Chapter 7
Invariants as Measurable Quantities

Abstract This chapter presents various applications to solid state physics of the mathematical results obtained in the earlier chapters. The topological invariants are connected to linear and nonlinear transport coefficients and the expected physical effects are discussed in depth for class A and class AIII of topological insulators, in several space dimensions. Then we follow with an in depth analysis of orbital polarization and magneto-electric effects, and virtual topological insulators are taken up as a more recent development. As a further novel implication, it is shown that the surface states of approximately chiral systems may exhibit a quantum Hall effect with a Hall conductance imposed by the bulk invariants.

7.1 Transport Coefficients of Homogeneous Solid State Systems

The topological invariants are closely related to the transport coefficients. These are briefly reviewed in this section within the operator algebra formalism developed so far. Let us consider a bulk homogeneous solid state system defined by the Hamiltonian $h \in M_N(\mathbb{C}) \otimes \mathcal{A}_d$. Following mainly [20, 195] (see also [168] for a computational perspective), let us assume an effective time evolution $e^{t\mathfrak{L}}$ on $M_N(\mathbb{C}) \otimes \mathcal{A}_d$ in the presence of a macroscopic electric field $\mathscr{E}$ and dissipation, generated by the densely defined derivation

$$\mathfrak{L}(a) = \mathrm{i}[a, h] + \langle \mathscr{E}, \partial a \rangle + \Gamma(a) \ ,$$

where Γ is the so called collision (super-) operator having adequate dissipation properties [195]. Recall that $\langle\ ,\ \rangle$ denotes the Euclidean scalar product. The temporal evolution of a density matrix is $\rho_t = e^{t\mathfrak{L}^*}\rho_0$ for a given an initial density matrix ρ_0. Now one is interested in computing (or measuring) the time average charge current density

$$\mathfrak{J} \;=\; \lim_{T\to\infty} \tfrac{1}{T} \int_0^T dt\ \mathcal{T}\big(\mathfrak{j}\, \rho_t\big)\ , \tag{7.1}$$

where $\mathfrak{j} = \partial h = \{\partial_j h\}_{j=1,\ldots,d}$ is the observable representing the charge current.

E. Prodan and H. Schulz-Baldes, *Bulk and Boundary Invariants for Complex Topological Insulators*, Mathematical Physics Studies,
DOI 10.1007/978-3-319-29351-6_7

Proposition 7.1.1 ([20, 195, 196]) *Assume the initial state of the system to be that of thermal equilibrium, namely the initial density matrix is the Fermi-Dirac function*

$$\rho_0 \;=\; f_{\beta,\mu}(h) \;=\; \frac{1}{1+\exp\big(\beta(h-\mu)\big)}\;.$$

Then:

(i) *The current density is given by* $\mathfrak{J}_i = \sum_{j=1}^{d} \sigma_{i,j}\mathscr{E}_j + o(\mathscr{E}^2)$, $i = 1, \ldots, d$, *with the linear conductivity tensor* σ *given by the Kubo formula*

$$\sigma_{i,j} \;=\; \mathcal{T}\Big((\partial_i h)\,\mathfrak{L}^{-1}\big(\partial_j f_{\beta,\mu}(h)\big)\Big)\;.$$

(ii) *If BGH or MBGH holds, the off-diagonal components of the linear conductivity tensor converge in the limit* $\beta \to \infty$ *and* $\Gamma \to 0$ *to*

$$\boxed{\sigma_{i,j} \;=\; \big\langle[\xi_{\{i,j\}}],[p_F]_0\big\rangle \;=\; \mathrm{Ch}_{\{i,j\}}(p_F)\;,} \tag{7.2}$$

for $1 \le i \ne j \le d$, *while the diagonal components vanish in this limit.*

The above statement provides a direct link between the 2-cocycles and the linear conductivity tensor. By taking derivatives with respect to the magnetic field of Eq. (7.2) and using the generalized Streda formulas from Corollary 5.6.4, we will be able to establish direct links between higher cocycles and non-linear transport coefficients. This will be quite relevant for the analysis in dimensions higher than $d = 2$.

We now turn our attention to the charge transport parallel the boundary of a solid state system defined by $\hat{h} = (h, \tilde{h}) \in M_N(\mathbb{C}) \otimes \widehat{\mathcal{A}}_d$. The observable representing the charge current parallel to the boundary is given by $\hat{\jmath} = \widehat{\partial}\hat{h}$, which indeed provides the expected expression when represented on the Hilbert space,

$$\widehat{\pi}_\omega(\hat{\jmath}) \;=\; \mathrm{i}[\widehat{H}_\omega, \widehat{X}]\;,$$

with $\widehat{X} = (X_1, \ldots, X_{d-1})$. Now, assume that BGH applies and let $f_{\mathrm{Exp}} : \mathbb{R} \to [0,1]$ be as in Proposition 4.3.1, that is, its derivative f'_{Exp} is positive and supported in the bulk gap and $\int dE\, f'_{\mathrm{Exp}}(E) = 1$, and

$$[\tilde{u}_\Delta]_1 \;=\; \mathrm{Exp}[p_F]_0 \;=\; [\exp(2\pi\mathrm{i} f_{\mathrm{Exp}}(\hat{h}))]_1\;.$$

The function $f'_{\mathrm{Exp}}(\hat{h})$ can be regarded as a density matrix, and since f'_{Exp} is smooth and with support inside the bulk gap, this function is an element from the boundary algebra and in fact from the smooth sub-algebra $\mathscr{E}_d$. Then

$$\widetilde{\mathfrak{J}} \;=\; \widetilde{\mathcal{T}}\big(f'_{\mathrm{Exp}}(\hat{h})\,\widehat{\partial}\hat{h}\big) \tag{7.3}$$

is the well-defined charge current density, flowing along the boundary when the quantum states are populated with a statistical weight given by $f'_{\text{Exp}}(E)$. We will refer to $\widetilde{\mathfrak{J}}$ as the boundary current.

Proposition 7.1.2 ([197, 107]) *The following identity holds for* $j = 1, \ldots, d-1$*:*

$$\mathrm{i}\,\widetilde{\mathcal{T}}\Big(\big(\exp(-2\pi\mathrm{i}f_{\text{Exp}}(\hat{h})) - \mathbf{1}\big)\,\widehat{\partial}_j \exp(2\pi\mathrm{i}f_{\text{Exp}}(\hat{h}))\Big) \;=\; -2\pi\;\widetilde{\mathcal{T}}\big(f'_{\text{Exp}}(\hat{h})\,\widehat{\partial}_j\hat{h}\big)\;. \quad (7.4)$$

Written differently,

$$\boxed{\widetilde{\text{Ch}}_{\{j\}}(\tilde{u}_\Delta) \;=\; -2\pi\;\widetilde{\mathfrak{J}}_j\;.} \quad (7.5)$$

Sketch of Proof Let Wind denote the quantity on the l.h.s. of (7.4). Expanding the exponential under the derivation as a series and using the Leibniz rule

$$\text{Wind} \;=\; \mathrm{i}\sum_{m=1}^{\infty}\frac{(2\pi\mathrm{i})^m}{m!}\sum_{l=0}^{m-1}\widehat{\mathcal{T}}\Big((\tilde{u}^*_\Delta - \mathbf{1})\,f_{\text{Exp}}(\hat{h})^l\,\widehat{\partial}_j f_{\text{Exp}}(\hat{h})\,f_{\text{Exp}}(\hat{h})^{m-l-1}\Big)\;,$$

where the trace and the infinite sum can be exchanged because $\tilde{u}_\Delta - \mathbf{1}$ belongs to the smooth sub-algebra $\mathscr{E}_d$. Due to cyclicity and the fact that $[\tilde{u}_\Delta, f_{\text{Exp}}(\hat{h})] = 0$, each summand is equal to $\widetilde{\mathcal{T}}((\tilde{u}^*_\Delta - 1)\,f_{\text{Exp}}(\hat{h})^{m-1}\,\widehat{\partial}_j f_{\text{Exp}}(\hat{h}))$. Exchanging the sum and the trace again and summing up the exponential,

$$\text{Wind} = \mathrm{i}\,\widetilde{\mathcal{T}}((\tilde{u}^*_\Delta - 1)\,\widehat{\partial}_j\tilde{u}_\Delta) \;=\; 2\pi\;\widetilde{\mathcal{T}}\Big((\mathbf{1} - \tilde{u}_\Delta)\,\widehat{\partial}_j f_{\text{Exp}}(\hat{h})\Big)\;.$$

Now let us use the homomorphism property of the pairing and repeat the same argument for $\tilde{u}^k_\Delta = \exp(2\pi\mathrm{i}\,k\,f_{\text{Exp}}(\hat{h}))$ with $k \neq 0$,

$$\text{Wind} \;=\; \frac{\mathrm{i}}{k}\,\widetilde{\mathcal{T}}\big((\tilde{u}^k_\Delta - \mathbf{1})^*\widehat{\partial}_j\hat{u}^k\big) \;=\; 2\pi\;\widetilde{\mathcal{T}}\Big((\mathbf{1} - \tilde{u}^k_\Delta)\,\widehat{\partial}_j f_{\text{Exp}}(\hat{h})\Big)\;.$$

Writing $f_{\text{Exp}}(E) = \int_{-\infty}^{\infty} dt\,\tilde{f}_{\text{Exp}}(t)\,e^{-E(1+\mathrm{i}t)}$ as a Laplace transform with an adequate function $\tilde{f}_{\text{Exp}}$, the last expression can be further processed using Duhamel's formula

$$\text{Wind} \;=\; 2\pi\int_{-\infty}^{\infty} dt\,\tilde{f}_{\text{Exp}}(t)\,(1+\mathrm{i}t)\int_0^1 dq\,\widetilde{\mathcal{T}}\Big((\hat{u}^k - \mathbf{1})\,e^{-(1-q)(1+\mathrm{i}t)\hat{h}}(\widehat{\partial}_j\hat{h})e^{-q(1+\mathrm{i}t)\hat{h}}\Big)\;.$$

Using the cyclic property of the trace and $f'_{\text{Exp}}(E) = -\int dt\,(1+\mathrm{i}t)\tilde{f}_{\text{Exp}}(t)\,e^{-E(1+\mathrm{i}t)}$, one therefore finds for $k \neq 0$,

$$\text{Wind} \;=\; 2\pi\;\widetilde{\mathcal{T}}\Big((\hat{u}^k - \mathbf{1})f'_{\text{Exp}}(\hat{h})\,\widehat{\partial}_j\hat{h}\Big)\;.$$

For $k = 0$, the r.h.s. vanishes, a fact which will be used below.

To conclude, let us choose a differentiable function $\phi : [0, 1] \to \mathbb{R}$ vanishing at the boundary points 0 and 1. Its Fourier coefficients will be denoted by $a_k = \int_0^1 dx\, e^{-2\pi \imath kx}\phi(x)$. Then $\sum_k a_k e^{2\pi \imath kx} = \phi(x)$ and thus $\sum_k a_k = 0$. Hence

$$\begin{aligned} a_0 \text{ Wind} &= -\sum_{k\neq 0} a_k \text{ Wind} \\ &= -2\pi \sum_k a_k\, \widetilde{\mathcal{T}}\Big((\mathbf{1} - \hat{u}^k) f'_{\text{Exp}}(\hat{h})\, \widehat{\partial}_j \hat{h}\Big) \\ &= -2\pi\, \widetilde{\mathcal{T}}\big(\phi(f_{\text{Exp}}(\hat{h})) f'_{\text{Exp}}(\hat{h})\, \widehat{\partial}_j \hat{h}\big)\,. \end{aligned}$$

Finally, we let ϕ converge to the indicator function of $[0, 1]$. Then $a_0 \to 1$, while on the other hand $\phi(f_{\text{Exp}}(\hat{h}))f'_{\text{Exp}}(\hat{h}) \to f'_{\text{Exp}}(\hat{h})$ (the Gibbs phenomenon is damped). This concludes the proof. □

The above statement establishes a direct link between the boundary 1-cocycles and the charge current density flowing along the boundary. By taking derivatives with respect to the magnetic field of Eq. (7.2) and using the generalized Streda formulas from Corollary 5.6.4, we will be able to establish direct links between higher cocycles and measurable physical quantities. This will again be quite relevant for the analysis in dimensions higher than $d = 2$. Furthermore, let us point out that the calculation of the above proof combined with a homotopy argument can be used to deal with quantized currents at interfaces of two materials with different topological invariants [124].

7.2 Topological Insulators from Class A in $d = 2$, 3 and 4

In dimension $d = 2$, the topological phases from the unitary class include the classical integer quantum Hall phases and there are many excellent accounts on the physics and mathematics of the integer quantum Hall effect in dimension $d = 2$, and we refrain from giving an incomplete list here. The papers of Bellissard [17, 18] present the bulk theory for tight-binding models and build up the algebraic formalism used in this work. A detailed account of this and an extension to the regime of a MBGH can be found in [20]. The bulk-boundary principle was first demonstrated by Hatsugai in [87] for the rational magnetic flux case, then [107, 197] used the Pimsner-Voiculescu sequence to extend this result to a more general context (see (iii) of Corollary 7.2.1). In particular, [197] also contains a detailed description of the physical interpretation and importance of this result as well as many citations to the physics literature. Later on, other rigorous proofs of bulk-boundary correspondence for tight-binding quantum Hall systems were found [58, 59] and the techniques were extended to models in continuous physical space [45, 108, 109]. An application of the machinery developed in [107, 197] to Chern insulators can be found in [166].

Below we summarize the main statements available for the topological phases from class A in dimension $d = 2$. They follow directly from [20, 107, 197] and they were also known in the physics literature [82], but here we view them as direct corollaries of the theory developed in the previous chapters. Of course, the input from the previous section is absolutely necessary.

Corollary 7.2.1 *Let $\hat{h} = (h, \tilde{h}) \in M_N(\mathbb{C}) \otimes \widehat{\mathcal{A}}_d$ with $d = 2$.*

(i) *If BGH holds, then the integrated density of states can take only the discrete values*

$$\mathfrak{T}(p_F) \;=\; \mathrm{Ch}_{\emptyset}(p_F) \;\in\; \mathbb{Z} \,+\, \frac{B_{1,2}}{2\pi}\,\mathbb{Z}\,.$$

(ii) *If MBGH holds, then the off-diagonal element of the bulk conductivity tensor is quantized by the strong bulk invariant*

$$\sigma_{1,2} \;=\; \mathrm{Ch}_2(p_F) \;\in\; \mathbb{Z}\,.$$

Furthermore, as long as MBGH holds, $\sigma_{1,2}$ remains quantized and invariant to the deformations of h defined by Definition 2.4.5.

(iii) *If BGH holds, then the boundary current is quantized by the bulk and boundary invariants*

$$2\pi\,\widetilde{\mathfrak{J}}_1 \;=\; -\,\widetilde{\mathrm{Ch}}_1(\tilde{u}_\Delta) \;=\; -\,\mathrm{Ch}_2(p_F) \;=\; \sigma_{1,2} \;\in\; \mathbb{Z}\,.$$

Furthermore, if $\mathrm{Ch}_2(p_F) \neq 0$, *the entire boundary spectrum is delocalized.*

Let us point out that (ii) assures us that the topological phases corresponding to the different values of $\mathrm{Ch}_2(p_F)$ are separated by a localization-delocalization phase transitions, which can be sharply identified experimentally via transport measurements, as demonstrated in [42].

In dimension $d = 3$ there are only weak topological phases. Among them are the quantum Hall phases in 3-dimensions. The available results for the latter [83, 119, 120, 122, 123, 142] are restricted to the cases where the entries in the **B** matrix (divided by 2π) are rational numbers. The following statements, which are again direct corollaries of the theory of the previous chapters, generalize them to arbitrary **B** and also include the disorder.

Corollary 7.2.2 *Let $\hat{h} = (h, \tilde{h}) \in M_N(\mathbb{C}) \otimes \widehat{\mathcal{A}}_d$ with $d = 3$ and assume that BGH holds. Then:*

(i) *The integrated density of states can take only the discrete values*

$$\mathfrak{T}(p_F) \;=\; \mathrm{Ch}_{\emptyset}(p_F) \;\in\; \mathbb{Z} \,+\, \sum_{1\leq i<j\leq 3} \frac{B_{i,j}}{2\pi}\,\mathbb{Z}\,.$$

(ii) *The off-diagonal elements of the bulk conductivity tensor are quantized*

$$\sigma_{i,j} \;=\; \mathrm{Ch}_{\{i,j\}}(p_F) \;\in\; \mathbb{Z}\,, \qquad 1 \leq i < j \leq 3\,.$$

Furthermore, as long as BGH holds, $\sigma_{i,j}$'s remains quantized and invariant to the deformations of h defined by Definition 2.4.5.

(iii) *The boundary currents are quantized too*

$$2\pi\;\widetilde{\mathfrak{I}}_j \;=\; -\,\widetilde{\mathrm{Ch}}_j(\tilde{u}_\Delta) \;=\; \mathrm{Ch}_{\{j,3\}}(p_F) \;=\; -\,\sigma_{j,3} \;\in\; \mathbb{Z}\,, \qquad j=1,2\,.$$

Since the weak Chern numbers do not accept an index formula, we cannot replace BGH with MBGH at point (i). In other words, with the methods developed here we cannot conclude that weak topological phases defined by the quantized values of $\sigma_{i,j}$'s are separated by phase boundaries where the localization length diverges, as it happens in $d = 2$. Also, at point (ii), we cannot say anything about the localized/delocalized character of the boundary spectrum, though we can say that is never gapped if any of $\sigma_{\{j,3\}}$ happens to be non-zero. Note that [15] predicted a certain delocalization of the boundary states, hence it will be important to further investigate the weak topological insulators.

Although purely fictitious, the quantum Hall effect in dimension $d = 4$ was conceptually very important in condensed matter theory [172, 228]. Below we summarize our predictions for the hypothetical topological insulators from class A in $d = 4$.

Corollary 7.2.3 *Let $\hat{h} = (h, \tilde{h}) \in M_N(\mathbb{C}) \otimes \widehat{\mathcal{A}}_d$ with $d = 4$.*

(i) *If BGH holds, the integrated density of states can take only the discrete values*

$$\mathfrak{T}(p_F) \;=\; \mathrm{Ch}_{\emptyset}(p_F) \in \mathbb{Z} \;+\; \sum_{\{i,j\}} \frac{B_{i,j}}{2\pi}\,\mathbb{Z} \;+\; \frac{\mathrm{Pf}(\mathbf{B})}{(2\pi)^2}\,\mathbb{Z}\,,$$

where all indices are assumed as being ordered.

(ii) *If BGH holds, the off-diagonal elements of the bulk conductivity tensor take only the discrete values*

$$\sigma_{i,j} \;=\; \mathrm{Ch}_{\{i,j\}}(p_F) \;\in\; \mathbb{Z} \;+\; \frac{B_{k,l}}{2\pi}\,\mathbb{Z}\,,$$

where $k < l$ and such that $\{i,j\} \cap \{k,l\} = \emptyset$. Furthermore, as long as BGH holds, $\sigma_{i,j}$'s remains quantized and invariant to the deformations of h defined by Definition 2.4.5.

(iii) *If MBGH holds, the derivatives of the Hall conductivities w.r.t. to the magnetic field are quantized by the strong invariant*

$$2\pi\;\partial_{B_{i,j}}\sigma_{k,l} \;=\; (-1)^\rho\,\mathrm{Ch}_4(p_F) \;\in\; \mathbb{Z}\,, \qquad \{i,j\} \cap \{k,l\} \;=\; \emptyset\,,$$

where ρ is the permutation which brings $\{i, j, k, l\}$ into $\{1, 2, 3, 4\}$. Furthermore, as long as MBGH holds, $\partial_{B_{i,j}}\sigma_{k,l}$'s remain quantized and invariant to the deformations of h defined by Definition 2.4.5.

(iv) *If BGH holds, then the boundary currents can take only the discrete values*

$$2\pi\,\widetilde{\mathfrak{J}}_j \;=\; -\,\widetilde{\mathrm{Ch}}_j(\tilde{u}_\Delta) \;=\; -\,\mathrm{Ch}_{\{j,4\}}(p_F) \in \mathbb{Z} \;+\; \frac{B_{k,l}}{2\pi}\,\mathbb{Z}\,, \qquad j = 1, 2, 3, \tag{7.6}$$

where $\{k, l\}$ are the unique set of indices such that $\{k, l\} \cap \{j, 4\} = \emptyset$.

(v) *If BGH holds, then the derivatives of the boundary currents w.r.t. the magnetic field are quantized*

$$(2\pi)^2\,\partial_{B_{i,j}}\widetilde{\mathfrak{J}}_k \;=\; -\,(-1)^\rho\,\widetilde{\mathrm{Ch}}_3(\tilde{u}_\Delta) \;=\; -\,(-1)^\rho\,\mathrm{Ch}_4(p_F) \;\in\; \mathbb{Z}, \tag{7.7}$$

where $i \neq j \neq k$ and ρ is the permutation which brings $\{i, j, k\}$ into $\{1, 2, 3\}$. Furthermore, if the above invariants are not zero, then the entire boundary spectrum is necessarily delocalized.

Note that $\partial_{B_{i,j}}\sigma_{k,l}$ represents the second-order response function $\partial^2\mathfrak{J}_k/\partial E_l \partial B_{i,j}$, hence point (iii) predicts the quantization of this physically measurable quantity, in agreement with the original finding in [228].

7.3 Topological Insulators from Class AIII in $d = 1, 2$ and 3

The experimentally measurable bulk properties relevant to the class of chiral symmetric solid state systems are the chiral (orbital) polarization P_{C} and the variations of P_{C} w.r.t. the magnetic field. For a chiral Hamiltonian $H = \{H_\omega\}_{\omega\in\Omega}$ of a solid state system with sub-lattice symmetry, the chiral polarization is defined as the difference between the electric dipole moments per unit cell of the two sub-lattices, which can be written as:

$$P_{\mathrm{C}} \;=\; \int_\Omega \mathbb{P}(d\omega)\;\mathrm{tr}\,\langle 0|P_\omega\, J\, X\, P_\omega|0\rangle\;, \quad P_\omega = \chi(H_\omega \leq 0). \tag{7.8}$$

Using $X|0\rangle = 0$, one can rewrite P_{C} with the non-commutative analysis tools as

$$P_{\mathrm{C}} \;=\; \mathrm{i}\,\mathcal{T}(p_F J \partial p_F)\;.$$

Let up point out that, without the chirality operator J, the r.h.s. would vanish identically. Hence, it is impossible to define the total dipole polarization in this manner. The real reason for this is that definition (7.8) will be ill behaved without J. Now, the following result show that P_{C} is actually of topological nature, namely given by a pairing of a K_1-group element with a 1-cocycle.

Proposition 7.3.1 *Let $h \in M_{2N}(\mathbb{C}) \otimes \mathcal{A}_d$ and assume CH and BGH hold. Then*

$$P_{\mathrm{C},j} \;=\; -\frac{1}{2}\,\big\langle [\xi_{\{j\}}], [u_F]_1 \big\rangle \;=\; -\frac{1}{2}\,\mathrm{Ch}_{\{j\}}(u_F)\;, \qquad j = 1, \ldots, d\;.$$

Proof Recall from (2.34) that

$$p_F \;=\; \frac{1}{2}\begin{pmatrix} \mathbf{1} & -u_F^* \\ -u_F & \mathbf{1} \end{pmatrix}, \qquad J \;=\; \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix}.$$

Thus

$$P_{\mathrm{C}} \;=\; \frac{\mathrm{i}}{4}\,\mathcal{T}\left(\begin{pmatrix} \mathbf{1} & u_F^* \\ -u_F & -\mathbf{1} \end{pmatrix}\begin{pmatrix} 0 & -\partial u_F^* \\ -\partial u_F & 0 \end{pmatrix}\right) \;=\; \frac{\mathrm{i}}{4}\,\mathcal{T}(-u_F^*\partial u_F + u_F \partial u_F^*)\;.$$

Now by Proposition 3.3.2(iv), $u_F(\partial u_F^*) = -(\partial u_F)u_F^*$, so that by cyclicity

$$P_{\mathrm{C}} \;=\; -\frac{\mathrm{i}}{2}\,\mathcal{T}(u_F^*\partial u_F)\;,$$

which is the precisely the claim. □

We now have all the tools to characterize the physics of the chiral symmetric solid state systems. The following statements were discussed extensively in Chap. 1, but we state them for completeness. In the published literature, one can find them in [139, 200].

Corollary 7.3.2 *Let $\hat{h} = (h, \tilde{h}) \in M_{2N}(\mathbb{C}) \otimes \widehat{\mathcal{A}}_d$ with $d = 1$. Assume that CH holds and recall that, for $d = 1$, the spectrum of $\hat{h}$ inside Δ is discrete whenever a bulk spectral gap exists.*

(i) *If the MBGH holds, then the chiral polarization is quantized by the strong bulk invariant*

$$P_{\mathrm{C}} \;=\; -\frac{1}{2}\,\mathrm{Ch}_1(u_F) \;\in\; \frac{1}{2}\,\mathbb{Z}\;.$$

Furthermore, as long as the MBGH holds, P_{C} remains quantized and invariant to the deformations of h defined by Definition 2.4.5.

(ii) *If the BGH holds and $P_{\mathrm{C}} \neq 0$, then by Corollary 4.3.4 there will necessarily be edge states exactly at $E = 0$, which are the zero modes discussed in Sect. 2.3. Furthermore*

$$N_+ \;-\; N_- \;=\; \widetilde{\mathrm{Ch}}_{\emptyset}(\tilde{p}_\Delta) \;=\; -\,\mathrm{Ch}_1(u_F) \;=\; 2\,P_{\mathrm{C}}\;,$$

where $N_\pm$ is the number of zero modes of $\pm$ chirality.

Let us stress that, as for the IQHE, topological phases corresponding to different values of P_{C} are separated by a localization-delocalization phase transition which can be determined experimentally via transport measurements. Next, in dimension $d = 2$, there are only weak chiral systems. Nevertheless, there are some interesting predictions for these systems.

Corollary 7.3.3 *Let $\hat{h} = (h, \tilde{h}) \in M_{2N}(\mathbb{C}) \otimes \widehat{\mathcal{A}}_d$ with $d = 2$ and assume that BGH and CH hold. Then everything said in Corollary 7.2.1 holds and, additionally:*

(i) *The components of the chiral polarization are quantized as*

$$P_{\mathrm{C},j} \;=\; -\tfrac{1}{2}\,\mathrm{Ch}_{\{j\}}(u_F) \;\in\; \tfrac{1}{2}\,\mathbb{Z}\,, \qquad j = 1, 2\,.$$

Furthermore, as long as BGH and CH hold, the components $P_{\mathrm{C},j}$ remain quantized and invariant under the deformations of h defined by Definition 2.4.5.

(ii) *The bulk-boundary principle gives*

$$\widetilde{\mathfrak{T}}(\tilde{p}_\Delta) \;=\; \widetilde{\mathrm{Ch}}_\emptyset(\tilde{p}_\Delta) \;=\; -\,\mathrm{Ch}_{\{2\}}(u_F) \;=\; 2\,P_{\mathrm{C},2}\,.$$

As a consequence, if $P_{\mathrm{C},2} \neq 0$, $\hat{h}$ will have essential spectrum at $E = 0$.

Proof We only need to show point (ii). If the spectrum at the origin is discrete, then we can choose an interval $[-\delta, \delta]$ as in Proposition 4.3.3, and $[-\delta, \delta]$ contains only discrete spectrum of $\hat{h}$. With the notations from Proposition 4.3.3, the bulk-boundary principle gives

$$\widetilde{\mathfrak{T}}\big(\tilde{p}_+(\delta)\big) \;-\; \widetilde{\mathfrak{T}}\big(\tilde{p}_-(\delta)\big) \;=\; 2\,P_{\mathrm{C},2}\,.$$

Hence for $\tilde{p}(\delta) = \tilde{p}_+(\delta) + \tilde{p}_-(\delta)$

$$\widetilde{\mathfrak{T}}\big(\tilde{p}(\delta)\big) \;\geq\; \Big|\widetilde{\mathfrak{T}}\big(\tilde{p}_+(\delta)\big) \;-\; \widetilde{\mathfrak{T}}\big(\tilde{p}_-(\delta)\big)\Big| \;=\; \big|2\,P_{\mathrm{C},2}\big|\,.$$

But for a spectral projector $\tilde{p}(\delta)$ onto discrete spectrum one has $\widetilde{\mathfrak{T}}\big(\tilde{p}(\delta)\big) = 0$, and this is a contradiction. □

The bulk invariants appearing in (i) of Corollary 7.3.3 are weak odd Chern numbers, hence we cannot replace the BGH by the MBGH. Consequently, with the methods developed so far, we cannot conclude that weak topological phases defined by the quantized values of $P_{\mathrm{C},j}$'s are separated by phase boundaries where the localization length diverges, as it happens in $d = 1$. Also, in item (ii), we cannot say anything about the localized or delocalized character of the boundary spectrum appearing at $E = 0$.

Corollary 7.3.4 *Let $\hat{h} = (h, \tilde{h}) \in M_{2N}(\mathbb{C}) \otimes \widehat{\mathcal{A}}_d$ with $d = 3$ and assume that the CH holds. Then:*

(i) *If the BGH holds, the components of the chiral polarization take discrete values*

$$P_{\mathrm{C},i} \;=\; -\tfrac{1}{2}\big\langle[\xi_{\{i\}}],[u_F]_1\big\rangle \;=\; -\tfrac{1}{2}\mathrm{Ch}_{\{i\}}(u_F) \;\in\; \tfrac{1}{2}\,\mathbb{Z} \;+\; \frac{B_{j,k}}{4\pi}\,\mathbb{Z}\,, \quad i \neq j \neq k \neq i\,.$$

Furthermore, as long as BGH holds, the components $P_{\mathrm{C},i}$ remain quantized and invariant to the deformations of h defined by Definition 2.4.5.

(ii) *If the MBGH holds, then the chiral magneto-electric response coefficients are quantized by a strong invariant*

$$\partial_{B_{i,j}} P_{\mathrm{C},k} \;=\; \frac{1}{4\pi}\,\big\langle[\xi_{\{i,j,k\}}],[u_F]_1\big\rangle \;=\; \frac{\eta}{4\pi}\,\mathrm{Ch}_3(u_F) \;\in\; \frac{1}{4\pi}\,\mathbb{Z}\,,$$

with η the sign of the permutation which brings i, j, k to the natural order. Furthermore, as long as the MBGH holds, $\partial_{B_{i,j}} P_{\mathrm{C},k}$ remains quantized and invariant to the deformations of h defined by Definition 2.4.5.

(iii) *If the BGH holds, then the bulk-boundary principle gives*

$$\widetilde{\mathfrak{T}}(\tilde{p}_\Delta) \;=\; \widetilde{\mathrm{Ch}}_\emptyset(\tilde{p}_\Delta) \;=\; -\mathrm{Ch}_{\{3\}}(u_F) \;=\; 2\,P_{\mathrm{C},3} \;\in\; \mathbb{Z} \;+\; \frac{B_{1,2}}{2\pi}\,\mathbb{Z}\,,$$

and

$$\widetilde{\mathrm{Ch}}_2(\tilde{p}_\Delta) \;=\; -\mathrm{Ch}_3(u_F) \;=\; 4\pi\,\partial_{B_{1,2}} P_{\mathrm{C},3} \;\in\; \mathbb{Z}\,.$$

As a consequence, if $P_{\mathrm{C},3} \neq 0$, then $\hat{h}$ will necessarily display essential spectrum at $E = 0$. If instead of or additionally to $P_{\mathrm{C},3} \neq 0$ we have $\partial_{B_{1,2}} P_{\mathrm{C},3} \neq 0$, then the boundary spectrum at $E = 0$ is necessarily delocalized.

(iv) *Assume the existence of an interval $[-\delta,\delta] \subset \Delta$ such that the ends $\pm\delta$ lie in a region of Anderson localized surface spectrum. Let $\tilde{p}(\delta) = \chi(-\delta \leq \hat{h} \leq \delta)$ be the associated spectral projection and decompose it as in Proposition 4.3.3 into chiral sectors $\tilde{p}(\delta) = \tilde{p}_+(\delta) + \tilde{p}_-(\delta)$ with $J\tilde{p}_\pm(\delta) = \pm\tilde{p}_\pm(\delta)$. Then*

$$\widetilde{\mathrm{Ch}}_2\big(\tilde{p}_+(\delta)\big) \;-\; \widetilde{\mathrm{Ch}}_2\big(\tilde{p}_-(\delta)\big) \;=\; -\mathrm{Ch}_3(u_F) \;=\; 4\pi\,\partial_{B_{1,2}} P_{\mathrm{C},3} \;\in\; \mathbb{Z}\,.$$

Among other things, this implies that, if the bulk invariant is odd, then necessarily

$$\mathbb{Z} \;\ni\; \widetilde{\mathrm{Ch}}_2\big(\tilde{p}(\delta)\big) \;\neq\; 0\,,$$

so that the surface will display the IQHE with the Hall conductance jumping at least by one unit in the interval $[-\delta,\delta]$.

Proof Item (ii) follows from Proposition 5.6.2 and (iv) by choosing the lift as in Proposition 4.3.3. □

Let us stress that (ii) assures that the topological phases corresponding to the different values of $\partial_{B_{i,j}} P_{C,k}$ are separated by a localization-delocalization phase transitions which is again visible in transport experiments. This has been confirmed numerically in [201]. The statement (iii) on the delocalized character of the surface states at $E = 0$ is in full agreement with the conclusions drawn in Ref. [65]. As already pointed out there, no such statement can be formulated about the states at other energies. For the IQHE predicted in (iv), the methods developed so far give no further information about the values of $\widetilde{\mathrm{Ch}}_2\big(\tilde{p}(\delta)\big)$. Hence we have no general prediction about the value of the Hall conductance of the surface states, though we will make a conjecture on these values in the next section. Nevertheless, let us note that the spectrum away from the origin is expected to be localized (see the discussion in [65]) and that (iv) can occur in the absence of a magnetic field. In the latter situation, item (iv) hence predicts an *anomalous* quantum Hall effect. Lastly, let us mention that the IQHE at the surface may be absent altogether for an even bulk invariant, as for example would happen if $\mathrm{Ch}_3(u_F) = 2$ and $\widetilde{\mathrm{Ch}}_2\big(\tilde{p}_\pm(\delta)\big) = \mp 1$. However, there are other interesting particular scenarios which are worth discussing and this is done in the next seciton.

7.4 Surface IQHE for Exact and Approximately Chiral Systems

Let us start by formulating a conjecture on the values of $\widetilde{\mathrm{Ch}}_2\big(\tilde{p}(\delta)\big)$ which is compatible with the bulk-boundary principle. For this, we introduce the concept of stable configuration which is best explained for $d = 1$. In this case, the bulk-boundary principle states that $N_+ - N_- = -\mathrm{Ch}_1(u_F)$, from where one can conclude that the number of edge zero modes $N = N_+ + N_-$ is necessarily larger than or equal to the absolute value of the bulk invariant, but one cannot say what exactly this number is, just from the bulk topology. However, under small perturbations or disorder, pairs of zero modes of opposite chirality can and usually will exit the zero-mode subspace, and this phenomenon will repeat itself until one of the chiral sectors is completely depleted of zero modes. The process cannot continue and the system reached what we call the stable configuration. In $d = 3$ and in the absence of disorder, something similar will happen because pairs of zero-energy Dirac points of opposite chirality in the boundary spectrum can annihilate each other or leave the zero-energy level, and a stable configuration can be reached only when one chiral sector is completely depleted of zero-energy Dirac points . For a general chiral system in dimension d, we define a stable configuration to be reached if there is a δ such that one of $\widetilde{\mathrm{Ch}}_{d-1}\big(\tilde{p}_\pm(\delta)\big)$ is zero. We are now ready to formulate our conjectures. The notations from Corollary 7.3.4 will be used throughout.

Conjecture ((Anomalous) Surface IQHE) *Let* $\hat{h} = (h, \tilde{h}) \in M_{2N}(\mathbb{C}) \times \widehat{\mathcal{A}}_d$ *in dimension* $d = 3$ *be such that BGH and CH apply, and assume* $\mathrm{Ch}_3(u_F) \neq 0$. *Then Corollary 7.3.4 assures us that the boundary spectrum is delocalized at* $E = 0$. *The* *first conjecture is that, in presence of disorder, the boundary spectrum is everywhere localized except at* $E = 0$ *for* $\mathbf{B} = 0$*, and for* $\mathbf{B} \neq 0$ *furthermore at a discrete set of Landau bands symmetrically located around* $E = 0$*. The second conjecture is that, in presence of disorder, the system is always in a stable configuration for all values of the magnetic field. In these conditions, the Hall conductance of the surface will display a plateau-plateau transition exactly at* $E = 0$*, with a jump equal precisely to* $\left|\mathrm{Ch}_3(u_F)\right|$*. For* $\mathbf{B} = 0$ *this is hence an anomalous surface IQHE with Hall conductance dictated by the bulk invariant.*

This conjecture can be probed numerically. For vanishing magnetic fields, our initial efforts in this direction unfortunately could not shed any light on these important issues. During these attempts, it became clear that resolving the localized/delocalized character of the surface states will be a large scale computational endeavor. We hope that this will be of interest to the experts in the field. We also hope that the possibility of observing the anomalous IQHE at the surface of a non-magnetic material will renew the experimental and theoretical efforts on identifying a topological solid state system from the AIII class in $d = 3$.

If an external magnetic field perpendicular to the surface is present, then the situation is more traceable because gaps in the surface spectrum open at weak disorder. Indeed, as it usually happens for two-dimensional electron systems, Landau bands are forming. If the bulk invariant is now odd, then based on item (iv) of Corollary 7.3.4 we know that a Landau band will be pinned at the origin and that the Hall conductance of the surface will jump by at least one unit as the Fermi level crosses this band. In this situation, we have verified the conjecture numerically for all topological phases of the model presented in Sect. 2.3.3 in $d = 3$, under relatively small magnetic fields. Note that there is one phase with even bulk invariant which hence also had a non-vanishing surface Hall conductance.

Let us further elaborate on the importance of the parity of the bulk invariant in the case of a non-vanishing magnetic field, hence supplementing statement (iv) of Corollary 7.3.4. Suppose that there is a Landau band at $E \neq 0$. Then, due to the chiral symmetry, there will be another Landau band at $-E$ and the Chern numbers of the two bands are equal. Under small perturbations, these paired Landau bands can, in principle, migrate towards $E = 0$ and then join the central Landau band, but note that such process will change the Chern number of the central band by an even number. If $\widetilde{\mathrm{Ch}}_2\big(\tilde{p}(\delta)\big)$ was odd in the first place, then the Chern number of the central Landau band cannot be canceled by the processes just described and it indeed remains odd.

The physics described in the above conjecture might remind one of the observations made on graphene at relatively small magnetic fields [147, 229] where the Hall conductance jumps by four units as the Fermi level crosses the Landau band pinned at the origin. However, this feature of graphene is not stable and at larger magnetic fields where the central Landau band splits into four Landau sub-bands and only jumps by one unit occur for the Hall conductance [226, 231].

We now turn our attention to the solid state systems with approximate chiral symmetry in dimension $d = 3$, that is, the ACH defined in Sect. 2.4 is supposed to hold. By Proposition 2.4.9, such a system is homotopically connected to a solid state system exhibiting an exact chiral symmetry and thus displaying the physics discussed above on its surface. Since the IQHE is robust against homotopies, we can automatically conclude that this interesting physics will also be observed under weak breaking of the chiral symmetry. More precisely:

Proposition 7.4.1 ((Anomalous) Surface IQHE under ACH) *Let* $\hat{h} = (h, \tilde{h}) \in M_{2N}(\mathbb{C}) \times \widehat{\mathcal{A}}_d$ *in dimension* $d = 3$ *be such that BGH and CH apply, and assume that the above Conjecture applies. Let* $t \in [0, 1] \mapsto \hat{h}(t)$ *be a continuous deformation of* $\hat{h}$ *(as defined in Definition 2.4.5) which breaks the chiral symmetry. Further assume that the interval* $[-\delta, \delta]$ *can be chosen such that its ends resides in a region of localized boundary spectrum for all* $t \in [0, 1]$ *(which is always possible for small deformations). Then the spectral projections* $\tilde{p}(\delta, t) = \chi(-\delta \leq \hat{h}(t) \leq \delta)$ *lead to a constant value* $\widetilde{\mathrm{Ch}}_2\big(\tilde{p}(\delta, t)\big)$ *during the deformations. As such, the system with weakly broken chiral symmetry will continue to display the surface IQHE, which is anomalous if the magnetic field vanishes. However, the divergence of the localization length is not necessarily at* $E = 0$ *any more.*

Proof From Proposition 2.4.11, it follows that $\tilde{p}(\delta, t)$ varies continuously in the non-commutative Sobolev space $M_N(\mathbb{C}) \otimes \mathcal{W}_{d-1,1}(\mathcal{E}_d, \widetilde{\mathcal{T}})$. Then the statement follows from Theorem 6.6.2. □

When the chiral symmetry is broken, the Hall conductance of the surface should continue to display a net jump of $|\mathrm{Ch}_3(u_F)|$ over the interval $[-\delta, \delta]$. This net jump, however, will very likely not happen suddenly at a single energy, but instead will be a sum of elementary jumps by one unit. As we already pointed out several times, the chiral symmetry is expected to hold only approximately in real solid state systems, hence the established stability of the physical effects also against weak symmetry breaking should facilitate the experimental observability of the surface IQHE in adequate materials.

7.5 Virtual Topological Insulators

The topological systems in $d = 4$ or higher dimensions are not entirely fictitious since additional dimensions can occur in a parameter space. A special place among such systems is held by the virtual topological insulators, introduced and characterized in [127]. Their defining characteristic is a strong topological invariant which is defined in $d+d'$ space dimensions, where d counts the physical dimensions and d' the virtual ones, with an invariant that is yet computable and experimentally measurable inside the d physical dimensions.

Let us briefly describe the virtual topological insulators from class A in 3 + 1 dimensions, introduced in [167]. For sake of simplicity, the disorder will be neglected. Then the virtual systems are generated by the algebra $\mathcal{A}_4 = C^*(u_1, \ldots, u_4)$ from

Definition 3.1.1 via the following faithful representation on $\ell^2(\mathbb{Z}^3)$ invoking only three magnetic translations U_1, U_2, U_3:

$$\pi_\theta(u_j) \;=\; U_j \;, \quad \text{for } j = 1,2,3 \;, \qquad \pi_\theta(u_4) \;=\; e^{\mathrm{i}(\langle \mathbf{B}_4, X\rangle + \theta)} \;,$$

where $\mathbf{B}_4 = (B_{1,4}, B_{2,4}, B_{3,4})$ now plays the role of frequencies of the perturbation and $\theta \in \mathbb{R}$ the phase of the representation. As a non-trivial example, let us take

$$h \;=\; \tfrac{1}{2\mathrm{i}} \sum_{j=1}^{4} \gamma_j \otimes (u_j - u_j^*) \;+\; \gamma_0 \otimes \Big(m + \tfrac{1}{2} \sum_{j=1}^{4} (u_j + u_j^*)\Big) \;\in\; M_4(\mathbb{C}) \otimes \mathcal{A}_4 \;,$$

which generates the model already analyzed in Sect. 2.2.4. There it was also shown to posses a strong topological invariant $\mathrm{Ch}_4(p_F) \neq 0$. Here focus is on the representations $H_\theta = \pi_\theta(h)$ on $\mathbb{C}^4 \otimes \ell^2(\mathbb{Z}^3)$ rather than $\mathbb{C}^4 \otimes \ell^2(\mathbb{Z}^4)$:

$$\begin{aligned} H_\theta \;&=\tfrac{1}{2\mathrm{i}} \sum_{j=1}^{3} \gamma_j \otimes (U_j - U_j^*) \;+\; \gamma_0 \otimes \Big(m + \tfrac{1}{2} \sum_{j=1}^{3} (u_j + u_j^*)\Big) \\ &\quad +\; \gamma_4 \otimes \sin(\langle \mathbf{B}_4, X\rangle + \theta) \;+\; \gamma_0 \otimes \cos(\langle \mathbf{B}_4, X\rangle + \theta) \;, \end{aligned}$$

which describes a periodic crystal subjected to a magnetic field and an additional incommensurate periodic potential, namely we require $\frac{1}{2\pi} B_{j,4}$ to be irrational. As H_θ acts on a Hilbert space over the three-dimensional lattice and and it depends on an additional parameter $\theta \in \mathbb{S}^1$ we refer to it as a model in $3+1$ dimensions. Let us now show that the topological invariant can be computed at fixed θ. First of all,

$$\begin{aligned} \mathcal{T}(a) \;=\; \int_{\mathbb{S}^1} \frac{d\theta}{2\pi}\, \mathrm{Tr}\, \langle 0|\pi_\theta(a)|0\rangle \;&=\; \lim_{|V|\to\infty} \frac{1}{|V|} \sum_{x\in V} \mathrm{Tr}\, \langle 0|\pi_{\theta + \langle \mathbf{B}_4, x\rangle}(a)|0\rangle \\ &=\; \lim_{|V|\to\infty} \frac{1}{|V|} \sum_{x\in V} \mathrm{Tr}\, \langle x|\pi_\theta(a)|x\rangle \;, \end{aligned}$$

where Birkhoff's theorem was used combined with $U_j \pi_\theta(a) U_j^* = \pi_{\theta + B_{j,4}}(a)$ and the irrationality of $B_{j,4}$. Hence the topological invariant can be indeed computed at fixed θ:

$$\mathrm{Ch}_4(p_F) \;=\; \Lambda_4 \sum_{\rho\in\mathcal{S}_4} (-1)^\rho\, \mathcal{T}\Big(P_\theta \prod_{j=1}^{4} \partial_j P_\theta\Big) \;,$$

where $P_\theta = \chi(H_\theta \leq \mu)$, $\partial_4 P_\theta = \partial_\theta P_\theta$ and $\partial_j P_\theta = \mathrm{i}[P_\theta, X_j]$ for $j = 1,2,3$. This bulk topological invariant was related in [167] to the magneto-electric response function, discussed in the following sections. Another interesting link can be established via the generalized Streda formulas. For example,

$$\mathrm{Ch}_4(p_F) \;=\; 2\pi\; \partial_{B_{3,4}} \sigma_{1,2} \;,$$

which implies the quantization of the variation of the bulk Hall conductance in the (1, 2) plane (i.e. the non-linear Hall conductivity) w.r.t. the modulation of the incommensurate potential (or of the original lattice) in the third direction. This is a piezo-magneto-electric effect and the prediction could be tested with cold atom physics. Furthermore, assume now a boundary, say at $x_1 = 0$. Then we can consider the topological invariant $\widetilde{\mathrm{Ch}}_3(\tilde{u}_\Delta)$ and by applying the statement (v) of Proposition 7.2.3 we obtain

$$(2\pi)^2\,\partial_{B_{3,4}}\widetilde{\mathfrak{J}}_2 \;=\; (2\pi)^2\,\partial_{B_{2,4}}\widetilde{\mathfrak{J}}_3 \;=\; -\,\widetilde{\mathrm{Ch}}_3(\tilde{u}_\Delta) \;=\; -\,\mathrm{Ch}_4(p_F) \;\in\; \mathbb{Z}\,.$$

This implies the existence of boundary currents in the second (third) direction whose variation w.r.t. the modulation of the incommensurate potential in the third (second) direction is quantized in units of $\frac{1}{(2\pi)^2}$.

7.6 Quantized Electric Polarization

The electric polarization has two contributions, one from the displacements of the nuclei and one from the electrons. Here we will be dealing only with the latter contribution, which is often called the orbital polarization $P = (P_1, \ldots, P_d)$. It has been realized in the 1990s that P itself is not a gauge-invariant and measurable quantity, but that the variation ΔP of the orbital polarization during adiabatic deformations of crystals is gauge-invariant and measurable which is directly related to the flow of charges induced by such deformations (see [179, 180] for a historical account). If the deformation is periodic in time, it turns out that the orbital polarization is of topological nature and is actually the same quantity considered in charge pumps [209]. This well known effect can now be placed in a broader context and several predictions can be made using the tools developed so far.

Let be given a closed differentiable path $t \in [0, T] \mapsto h(t) \in \mathcal{A}_d$, $h(T) = h(0)$, of Hamiltonians satisfying the BGH at a fixed Fermi lelve μ, and set $p_A(t) = \chi(h(t) \leq \mu)$ to be the instantaneous Fermi projection. Then it is shown in [198] that, up to arbitrarily small corrections in the adiabatic limit, the change in the electric polarization during one adiabatic cycle is

$$\Delta P_j \;=\; \mathrm{i}\int_0^T dt\;\mathcal{T}\Big(p_A(t)\,\big[\partial_t p_A(t),\,\partial_j p_A(t)\big]\Big)\,. \tag{7.9}$$

This is the disordered version of the King-Smith-Vanderbilt formula for the orbital polarization [114]. Note that Eq. (7.9) is invariant to the scaling of the time, hence t can be seen as taking values on the unit circle $\mathbb{S}^1 \cong [0, 2\pi)$. The r.h.s. is, up to a constant, the pairing of the projection $p_A = \{p_A(t)\}_{t\in\mathbb{S}^1}$ with a 2-cocyle over the algebra $C(\mathbb{S}^1, \mathcal{A}_d)$, which is isomorphic to $\mathcal{A}_{d+1}$ if the periodic time dependence is interpreted as an extra space direction. To avoid confusion, we choose the time to be in the 0th direction. Then, from (7.9),

$$\Delta P_j \;=\; 2\pi \left\langle [\xi_{\{0,j\}}], [p_A]_0 \right\rangle \;=\; 2\pi \;\mathrm{Ch}_{\{0,j\}}(p_A)\;. \tag{7.10}$$

Based on (7.10), Theorem 5.7.1 and Corollary 5.7.2 gives the following prediction.

Corollary 7.6.1 *The change in the components of the bulk electric polarization, after and adiabatic periodic cycle, depends only on the class $[p_A]_0 \in K_0(\mathcal{A}_{d+1})$ of the Fermi projection, and is equal to:*

$$\Delta P_j \;=\; \sum_{\{0,j\}\subseteq J\subseteq\{0,\ldots,d\}} \beta_J \,(2\pi)^{1-\frac{|J|}{2}}\;\mathrm{Pf}\left(\mathbf{B}_{J\setminus\{0,j\}}\right)\,,$$

with $|J|$ even and β_J the integer numbers appearing in the decomposition of $[p_A]_0$ into the generators of the $K_0(\mathcal{A}_{d+1})$ group,

$$[p_A]_0 \;=\; \sum_{J\subset\{0,\ldots,d\}} \beta_J[e_J]_0\;,$$

as elaborated in Sect. 4.2.3. Above, it is assumed that $\mathrm{Pf}(\mathbf{B}_\emptyset)=1$.

According to the above statement, ΔP_j can take only discrete values but these values are not necessarily integer. For example, for $d=1$ and $d=2$ the set J can only be $\{0,j\}$, hence $\Delta P_j=\beta_{\{0,j\}}$ is always an integer, while for $d=3$ we have in general

$$\Delta P_j \;=\; \beta_{\{0,j\}} \;+\; \beta_{\{1,2,3\}\setminus\{j\}}B_{\{1,2,3\}\setminus\{j\}}\;,\qquad j=1,2,3\;.$$

Note, however, that the variation of the magneto-electric response coefficient

$$\partial_{B_{\{1,2,3\}\setminus\{j\}}}\Delta P_j \;=\; \beta_{\{1,2,3\}\setminus\{j\}}\;,\qquad j=1,2,3\;,$$

is an integer, a fact which will be addressed in more detail in Sect. 7.8. Let us mention that, for $d=1$, the above quantization already appeared in the work of Thouless [209], while, for $d=2$, a non-trivial example manifesting this quantization is constructed in [55], where an adequate loop of next-nearest hopping Hamiltonians on the hexagonal lattice is constructed. It will definitely be very interesting to test the prediction of Corollary 7.6.1 in dimension $d=3$.

Next let us show how the K-theoretic result of Sect. 4.3.4 can be applied to obtain a further formula for the polarization. Invoking (5.19) in Theorem 5.4.1 on the duality of pairings under the suspension map combined with Proposition 4.3.7, on obtains:

$$\begin{aligned}\left\langle [\xi_{\{0,j\}}], [p_A]_0\right\rangle \;&=\; \left\langle [\xi_{\{0,j\}}], [p_A]_0-[p_F]_0\right\rangle\\ &=\; \left\langle [\xi_{\{j\}}], [p_F v_{A,2\pi} p_F + \mathbf{1}_N - p_F]_1\right\rangle\,,\end{aligned}$$

where $v_{A,2\pi}$ is the Poincaré map of the adiabatic time evolution over one cycle, see Sect. 4.3.4. Now the r.h.s. can be written out more explicitly (using the identity $v_{A,2\pi}p_F = p_F v_{A,2\pi}p_F$):

$$\Delta P_j \;=\; 2\pi\,\mathrm{i}\,\mathcal{T}\left(p_F v^*_{A,2\pi} p_F\,\partial_j\big(p_F v_{A,2\pi} p_F\big)\right)\;.$$

This is the stroboscopic interpretation of the polarization, expressing it in terms of the winding number of the adiabatic evolution over one cycle restricted to the range of the Fermi projection. Yet another formula for the polarization will be given in the next section.

Next let us come to periodic loops of chiral systems. The following shows that their polarization vanishes.

Proposition 7.6.2 *Suppose that $t \in \mathbb{S}^1 \cong [0, 2\pi) \mapsto h(t) \in \mathcal{A}_d$ is a loop of Hamiltonian satisfying the CH. Then ΔP given by (7.9) vanishes.*

Proof Inserting $J^2 = \mathbf{1}$ and using $Jp_AJ = \mathbf{1} - p_A$ on the r.h.s. of (7.9) shows $-\Delta P_j = 2\pi\ \mathrm{Ch}_{\{0,j\}}(\mathbf{1} - p_A)$. But the homomorphism property of the pairing implies $\mathrm{Ch}_{\{0,j\}}(p_A) + \mathrm{Ch}_{\{0,j\}}(\mathbf{1} - p_A) = \mathrm{Ch}_{\{0,j\}}(\mathbf{1}) = 0$ so that $\Delta P_j = -\Delta P_j = 0$. □

Nevertheless, it is possible to associate a topological quantity to a loop of chiral systems, namely the chiral time polarization defined by

$$P_{\mathrm{CT}} \;=\; \mathrm{i}\int_0^{2\pi} dt\,\mathcal{T}(p_F(t)\,J\,\partial_t p_F(t))\;.$$

The chiral polarization P_{C} defined for a given chiral Hamiltonian (and not a loop of them) in Sect. 7.3 is quite similar. Following the calculation in the proof of Proposition 7.3.1 shows

$$P_{\mathrm{CT}} \;=\; \tfrac{1}{2\mathrm{i}}\int_0^{2\pi} dt\,\mathcal{T}(u_F(t)^*\partial_t u_F(t)) \;=\; -\tfrac{1}{2}\left\langle [\xi^s_{\emptyset}], [u_F(t)_{t\in[0,2\pi)}]_1\right\rangle .$$

The r.h.s. is, up to a factor, the winding number of the time-varying Fermi unitary operator, hence it is a stable topological number. Using the Streda formula, one deduces for $1 \le i, j \le d$

$$\partial_{B_{i,j}} P_{\mathrm{CT}} \;=\; -\tfrac{1}{4\pi}\left\langle [\xi^s_{\{i,j\}}], [u_F(t)_{t\in[0,2\pi)}]_1\right\rangle . \tag{7.11}$$

In $d = 2$, the r.h.s. is integer valued by the odd index theorem. For $d = 3$ it is an integer valued weak invariant under the BGH.

7.7 Boundary Phenomena for Periodically Driven Systems

In this section investigates the implications of the bulk-boundary correspondence for the periodically driven systems used for the definition of the orbital polarization in Sect. 7.6. Thus let us consider a time-periodic family of half-space Hamiltonians

$$t \in \mathbb{S}^1 \cong [0, 2\pi) \;\mapsto\; \widehat{h}(t) \;=\; \big(h(t), \tilde{h}(t)\big) \;\in\; \widehat{\mathcal{A}}_d \;.$$

This family is a lift of $t \in \mathbb{S}^1 \mapsto h(t)$ in the exact sequence of time period systems

$$0 \longrightarrow C(\mathbb{S}^1, \mathcal{E}_d) \overset{i}{\to} C(\mathbb{S}^1, \widehat{\mathcal{A}}_d) \overset{\text{ev}}{\to} C(\mathbb{S}^1, \mathcal{A}_d) \longrightarrow 0 \,, \tag{7.12}$$

which is just a reformulation of (3.36). In fact, if we see the time as another space direction, then (7.12) is exactly (3.36). Now the bulk-boundary correspondence (5.27) implies

$$\Delta P_d \;=\; 2\pi \,\text{Ch}_{\{0,d\}}(p_A) \;=\; 2\pi \,\widetilde{\text{Ch}}_{\{0\}}(\tilde{u}_\Delta) \;,$$

where the 0th component is still time and $[\tilde{u}_\Delta]_1 = \text{Exp}[p_A]_0$. Our goal here is to give a physical interpretation of the 1-cocycle appearing on the r.h.s.. According to Proposition 7.1.2

$$\widetilde{\text{Ch}}_{\{0\}}(\tilde{u}_\Delta) \;=\; -2\pi \int_0^{2\pi} dt\; \widetilde{\mathcal{T}}\Big(f'_{\text{Exp}}\big(\hat{h}(t)\big)\,\partial_t \hat{h}(t)\Big) \,. \tag{7.13}$$

Following an argument from [56] (see Proposition 4 there), in the case $d = 1$, the r.h.s. of (7.13) is just 2π times the classical spectral flow [158] of boundary eigenvalues of the path $t \in \mathbb{S}^1 \mapsto \hat{h}(t)$ through the bulk gap at μ,

$$\Delta P_1 \;=\; -2\pi \;\text{Sf}\big(t \in \mathbb{S}^1 \mapsto \hat{h}(t) \text{ by } \mu\big) \,.$$

The spectral flow counts the number of eigenvalues crossing the Fermi level from below minus the number of eigenvalues crossing from above during the adiabatic cycle. As one can immediately see, this is precisely the amount of charge pumped from the valence to the conduction states. For $d > 1$, the spectral flow in the above bulk-boundary correspondence has to be understood in a generalized sense of Breuer-Fredholm operators (see [22]), but its physical interpretation remains the same, as the charge per the unit area pumped during the adiabatic cycle. We will use the symbol Sf also for the spectral flow in this generalized sense.

Let us briefly comment on the bulk-boundary correspondence for the chiral time polarization P_{CT} for paths of chiral Hamiltonians. As P_{CT} itself is given by the pairing with a 0-cocycle, there is no bulk-boundary correspondence for it. On the other hand, for its derivatives w.r.t. a magnetic field perpendicular to the surface one has due to (7.11):

$$\begin{aligned}\partial_{B_{i,d}} P_{\mathrm{CT}} &= -\tfrac{1}{4\pi}\,\big\langle[\xi^s_{\{i\}}],\,[\tilde{p}_\Delta(t)_{t\in[0,2\pi)}]_0\big\rangle \\ &= -\tfrac{1}{4\pi}\,\Big(\big\langle[\xi^s_{\{i\}}],\,[\tilde{p}_+(\delta,t)_{t\in[0,2\pi)}]_0\big\rangle - \big\langle[\xi^s_{\{i\}}],\,[\tilde{p}_-(\delta,t)_{t\in[0,2\pi)}]_0\big\rangle\Big)\,,\end{aligned}$$

where in the second identity it was supposed that $\pm\delta$ lie in gaps of the surface spectrum (e.g. opened by the magnetic field).

7.8 The Magneto-Electric Response in $d = 3$

The magneto-electic effect in an insulating material consists in the change of its electric polarization under a variation of the external magnetic field or, alternatively, the change of the magnetization under a variation of an electro-static potential. As in the previous section, we will be dealing only with the electron contributions to the effect. Now, let us consider a periodically driven system in dimension $d = 3$ for which the orbital polarization is given by (7.9). Then the change in the magneto-electric response coefficients per cycle is

$$\Delta\,\alpha_{i,j,k} \;=\; \partial_{B_{i,j}}\,\Delta P_k\;, \qquad \{i,j,k\} = \{1,2,3\}\;.$$

By using the connection given in (7.10) and applying the generalized Streda formula from Theorem 5.6.3, we obtain

$$\Delta\,\alpha_{i,j,k} \;=\; (-1)^\rho\,\big\langle[\xi_{\{0,1,2,3\}}],\,[p_F]_0\big\rangle \;=\; (-1)^\rho\,\mathrm{Ch}_4(p_F) \in \mathbb{Z}\;,$$

where ρ is the permutations which sends $\{i, j, 0, k\}$ into $\{0, 1, 2, 3\}$. The r.h.s. is the strong even pairing over the algebra $\mathcal{A}_{3+1}$ and hence integer-valued. A formula of this type already appeared in [169], but there an average over the space direction k was taken and used. The above statement shows that all 3 terms are in fact equal to the same invariant. In dimension $d = 4$, which will be relevant for the virtual topological insulator discussed above, a similar statement holds, but the even pairing is only a weak invariant in this case.

For a crystal with surface in $d = 3$, we can use the bulk-boundary principle of (5.27) in the following way

$$\Delta\alpha_{1,2,3} \;=\; \partial_{B_{1,2}}\Delta P_3 \;=\; \partial_{B_{1,2}}\,\widetilde{\mathrm{Ch}}_{\{0\}}(\tilde{u}_\Delta) \;=\; -\,2\pi\;\partial_{B_{1,2}}\mathrm{Sf}\big(t\in\mathbb{S}^1\mapsto\hat{h}(t)\text{ by }\mu\big)\;.$$

Hence, the spectral flow is not quantized but its variation with respect to the component of the magnetic field perpendicular to the surface is quantized:

$$-\,2\pi\;\partial_{B_{1,2}}\;\mathrm{Sf}\big(t\in\mathbb{S}^1\mapsto\hat{h}(t)\text{ by }\mu\big) \;=\; \mathrm{Ch}_4(p_F)\;.$$

This relations tells that, if $\mathrm{Ch}_4(p_F) \neq 0$, there is a spectral flow no matter where we place the Fermi level in the bulk gap. This implies that essential spectrum moves across the bulk gap as the time evolves, connecting the upper and lower parts of the bulk spectrum.