbb{Z}$ in Table 1.1 are given by the top even Chern number applied to P_F , for even space dimensions, and by the top odd Chern number applied to U_F , for odd dimensions [27]. They will be further elaborated in Sect. 2.4 and, for now, let us present two examples of topological models, which can be solved explicitly in the bulk as well as with a boundary. The explicit calculations can be found in [26].

Example 2.1 (A topological insulator from class A) Assume the space dimension even and let $\{\gamma_j\}_{j=1,d}$ be the irreducible representation of the even complex Clifford algebra \mathcal{Cl}_d on $\mathbb{C}^{2^{\frac{d}{2}}}$ and γ_0 be its standard inner grading. Consider the following Hamiltonian on the Hilbert space $\mathbb{C}^{2^{\frac{d}{2}}} \otimes \ell^2(\mathbb{Z}^d)$:

$$H = \frac{1}{2i} \sum_{j=1}^d \gamma_j \otimes (S_j - S_j^*) + \gamma_0 \otimes \left(m + \frac{1}{2} \sum_{j=1}^d (S_j + S_j^*) \right), \quad (2.7)$$

with Fermi level fixed at the origin. Then H has a spectral gap at the Fermi level, except when $m \in \{-d, -d+2, \dots, d-2, d\}$. If $m \in (-d+2n, -d+2n+2)$, with $n = 0, \dots, \frac{d-2}{2}$, the model is in a topological insulating phase labeled by its top even Chern number which takes the value $(-1)^n \binom{d-1}{n}$. \diamond

Remark 2.2 If $d = 4$, the above model is in fact time-reversal symmetric, hence it can be as well considered from the class AII. \diamond

Example 2.3 (A topological insulator from class AIII) Assume the space dimension odd and let $\{\gamma_j\}_{j=1, \overline{d+1}}$ be the irreducible representation of the even complex Clifford algebra \mathcal{Cl}_{d+1} on $\mathbb{C}^{2^{\frac{d+1}{2}}}$. Consider the following Hamiltonian on the Hilbert space $\mathbb{C}^{2^{\frac{d+1}{2}}} \otimes \ell^2(\mathbb{Z}^d)$:

$$H = \frac{1}{2i} \sum_{j=1}^d \gamma_j \otimes (S_j - S_j^*) + \gamma_{d+1} \otimes \left(m + \frac{1}{2} \sum_{j=1}^d (S_j + S_j^*) \right), \quad (2.8)$$

with Fermi level fixed at the origin. Then H has the chiral symmetry $\gamma_0 H \gamma_0^* = -H$ and the model displays a spectral gap at the Fermi level, except when $m \in \{-d, -d+2, \dots, d-2, d\}$. If $m \in (-d+2n, -d+2n+2)$, with $n = 0, \dots, \frac{d-1}{2}$, the model is in a topological phase labeled by its top odd Chern number which takes the value $(-1)^n \binom{d-1}{n}$. \diamond

The presence of a uniform magnetic field is incorporated in the lattice models by using the Peierls substitution [21], which amounts to replacing the ordinary shift operators with the dual magnetic translations:

$$S_y \mapsto U_y = e^{iy \wedge X} S_y = S_y e^{iy \wedge X}. \quad (2.9)$$

Throughout:

$$x \wedge x' = \frac{1}{2} \sum_{i,j=1}^d \phi_{ij} x_i x'_j, \quad \forall x, x' \in \mathbb{R}^d, \quad (2.10)$$

where ϕ is a real anti-symmetric $d \times d$ matrix with entries from $[0, 2\pi)$, encoding the magnetic fluxes through the facets of the primitive cell, in units of flux quantum $\phi_0 = h/e$. When the dependence on the magnetic flux needs to be emphasized we will use \wedge_ϕ . With this substitution, the lattice Hamiltonians become:

$$H = \sum_{y \in \mathbb{Z}^d} w_y \otimes U_y = \sum_{x, y \in \mathbb{Z}^d} e^{iy \wedge x} w_y \otimes |x\rangle \langle x - y|. \quad (2.11)$$

They are no longer invariant w.r.t. the ordinary shifts but they are invariant w.r.t. the magnetic translations:

$$V_y H V_y^* = H, \quad V_y = e^{-iy \wedge X} S_y = S_y e^{-iy \wedge X}. \quad (2.12)$$

It is important to note that the unitary classes of topological insulators, namely the classes A and AIII, can incorporate magnetic fields because time-reversal symmetry is not required.

The next step incorporates the disorder. As we have seen in the previous chapter, a homogeneous disorder is described by a measure-preserving ergodic dynamical system $(\Omega, \tau, \mathbb{Z}^d, d\mathbb{P})$. Below is an important example.

Example 2.4 (Disorder induced by thermal fluctuations) Assume we are dealing with a chemically pure crystal with the atoms arranged in a perfectly periodic lattice at zero temperature. At finite temperature, though, the atoms wander around the equilibrium positions and the crystal is in a disordered state. If R_x^α is the displacement from equilibrium position of atom α in the primitive cell x at an instantaneous time, then the disorder configuration at that time is encoded in $\omega = \{R_x^\alpha\}_{x \in \mathbb{Z}^d}^{\alpha=1, N_a}$, where N_a is the number of atoms in the repeating cell. One assumption is that each atom wanders only in a finite neighborhood Ω_x^α of its equilibrium position. Then homogeneity requires that $\Omega_x^\alpha = \Omega_0^\alpha$, and the space of disorder configurations and the \mathbb{Z}^d -action are given by:

$$\Omega = \prod_{x \in \mathbb{Z}^d} \prod_{\alpha=1}^{N_a} \Omega_0^\alpha = \prod_{x \in \mathbb{Z}^d} \Omega_0, \quad \tau_y \omega = \tau_y \{R_x^\alpha\} = \{R_{x-y}^\alpha\}. \quad (2.13)$$

Note that Ω is a Tychononov space, hence compact and metrizable, and that τ is continuous and invertible hence $(\Omega, \tau, \mathbb{Z}^d)$ is indeed a topological classical dynamical system. The Gibbs measure governing the classical statistical mechanics of the atoms is defined as the thermodynamic limit of the finite volume probability measures:

$$d\mathbb{P}_V(\omega) = \mathcal{Z}_V^{-1} e^{-\beta \mathcal{V}_V(\omega)} \prod_{x \in V \subset \mathbb{Z}^d} \prod_{\alpha=1}^{N_a} d\omega_x^\alpha, \quad (2.14)$$

where \mathcal{V}_V is a classical potential for the atomic degrees of freedom and $\beta = \frac{1}{kT}$, where k is Boltzmann's constant and T is the temperature. When the electronic and atomic degrees of freedom decouple as in the Born-Oppenheimer regime, the potential \mathcal{V}_V can be mapped explicitly from the ground state of the electrons. \diamond

As we have already seen, central to the theory of homogeneous aperiodic solids is the notion of covariance of physical observables, which in the presence of a uniform magnetic field takes the form:

$$V_y F_\omega V_y^* = F_{\tau_y \omega}. \quad (2.15)$$

We will always assume that the matrix elements $\langle x | F_\omega | y \rangle$ are measurable functions of ω , which is indeed the case for the applications considered here.

Proposition 2.5 *Let $F_\omega, F'_\omega, \dots$ be covariant operators. Then \mathbb{P} -almost surely:*

$$\lim_{|V| \rightarrow \infty} \text{tr}_V (\Pi_V F_\omega F'_\omega \dots \Pi_V^*) = \int_\Omega d\mathbb{P}(\omega) \text{tr}(\langle 0 | F_\omega F'_\omega \dots | 0 \rangle), \quad (2.16)$$

where V is a cube from \mathbb{Z}^d and $|V|$ is its cardinality. The functional on the righthand side defines the trace per volume, which will be denoted by $\mathcal{T}(\cdot)$ throughout.

Proof We have:

$$\mathrm{tr}_V(\Pi_V(F_\omega F'_\omega \dots)\Pi_V) = \frac{1}{|V|} \sum_{x \in V} \mathrm{tr}(\langle x | F_\omega F'_\omega \dots | x \rangle), \quad (2.17)$$

and the last term can be written equivalently as:

$$\frac{1}{|V|} \sum_{x \in V} \mathrm{tr}(\langle 0 | V_x^*(F_\omega F'_\omega \dots) V_x | 0 \rangle) = \frac{1}{|V|} \sum_{x \in V} \mathrm{tr}(\langle 0 | F_{\tau_{-x}\omega} F'_{\tau_{-x}\omega} \dots | 0 \rangle). \quad (2.18)$$

Then we are in the conditions of Birkhoff ergodic theorem [10] and the statement follows. \square

Remark 2.6 One important implication of the above statement is that the intensive thermodynamic coefficients connected to the covariant physical observables do not fluctuate from one disorder configuration to another or, in other words, it has the self-averaging property in the thermodynamic limit. \diamond

When disorder is present, all the coefficients of the Hamiltonians develop a random component. The most general form of a covariant Hamiltonian on a lattice takes the form:

$$H_\omega = \sum_{x,y \in \mathbb{Z}^d} w_y(\tau_x \omega) \otimes |x\rangle \langle x| U_y = \sum_{x,y \in \mathbb{Z}^d} e^{i y \wedge x} w_y(\tau_x \omega) \otimes |x\rangle \langle x - y|. \quad (2.19)$$

We will assume that the hopping matrices w_y are continuous functions over Ω with values in $M_N(\mathbb{C})$. We will also assume a certain rapid decay of w_y with y , to be precisely quantified in Sect. 6.1. These assumptions are quite natural and fulfilled by most model Hamiltonians.

Example 2.7 (“Linearized” disordered models) Most of the numerical simulations found in the physics literature consider linearizations of the coefficients:

$$w_y(\omega) = w_y + \sum_{\alpha} \omega_0^\alpha \lambda_y^\alpha, \quad (2.20)$$

where w_y and λ_y^α are non-stochastic $N \times N$ matrices. Furthermore, ω_x^α are drawn randomly and independently from the interval $[-\frac{1}{2}, \frac{1}{2}]$. Hence, the disorder configuration space is just the Hilbert cube whose topology is discussed in great detail in e.g. [14, Chap. 5]. Inserting these expressions in (2.19) leads to:

$$H_\omega = \sum_{x,y \in \mathbb{Z}^d} \left(w_y + \sum_{\alpha} \omega_x^\alpha \lambda_y^\alpha \right) \otimes |x\rangle \langle x| U_y. \quad (2.21)$$

In the physicists' jargon, the random fluctuations in the coefficients $w_{y \neq 0}$ are often referred to as bond disorder, while to those in $w_{y=0}$ as on-site disorder. \diamond

2.3 Disorder Regimes

Consider the following simplified Hamiltonian on the Hilbert space $\ell^2(\mathbb{Z}^d)$:

$$H_\omega = \lambda_0 H_0 + \lambda_1 \sum_{x \in \mathbb{Z}^d} \omega_x |x\rangle \langle x|, \quad (2.22)$$

where H_0 is a non-stochastic periodic Hamiltonian and λ 's are just real numbers. There are two extreme limits where the spectral properties of H_ω can be readily understood. One is $\lambda_1 = 0$ when Bloch-Floquet theory can be applied, in which case the spectrum is absolutely continuous and can be graphed as energy bands versus quasi-momentum. The other extreme is $\lambda_0 = 0$, when the Hamiltonian is already diagonal and the spectrum is pure-point, with eigenvalues $\{\lambda_1 \omega_x\}_{x \in \mathbb{Z}^d}$ and corresponding eigenvectors localized on the lattice's sites $\{|x\rangle\}_{x \in \mathbb{Z}^d}$. Note that the set of eigenvalues is a countable subset of the real axis, hence of zero Lebesgue measure, yet the set is \mathbb{P} -almost sure dense in its interval. These are the trades of the Anderson localized spectrum.

Definition 2.8 The part of the *essential* spectrum which is pure-point and has corresponding eigenvectors that are exponentially localized in space is called the Anderson localized spectrum. The complement part of the essential spectrum will be called the Anderson delocalized spectrum.

In the intermediate regimes where both randomly fluctuating and non-fluctuating components are present in a Hamiltonian, both Anderson localized and delocalized spectra are expected to be present. If the space dimension is low, specifically for $d = 1$ and 2, Anderson and collaborators [1] found that sometimes even small random fluctuations can localize the entire energy spectrum. In fact, this was believed to be the rule rather than the exception because, until the discovery of the topological insulators, there were only a handful of known exceptions. The situation is somewhat different in higher dimensions, where typically only the regions around the spectral edges are localized while the spectral regions deep inside the bands remain delocalized, though, the spectrum is expected to become entirely localized for extremely strong disorder. Below we briefly discuss the regimes of weak and strong disorder. For an in-depth treatment of the subject, the reader can consult the monograph [5].

Remark 2.9 Perhaps now it becomes more clear how extraordinary are the claims contained in the classification table. If the topology is nontrivial, then, even in lower dimensions, regions of extended spectrum can exist in the presence of large random fluctuations and the entire boundary spectrum can avoid the Anderson localization phenomenon. \diamond

Let us now assume that, in the absence of disorder, we are dealing with an insulator, hence the Hamiltonian has a spectral gap in its spectrum and the Fermi level is pinned in the middle of this gap. Note that the spectrum of covariant Hamiltonians is non-random and, quite generally, the edges of the energy spectrum depend continuously on the amplitudes of the random fluctuations. Hence, if the random fluctuations are small, such as when $\lambda_1 \ll \lambda_0$ in the example (2.22), the spectral gap persists and the Fermi level continues to be located in a region free of spectrum. One refers to this regime as the regime of weak disorder. In this regime, the matrix elements $\langle x | P_F(\omega) | y \rangle$ of the Fermi projection are rapidly decaying with the separation $|x - y|$, uniformly in ω . If the Hamiltonian is of finite-range, *i.e.* $w_y = 0$ outside a finite neighborhood of the origin, or if w_y decays with y exponentially fast, then:

$$\sup_{\omega \in \Omega} \|\langle x | P_F(\omega) | y \rangle\| \leq A e^{-\beta|x-y|}, \quad 0 < A, \beta < \infty. \quad (2.23)$$

The inequality can be established by a straightforward application of the Combes–Thomas technique [12]. The ordinary perturbation theory is available in this regime and can be used to investigate the behavior of the Fermi projection under various deformations of the models. In particular, to establish that $P_F(\omega)$ varies continuously in the topology of $\mathbb{B}(\mathcal{H})$ induced by the operator norm.

When the amplitudes of the random fluctuations become large, the spectral gap closes but a region of Anderson localized spectrum may still survive. This region is typically sandwiched between two regions of Anderson delocalized spectrum and in such situations one speaks of a mobility gap. One refers to this regime as the regime of strong disorder. Note that the Fermi level is now located in the essential spectrum but the quantum diffusion is absent. In this regime the ordinary perturbation theory does not apply. Also, the location of the eigenvalues in the Anderson localized spectrum fluctuate from one disorder configuration to another, and when a model is deformed continuously, these eigenvalues shift and inherently cross the Fermi level. These crossings can come simultaneously from below and above, hence they cannot be avoided, *e.g.* by shifting the Fermi level. As a result, the Fermi projection does not vary continuously under the deformations of the models, in neither of the natural topologies of $\mathbb{B}(\mathcal{H})$.

Remark 2.10 The above phenomenon happens also when one tries to compute the bulk invariants using twisted boundary conditions [16]. As a result, the numerical values of the invariants, as computed by such methods, fluctuate from one disorder configuration to another and the quantization can be seen only after the disorder average is taken. As we shall see, this is not the case for the computational methods reviewed here, where the self-averaging property manifests explicitly. \diamond

A convenient and effective way to describe the Anderson localized spectrum is through the Aizenman–Molchanov bound on the resolvent [4]:

$$\int_{\Omega} d\mathbb{P}(\omega) \|\langle x | (\varepsilon + i\delta - H_{\omega})^{-1} | y \rangle\|^s \leq A_s e^{-\beta_s|x-y|}, \quad s \in (0, 1), \quad (2.24)$$

assumed to hold uniformly in $\delta \in (0, \infty)$. Above, A_s and β_s are strictly positive and finite parameters. The Aizenman–Molchanov bound automatically implies all characteristics of the Anderson localization [2, 3, 5], such as absence of diffusion, pure-point nature of the spectrum, exponential decay of the eigenvectors at infinity and exponential decay of the averaged matrix elements of the Fermi projection:

$$\int_{\Omega} d\mathbb{P}(\omega) \left\| \langle x | P_F(\omega) | y \rangle \right\| \leq A e^{-\gamma|x-y|}, \quad 0 < A, \gamma < \infty. \quad (2.25)$$

Note that without the average, the inequality (2.25) fails for ω in a set of strictly positive measure, no matter how large we pick the constant A . The bound (2.24) is known to hold for finite-range Hamiltonians in all situations where Anderson localization was established with mathematical rigor [5].

2.4 Topological Invariants

The theory of the topological bulk invariants for the phases classified by \mathbb{Z} or $2\mathbb{Z}$ in Table 1.1 was developed in [8, 24, 25] for the regime of strong disorder. The recent work [11] by Bourne and Rennie extended these result to continuum models. Below we briefly state the main results for the discrete case, which are covered extensively in [26]. A brisk review of the methods involved by these works can be found in [22].

For periodic models, the Bloch-Floquet transformation \mathcal{F} over the d -dimensional Brillouin torus \mathbb{T}^d gives:

$$\mathcal{F} H \mathcal{F}^* = \int_{\mathbb{T}^d}^{\oplus} dk H_k, \quad \mathcal{F} P_F \mathcal{F}^* = \int_{\mathbb{T}^d}^{\oplus} dk P_F(k). \quad (2.26)$$

The analysis is then reduced to that of smooth families of $N \times N$ matrices:

$$H_k : \mathbb{C}^N \rightarrow \mathbb{C}^N, \quad H_k = \sum_{y \in \mathbb{Z}} e^{i y \cdot k} w_y, \quad P_F(k) = \chi(H_k \leq \varepsilon_F).$$

Throughout, $x \cdot x'$ will denote the Euclidean scalar product. In this simplified setting, the top even Chern number takes the familiar form [6] ($d = \text{even}$):

$$\text{Ch}_d(P_F) = \frac{(2\pi i)^{\frac{d}{2}}}{(\frac{d}{2})!} N \sum_{\rho \in \mathcal{S}_d} (-1)^\rho \int_{\mathbb{T}^d} \frac{dk}{(2\pi)^d} \text{tr} \left(P_F(k) \prod_{j=1}^d \frac{\partial P_F(k)}{\partial k_{\rho_j}} \right). \quad (2.27)$$

Similarly, the top odd Chern number takes the familiar form [27] ($d = \text{odd}$):

$$\text{Ch}_d(U_F) = \frac{i(\pi)^{\frac{d-1}{2}}}{d!!} N \sum_{\rho \in S_d} (-1)^\rho \int_{\mathbb{T}^d} \frac{dk}{(2\pi)^d} \text{tr} \left(\prod_{j=1}^d U_F^*(k) \frac{\partial U_F(k)}{\partial k_{\rho_j}} \right). \quad (2.28)$$

Throughout, S_I will denote the group of permutations of the finite set I . In particular S_d denotes the permutation group of $\{1, \dots, d\}$.

For the generic models (2.19), the top even Chern number can be formulated [8, 24] using a real-space representation of the operators and the trace per volume $\mathcal{T}(\cdot) = \lim_{V \rightarrow \infty} \text{tr}_V(\cdot)$ from Proposition 2.5:

$$\text{Ch}_d(P_F) = \frac{(2\pi i)^{\frac{d}{2}}}{(\frac{d}{2})!} N \sum_{\rho \in S_d} (-1)^\rho \mathcal{T} \left(P_F(\omega) \prod_{j=1}^d (i[P_F(\omega), X_{\rho_j}]) \right). \quad (2.29)$$

When the disorder and the magnetic fields are turned off, this expression become identically with (2.27). In the general case, the quantization of (2.29) follows from:

Theorem 2.11 ([8, 24]) *Let d be even and let $\{P_\omega\}_{\omega \in \Omega}$ be a family of covariant projections over $\mathbb{C}^N \otimes \ell^2(\mathbb{Z}^d)$ such that:*

$$\sum_{x \in \mathbb{Z}^d} (1 + |x|)^{d+1} \int_{\Omega} d\mathbb{P}(\omega) \text{tr}(|\langle 0 | P_\omega | x \rangle|^{d+1}) < \infty. \quad (2.30)$$

Consider the family of operators on $\mathbb{C}^{2^{\frac{d}{2}}} \otimes \mathbb{C}^N \otimes \ell^2(\mathbb{Z}^d)$:

$$F_{\omega, x_0} = I \otimes P_\omega \left(\frac{\Gamma \cdot (X + x_0)}{|X + x_0|} \right) I \otimes P_\omega = \begin{pmatrix} 0 & G_{\omega, x_0}^* \\ G_{\omega, x_0} & 0 \end{pmatrix}, \quad x_0 \in (0, 1)^d, \quad (2.31)$$

where $\Gamma = (\Gamma_1, \dots, \Gamma_d)$ is an irreducible representation of the even d -dimensional complex Clifford algebra Cl_d and $\Gamma \cdot (X + x_0)$ is a shorthand for $\sum_{j=1}^d \Gamma_j \otimes I \otimes (X + x_0)_j$. Also, the second equality in (2.31) gives the decomposition of F_{ω, x_0} w.r.t. to the natural inner grading of Cl_d . Then G_{ω, x_0} is \mathbb{P} -almost surely a Fredholm operator on the range of $I \otimes P_\omega$. Its almost sure Fredholm index is independent of x_0 and \mathbb{P} -almost surely independent of $\omega \in \Omega$, and is given by the formula:

$$\text{Index } G_{\omega, x_0} = \frac{(2i\pi)^{\frac{d}{2}}}{(\frac{d}{2})!} N \sum_{\rho \in S_d} (-1)^\rho \mathcal{T} \left(P_\omega \prod_{j=1}^d i[P_\omega, X_{\rho_j}] \right). \quad (2.32)$$

Remark 2.12 In the regime of strong disorder when the Fermi level lies in the essential spectrum, the physical interpretation of the top even Chern number in dimension $d = 2$ has been elucidated in [8]. There, the reader can find a derivation of the finite-temperature Kubo-formula for the conductivity tensor in the presence of disorder and dissipation, together with a proof of the following limit:

$$\lim_{T \rightarrow 0} \sigma_{12}(T, \varepsilon_F) = \text{Ch}_2(P_F) , \quad (2.33)$$

provided the conditions of the Theorem 2.11 are satisfied. Here, σ_{12} denotes the off-diagonal or the Hall component of the linear conductivity tensor $\{\sigma_{ij}\}_{i,j=\overline{1,d}}$. The latter provides the linear link between the current-density J set in motion by an externally applied electric field E :

$$J_i = \sum_{j=1}^d \sigma_{ij} E_j . \quad (2.34)$$

In higher dimensions, it was shown in [26] that, up to an un-interesting constant:

$$\text{Ch}_d(P_F) = \frac{\partial^{\frac{d}{2}-1} \sigma_{i_{d-1} i_d}}{\partial \phi_{i_1 i_2} \dots \partial \phi_{i_{d-3} i_{d-2}}} , \quad (2.35)$$

where the set of indices at the righthand side is such that $\{i_1, \dots, i_d\} = \{1, \dots, d\}$. According to this result, the top even Chern numbers can be interpreted as non-linear magneto-electric transport coefficients. \diamond

Similarly, in odd dimensions, the top odd Chern number can be formulated for generic disordered models with chiral symmetry as [19]:

$$\text{Ch}_d(U_F) = \frac{i(i\pi)^{\frac{d-1}{2}}}{d!!} N \sum_{\rho \in \mathcal{S}_d} (-1)^\rho \mathcal{T} \left(\prod_{j=1}^d U_F^*(\omega) i[U_F(\omega), X_{\rho_j}] \right) . \quad (2.36)$$

When the disorder and the magnetic fields are turned off, this expression become identically with (2.28). In the general case, the quantization of (2.36) follows from:

Theorem 2.13 ([25]) *Let d be odd and let $\{U_\omega\}_{\omega \in \Omega}$ be a family of covariant unitary operators over $\mathbb{C}^N \otimes \ell^2(\mathbb{Z}^d)$ such that:*

$$\sum_{x \in \mathbb{Z}^d} (1 + |x|)^{d+1} \int_{\Omega} d\mathbb{P}(\omega) \text{tr} \left(|\langle 0 | U_\omega | x \rangle|^{d+1} \right) < \infty . \quad (2.37)$$

Consider the family of operators on $\mathbb{C}^{2^{\frac{d-1}{2}}} \otimes \mathbb{C}^N \otimes \ell^2(\mathbb{Z}^d)$:

$$F_{\omega, x_0} = \frac{1}{4} \left(I + \frac{\Sigma \cdot (X + x_0)}{|X + x_0|} \right) (I \otimes U_\omega) \left(I + \frac{\Sigma \cdot (X + x_0)}{|X + x_0|} \right) , \quad x_0 \in (0, 1)^d , \quad (2.38)$$

where $\Sigma = (\Sigma_1, \dots, \Sigma_d)$ is an irreducible representation of the odd d -dimensional complex Clifford algebra Cl_d and $\Sigma \cdot (X + x_0)$ is a shorthand for $\sum_{j=1}^d \Sigma_j \otimes I \otimes (X + x_0)_j$. Then F_{ω, x_0} is \mathbb{P} -almost surely a Fredholm operator. Its almost sure Fredholm

index is independent of x_0 and \mathbb{P} -almost surely independent of $\omega \in \Omega$, and is given by the formula:

$$\text{Index } F_{\omega, x_0} = \frac{i(i\pi)^{\frac{d-1}{2}}}{d!!} N \sum_{\rho} (-1)^{\rho} \mathcal{T} \left(\prod_{j=1}^d U_{\omega}^* i[U_{\omega}, X_{\rho_j}] \right). \quad (2.39)$$

Remark 2.14 The physical interpretation of the top odd Chern numbers has been elucidated in [26]. If P^c denotes the vector of chiral polarization, that is, the difference between the electric polarizations corresponding to the two chiral sectors, then, for d odd:

$$\text{Ch}_d(P_F) = \frac{\partial^{\frac{d-1}{2}} P_{i_d}^c}{\partial \phi_{i_1 i_2} \dots \partial \phi_{i_{d-2} i_{d-1}}}, \quad (2.40)$$

where the set of indices at the righthand side is such that $\{i_1, \dots, i_d\} = \{1, \dots, d\}$. According to this result, the top odd Chern numbers can be interpreted as non-linear magneto-electric response coefficients. \diamond

Remark 2.15 Note that the Dirac operators and the appended Hilbert space in the index theorems for both even and odd Chern numbers are just auxiliary mathematical constructs and have no direct connection with the physics. \diamond

As we already mentioned, in the regime of strong disorder, the Fermi projection, hence also the Fermi unitary operator when chiral symmetry is present, do not vary continuously in norm under the deformations of the models. As such, the invariance of the Fredholm index w.r.t. norm-deformations cannot be used in this context. However, under the Aizenman–Molchanov condition, the righthand side of (2.32) (or of (2.39)) varies continuously with the deformations of the models [24, 25]. As such, using both sides of (2.32) and (2.39), one can indeed establish the quantization and invariance of the bulk topological numbers under the Anderson localization assumption. Given all the above, we can conclude at once that the only way to change the bulk topological invariants is by violating the Aizenman–Molchanov condition, that is, through an Anderson localization-delocalization transition.

The derivations of Theorems 2.11 and 2.13 together with the context in which they naturally occur, which is Alain Connes’ non-commutative geometry [13], is the subject of the monograph [26]. In the present work, we are primarily concerned with how to compute the topological invariants once we are given a concrete disordered model. It turns out that the algebraic framework introduced by Jean Bellissard [7], and used in [26] for quite different purposes, provides just the right framework for the computer assisted calculations as well as for the analysis of the error bounds.

References

1. Abrahams, E., Anderson, P.W., Licciardello, D., Ramakrishnan, T.: Scaling theory of localization: absence of quantum diffusion in two dimensions. *Phys. Rev. Lett.* **42**, 673–676 (1979)
2. Aizenman, M.: Localization at weak disorder: some elementary bounds. *Rev. Math. Phys.* **6**, 1163–1182 (1994)
3. Aizenman, M., Elgart, A., Naboko, S., Schenker, J.H., Stolz, G.: Moment analysis for localization in random Schrödinger operators. *Invent. Math.* **163**, 343–413 (2006)
4. Aizenman, M., Molchanov, S.: Localization at large disorder and at extreme energies: an elementary derivation. *Commun. Math. Phys.* **157**, 245–278 (1993)
5. Aizenman, M., Warzel, S.: Random operators: disorder effects on quantum spectra and dynamics. AMS, Providence (2015)
6. Avron, J.E., Sadun, L., Segert, J., Simon, B.: Chern numbers, quaternions, and Berry's phases in Fermi systems. *Commun. Math. Phys.* **124**, 595–727 (1989)
7. Bellissard, J.: K -theory of C^* -algebras in solid state physics. In: Dorlas, T., Hugenholtz, M., Winnink, M. (eds.) *Lecture Notes in Physics*, vol. 257, pp. 99–156. Springer, Berlin (1986)
8. Bellissard, J., van Elst, A., Schulz-Baldes, H.: The non-commutative geometry of the quantum Hall effect. *J. Math. Phys.* **35**, 5373–5451 (1994)
9. Bernevig, B.A., Hughes, T.L., Zhang, S.-C.: Quantum spin Hall effect and topological phase transition in HgTe quantum wells. *Science* **314**, 1757–1761 (2006)
10. Birkhoff, G.D.: Proof of the ergodic theorem. *Proc. Natl. Acad. Sci. USA* **17**, 656–660 (1931)
11. Bourne, C., Rennie, A.: Chern Numbers, Localisation and the bulk-edge correspondence for continuous models of topological phases (2016). [arXiv:1611.06016](https://arxiv.org/abs/1611.06016)
12. Combes, J., Thomas, L.: Asymptotic behaviour of eigenfunctions for multiparticle Schrödinger operators. *Commun. Math. Phys.* **34**, 251–270 (1973)
13. Connes, A.: Noncommutative geometry. Academic Press, San Diego (1994)
14. Ingram, W.T., Mahavier, W.S.: Inverse limits. Springer, New York (2012)
15. König, M., Buhmann, H., Molenkamp, L.W., Hughes, T., Liu, C.-X., Qi, X.-L., Zhang, S.-C.: The quantum spin Hall effect: theory and experiment. *J. Phys. Soc. Jpn.* **77**, 031007 (2008)
16. Leung, B., Prodan, E.: Effect of strong disorder in a 3-dimensional topological insulator: phase diagram and maps of the \mathbb{Z}_2 invariant. *Phys. Rev. B* **85**, 205136 (2012)
17. Liu, C.-X., Qi, X.-L., Zhang, H., Dai, X., Fang, Z., Zhang, S.-C.: Model Hamiltonian for topological insulators. *Phys. Rev. B* **82**, 045122 (2010)
18. Marzari, N., Mostofi, A.A., Yates, J.R., Souza, I., Vanderbilt, D.: Maximally localized Wannier functions: theory and applications. *Rev. Mod. Phys.* **84**, 1419–1475 (2012)
19. Mondragon-Shem, I., Song, J., Hughes, T.L., Prodan, E.: Topological criticality in the chiral-symmetric AIII class at strong disorder. *Phys. Rev. Lett.* **113**, 046802 (2014)
20. Ortmann, F., Roche, S., Valenzuela, S.O. (eds.): Topological insulators: fundamentals and perspectives. Wiley-VCH Verlag, Weinheim (2015)
21. Peierls, R.E.: Zur Theorie des diamagnetismus von leitungselektronen. *Zeitschrift für Phys.* **80**, 763–791 (1933)
22. Prodan, E.: The non-commutative geometry of the complex classes of topological insulators. *Topol. Quantum Matter* **1**, 1116 (2014)
23. Prodan, E.: Virtual topological insulators with real quantized physics. *Phys. Rev. B* **91**, 245104 (2015)
24. Prodan, E., Leung, B., Bellissard, J.: The non-commutative n -th Chern number ($n \geq 1$). *J. Phys. A: Math. Theor.* **46**, 485202 (2013)
25. Prodan, E., Schulz-Baldes, H.: Non-commutative odd Chern numbers and topological phases of disordered chiral systems. *J. Funct. Anal.* **271**, 1150–1176 (2016)
26. Prodan, E., Schulz-Baldes, H.: Bulk and boundary invariants for complex topological insulators: From K -Theory to physics. Springer, Berlin (2016)
27. Ryu, S., Schnyder, A.P., Furusaki, A., Ludwig, A.W.W.: Topological insulators and superconductors: tenfold way and dimensional hierarchy. *New J. Phys.* **12**, 065010 (2010)

28. Weng, H., Dai, X., Fang, Z.: Exploration and prediction of topological electronic materials based on first-principles calculations. *MRS Bull.* **39**, 849–858 (2014)
29. Zhang, W., Yu, R., Zhang, H.J., Dai, X., Fang, Z.: First-principles studies of the three-dimensional strong topological insulators Bi_2Te_3 , Bi_2Se_3 and Sb_2Te_3 . *New J. Phys.* **12**, 065013 (2010)

A Computational Non-commutative Geometry Program
for Disordered Topological Insulators

Prodan, E.

2017, X, 118 p. 19 illus. in color., Softcover

ISBN: 978-3-319-55022-0