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Harmonic Analysis in Operator Algebras and its Applications to Index Theory and Topological Solid State Systems

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Preface and Overview

The central theme of classical harmonic analysis is to characterize regularity properties of functions $f : \mathbb{R}^n \to \mathbb{R}$ or $f : \mathbb{T}^n \to \mathbb{R}$ such as (weak) differentiability, integrability and mixtures of these two properties. If these functions are seen as (parts of) symbols of (possibly singular) integral operators (with Calderon-Zygmund kernels), it is then of crucial interest to characterize boundedness and trace class properties of these operators in terms of the regularity of their symbols. This naturally leads to a wealth of function spaces like: Hölder, L^p, Sobolev, Besov and BMO spaces. There are numerous modern accounts of the subject, each with different point of view [1, 2, 3, 4]. Some of the key elements are Littlewood-Paley decompositions, Fourier multipliers and maximal functions. The theory also extends to functions on Riemannian manifolds [2].

Of relevance for the present work is the particular case of classical Hankel operators of the form $H_f = Pf(1-P)$ where P is the Hardy projection in $L^2(\mathbb{T}^1)$ onto functions on the torus $\mathbb{T}^1 = [0, 1)$ with positive frequencies and f is viewed as the multiplication operator with a function $f : \mathbb{T}^1 \to \mathbb{R}$. The following classical results are then well-known and nicely exposed in [5, 6]. Kronecker proved that H_f is of finite rank if and only if f is rational. On the other hand, results of Nehari [7] and Feffermann [8] imply that H_f is bounded if and only if f is BMO. Furthermore, Peller showed that H_f is in the Schatten ideal $\mathscr{L}^p$ if and only if f is in the Besov space $B^{\frac{1}{p}}_{p,p}$. In particular, H_f is trace class if $f \in B^1_{1,1}$. For invertible such functions, the associated Toeplitz operator $T_f = PfP$ is a Fredholm operator on $\mathrm{Ran}(P)$ and its index is given by

$$\mathrm{Ind}(T_f) = -\mathrm{Tr}(f^{-1}[P, f]) = -\int_{\mathbb{T}^1} f^{-1} df, \tag{0.1}$$

where latter equality follows from Noether-Gohberg-Krein index theorem for the winding number of a differentiable function f.

The Peller criterion has been generalized in many directions. Peller himself extended it to vector-valued functions [9] and Janson and Wolff to higher dimensions [10]. Janson and Peetre proved it for paracommutators [11] and Zhu for Hankel operators on Bergman spaces [12]. Necessary and sufficient conditions for the Hankel operators to be of Dixmier trace-class were given by Engliš and Rochberg [13]. This was generalized by Goffeng and Usachev who showed how Besov spaces can be used to characterize Hankel operators in Macaev ideals [14].

This work further extends the definition of Besov spaces and associated Peller criteria to noncommutative von Neumann algebras $\mathscr{M}$ equipped with a weakly continuous G-action α and an α-invariant semi-finite, normal, faithful (s.n.f.) trace $\mathscr{T}$ where $G = \mathbb{T}^{n_1} \times \mathbb{R}^{n_2}$ with $n_1 + n_2 = n$. The main application here is not a trace formula in this context, but rather a generalization of the index formula (0.1) in the spirit of Connes' non-commutative geometry [6]. In that framework, a natural cyclic cocycle on sufficiently smooth elements $a_0, \ldots, a_n$ of $\mathscr{M}$ is defined by

$$\mathrm{Ch}_{\mathscr{T},\alpha}(a_0, \ldots, a_n) = c_n \sum_{\rho \in S_n} (-1)^{\rho} \mathscr{T}(a_0 \nabla_{\rho(1)} a_1 \cdots \nabla_{\rho(n)} a_n),$$

where the sum carries over the symmetric group S_n and $(-1)^{\sigma}$ is the signature of the permutation σ, the ∇_j are the derivations associated to the G-actions and finally the normalization constants c_n are chosen as in Definition 4.3.4 below. It then follows from semi-finite index theory (a history of relevant contributions follows shortly) that, if n is odd and $u \in \mathscr{M}$ a sufficiently smooth unitary,

$$\widehat{\mathscr{T}}_{\alpha} - \mathrm{Ind}(\mathbf{P}\pi(u)\mathbf{P} + 1 - \mathbf{P}) = \mathrm{Ch}_{\mathscr{T},\alpha}\big(u^* - 1, u - 1, \ldots, u^* - 1, u - 1\big), \quad (0.2)$$

where the index is understood in the Breuer-Fredholm sense w.r.t. the dual trace $\widehat{\mathscr{T}}_{\alpha}$ on the von Neumann crossed product $\mathscr{M} \rtimes_{\alpha} G$ and $\mathbf{P} = \chi(\mathbf{D} > 0)$ is the Hardy projection of the Dirac operator constructed from the generators $\gamma_1, \ldots, \gamma_n$ of the complex Clifford algebra via

$$\mathbf{D} = \sum_{i=1}^{n} \gamma_i \otimes D_i,$$

with $D_1, \ldots, D_n$ being the self-adjoint generators of the action α in a covariant representation π. Phrased differently, one considers the Toeplitz operator $\mathbf{P}\boldsymbol{\pi}(u)\mathbf{P}$ for non-commutative symbols u contained in a suitable smooth subalgebra $\mathcal{A} \subset \mathscr{M}$ and finds that its (Breuer)-index is given by a higher-dimensional analogue of the winding number. This is a non-commutative generalization of the Noether-Gohberg-Krein theorem. In a C^*-algebraic setting of such a norm continuous action and for $G = \mathbb{R}$, Connes proved a precursor of (0.2) for smooth unitaries u in the form of a trace formula using the Connes-Thom isomorphism [15]. The interpretation as a semi-finite Breuer-Fredholm index was then refined in [16] and [17]. Newer works such as [18, 19, 20, 21, 22, 23, 24, 25] further extend these results and interpret them in terms of semi-finite spectral triples and spectral flow. Let us note, however, that all purely C^*-algebraic approaches to index theory require some smoothness w.r.t. the operator norm topology, notably in the cases described above, u has to be at least norm-differentiable w.r.t. the action α (and satisfy additional summability conditions). Also the approach using unbounded spectral triples [19, 21] usually requires at least that the $\nabla_i u$ define bounded operators. This is already too restrictive for some applications (in physical systems that will be described below).

This work (see Chap. 3) proves (0.2) and also its even analogue for differentiable symbols, but the main point is that it provides more general and natural regularity assumptions on the symbols for the validity of this index theorem which do not require the symbols to be either differentiable or continuous (*i.e.* lie in an underlying C^*-algebra). Generalizing the classical theory sketched above, one introduces Besov spaces for a quadruple $(\mathscr{M}, \alpha, G, \mathscr{T})$ consisting of a W^*-dynamical system with an invariant trace. A lot is known for such W^*-dynamical systems, its W^*-crossed product $\mathscr{M} \rtimes_\alpha G$ and the associated non-commutative L^p-spaces $L^p(\mathscr{M})$ and $L^p(\mathscr{M} \rtimes_\alpha G)$ [26, 27], see Sect. 1 and the appendices. Recalling that $\mathscr{M}$ is considered as the space of symbols, the Toeplitz operators $T_a = \mathbf{P}\boldsymbol{\pi}(a)\mathbf{P}$ are by construction elements of the W^*-crossed product algebra $\mathscr{M} \rtimes_\alpha G$ and applicability of the index theorem turns out to be governed by the regularity of the Hankel operator $H_a = \mathbf{P}\boldsymbol{\pi}(a)(1 - \mathbf{P}) \in \mathscr{M} \rtimes_\alpha G$. In particular, the index theorem can be established for $H_a \in L^{n+1}(\mathscr{M} \rtimes_\alpha G)$, *i.e.* if the commutator $[\mathbf{P}, \boldsymbol{\pi}(a)]$ is n-summable. This justifies the search for a generalization of Peller's criterion.

The approach to harmonic analysis on operator algebras is based on the theory of abelian groups of automorphisms by Arveson [29] (see also [29] and [26]), in which the analogue of a Fourier multiplier $f \in \mathscr{F}(L^1(G))$ acts by convolution of the G-action α with the inverse Fourier transform of f by

$$\hat{f} * a = \int_G \big(\mathscr{F}^{-1} f\big)(-t)\alpha_t(a)\mathrm{d}t, \quad a \in \mathscr{M}.$$

For some smooth function $\varphi : \mathbb{R} \to [0, 1]$ with support $[2^{-1}, 2]$ and such that $\sum_{j\in\mathbb{Z}} \varphi(2^{-j}x) = 1$ for all $x \in \mathbb{R}^+$, one introduces the dyadic Littlewood-Paley decomposition $(W_j)_{j\in\mathbb{N}}$ by

$$W_j(t) = \varphi\big(2^{-j}|t|\big) \text{ for } t \in \mathbb{R}^n,\ j > 0, \qquad W_0 = 1 - \sum_{j>0} W_j,$$

and then defines, given $p, q \in [1, \infty)$ and $s > 0$, the Besov norm of $a \in \mathscr{M}$ in generalization of the classical multiplier definition by

$$\|a\|_{B^s_{p,q}} = \left(\sum_{j\geq 0} 2^{qsj} \left\| \hat{W}_j * a \right\|^q_{L^p(\mathscr{M})}\right)^{\frac{1}{q}}.$$

Chapter 2 shows that elements of $L^p(\mathscr{M})$ with bounded Besov norm form a Banach space $B^s_{p,q}(\mathscr{M})$ and that $\mathscr{M} \cap B^s_{p,q}(\mathscr{M})$ is a $*$-algebra. It provides an equivalent norm in terms of finite differences of functions (as in the classical case), uses interpolation theory [30, 31] to derive properties of the full scale of Besov spaces and establishes connections to the domains of the derivations $\nabla_1, \ldots, \nabla_n$ and the noncommutative Sobolev spaces $W^m_p(\mathscr{M})$. Most importantly, Theorem 3.2.1 proves a Peller criterion and Theorem 3.3.1 characterizes trace class properties of Hankel operators in terms of Besov space (just as in the classical case [5, 12]). A particular form of the Peller criterion is part of the following main result of this work (see Chap. 3 and, in particular, Theorem 3.4.9 for a detailed statement that also covers the case of even pairings):

Theorem 0.0.1 (Sobolev index theorem). *Let n be odd and $p > n$. Suppose that $u - 1 \in \mathscr{M} \cap W^1_p(\mathscr{M})$. Then the Hankel operator H_u is in $L^{n+1}(\mathscr{M} \rtimes_\alpha G)$ and the index formula* (0.2) *holds.*

Let us stress that the stated Sobolev property is not necessary for the index formula (0.2) to hold. In fact, for the case of even and integer-valued pairings, it has been shown that the Hankel operators only need to lie in a Macaev ideal that allows supplementary logarithmic divergences [32, 33]. This is based on an identity for the Dixmier trace. The recent contribution [34] shows a similar result for the rotation algebra. Here a more analytical reasoning closer to Peller's original argument is presented.

Apart from the Sobolev index theorem, this work contains in Chap. 4 another result of pure mathematics that is worth mentioning in this introduction. If $\mathscr{A}$ is a C^*-algebra and ξ is norm continuous $\mathbb{R}$-action, then the Connes-Thom isomorphisms $\partial^\xi_i : K_i(\mathscr{A}) \to K_{i+1}(\mathscr{A} \rtimes_{\alpha\xi} \mathbb{R})$ connect the K-theory of $\mathscr{A}$ to that of the C^*-crossed product $\mathscr{A} \rtimes_\xi \mathbb{R}$ [15]. If one has another norm-continuous G-action θ commuting with ξ and a s.n.f. trace $\mathscr{T}$ that is invariant under both ξ and θ, one also obtains a $(G \times \mathbb{R})$-action $\theta \times \xi$. There exist natural dense Fréchet subalgebras of $\mathscr{A}$ and $\mathscr{A} \rtimes_\xi \mathbb{R}$ which can be used to define cocycles $\mathrm{Ch}_{\mathscr{T},\theta\times\xi}$ and $\mathrm{Ch}_{\widehat{\mathscr{T}}_\xi,\theta}$ that provide well-defined pairings with K-theory. Note that if n is even, then $\mathrm{Ch}_{\mathscr{T},\theta\times\xi}$ is an odd cocycle which pairs with odd K-theory.

Theorem 0.0.2 (Duality theorem). *For $[u]_1 \in K_1(\mathscr{A})$ and n even,*

$$\langle \mathrm{Ch}_{\mathscr{T},\theta\times\xi}, [u]_1 \rangle = -\langle \mathrm{Ch}_{\widehat{\mathscr{T}}_\xi,\theta}, \partial^\xi_1 [u]_1 \rangle,$$

where $\widehat{\mathscr{T}}_\xi$ is the dual trace on $\mathscr{A} \rtimes_\xi \mathbb{R}$.

Chapter 4 (see, in particular, Theorem 4.5.3) contains a proof of this statement and also a similar one for even n. While Theorem 0.0.2 essentially follows by combining results from the literature [35, 36, 37, 38] and certainly can also be proved by KK-theory (such as in [1, 19]), we provide a self-contained proof based on cyclic cohomology. For this we review and slightly generalize the approach of [35] which relates the pairings of $K_i(\mathscr{A})$ with a cyclic cocycle φ densely defined on a Fréchet subalgebra $\mathscr{A}$ of $\mathscr{A}$ to those of $K_{1-i}(\mathscr{A} \rtimes_\alpha \mathbb{R})$ with a dual cocycle $\#_\alpha \varphi$ densely defined on a subalgebra of $\mathscr{A} \rtimes_\alpha \mathbb{R}$. An important technical issue is that those dense subalgebras must be spectrally invariant in $\mathscr{A}$ respectively $\mathscr{A} \rtimes_\alpha \mathbb{R}$ such that the K-theoretical index pairings are well-defined. Therefore the arguments of [35] are adapted in such a way that Schweitzer's notion of strong spectral invariance of $\mathcal{A}$ in $\mathscr{A}$ [41] can be applied as a (constructive) sufficient condition.

For applications of this formula, it is often desirable to replace the abstract Connes-Thom isomorphism by the connecting map of a more concrete exact sequence of C^*-algebras such as the Wiener-Hopf extension. Likewise, many applications require analogous formulas for crossed products with $\mathbb{Z}$-actions based on the connecting maps of the Pimsner-Voiculescu sequence, which have to be proved independently. All of these issues can be addressed in a unified manner by noting that associated to the data $(\mathscr{A}, \xi, \mathbb{R})$ is an exact sequence of C^*-algebras

$$0 \to \mathscr{A} \rtimes_\xi \mathbb{R} \hookrightarrow \mathrm{T}(\mathscr{A}, \mathbb{R}, \xi) \to \mathscr{A} \to 0.$$

where the middle algebra is the smooth Toeplitz extension introduced by [42]. This was used *e.g.* in [16] to generalize the index theory of Toeplitz operators to flows in non-commutative symbol algebras. The K-theoretical connecting maps of the Toeplitz extensions are known to give isomorphisms related to the Connes-Thom isomorphisms and the connecting maps of Rieffel's Wiener-Hopf extension [43]. This is revisited in Sect. 4.2 which also studies an analogous extension for $\mathbb{T}$-actions, a generalization of the discrete Toeplitz extension used by Pimsner and Voiculescu [44]. By applying the interrelations between these K-theoretical maps and combining them with Takai duality, the above duality theorem appears as one of several such results for a fairly flexible class of extensions. As an additional result, the analogue of the duality theorem for $\mathbb{Z}$-actions also follows directly from Theorem 0.0.2 already. Section 5.4 later on provides an application of these results to the bulk-boundary-correspondence for half-spaces with irrational cutting angles.

The remainder of this introduction describes the application of the above theory and results to the mathematical physics of solid state systems. This makes up Chap. 5. Let us begin with a short historic account and by documenting some of the enormous recent activity in the field. This work is placed within the operator algebraic framework developed by Bellissard in the early 1980s which allowed to understand quantum Hall systems as examples of Connes' noncommutative geometry [45]. More recent accounts thereof are [32] and [46]. For physical reasons, namely in order to deal with Anderson localized systems without a spectral gap, it was necessary to go beyond the standard C^*-algebraic formulation and prove index theorems for certain elements of the enveloping von Neumann algebra, see again [32]. Another advance was to understand the bulk-boundary correspondence (BBC) in quantum Hall systems as a result of the K-theoretic exponential map of Pimsner-Voiculescu exact sequence for the discrete Toeplitz extension and the corresponding duality theory [37, 47]. Being such a robust mathematical concept, the BBC could then be extended to other dimensions and therefore allowed to describe numerous situations of physical interest in the growing field of topological insulators [46, 48, 49, 50, 51, 52, 53, 54, 55], some by extending or modifying the initially proposed framework of [45]. There are also countless more analytical contributions for these systems and, while it is impossible to cite them all here, let us mention contributions proving the BBC in presence of a mobility gap regime by Elgart, Graf and Schenker [56] as well as Graf and Shapiro [57] and for semimetals by Mathai and Thiang [58] and Carey and Thiang [59], all of which have not yet (prior to this work) been dealt with within the operator algebraic approach.

There are four main novel contributions of this work:

- The first is to provide sufficient conditions for the existence of the weak bulk Chern numbers. This covers the mobility gap (for Anderson localized systems) and pseudo-gap regime (for certain semimetals). It uses the index theoretical approach with Besov symbols (Theorem 0.0.1), but requires a substantial amount of supplementary analytical preparations.
- The second contribution, less substantial, is an extension of the range of applicability of the BBC for spectrally gapped insulators to half-spaces with arbitrary orientation w.r.t. the lattice directions. This is based on the duality result Theorem 0.0.2.
- The third proves that the surface states associated to non-vanishing weak Chern numbers cannot be localized.
- The fourth contribution is to establish the BBC for the weak winding number invariants of chiral Hamiltonians in the absence of a bulk gap (again for the mobility gap and pseudogap regime). This implies the existence of flat bands of surface states in these systems and is also based on the Sobolev index theorem.

Detailed descriptions of these results are given in Sects. 5.3, 5.4, 5.5 and 5.6 respectively. This introduction gives a flavor of these results and the techniques involved, but only states one result (Theorem 0.0.3) in some detail.

The algebraic set-up for the description of solid state systems is as follows [45, 46] (see Sect. 5.1). The set of configurations of the solid is a compact probability space $(\Omega, \mathbb{P})$ which is equipped with an invariant and ergodic $\mathbb{Z}^d$-action. The bulk observables are then elements of the disordered rotation algebra $\mathbb{T}^d_{\mathbf{B},\Omega} = C(\Omega) \rtimes_{\mathbf{B}} \mathbb{Z}^d$, a twisted crossed product associated to an anti-symmetric real matrix $\mathbf{B}$ of constant magnetic fields. Associated to the probability measure $\mathbb{P}$ on Ω is a tracial state $\mathscr{T}$ on $\mathbb{T}^d_{\mathbf{B},\Omega}$ whose GNS representation allows to identify an element $a \in \mathbb{T}^d_{\mathbf{B},\Omega}$ with a covariant family $(a_\omega)_{\omega\in\Omega}$ of bounded operators on $\ell^2(\mathbb{Z}^d)$. In this faithful representation, $\mathbb{T}^d_{\mathbf{B},\Omega}$ is generated by the magnetic translations on $\ell^2(\mathbb{Z}^d)$ and multiplication operators (potentials) obtained by shifting functions $f \in C(\Omega)$. Furthermore, there is a dual action ρ of the torus $\mathbb{T}^d$ whose unbounded generators are the position operators $X_1, \dots, X_d$ on the lattice $\mathbb{Z}^d$ and which induce derivations $\nabla_1, \dots, \nabla_d$ on $\mathbb{T}^d_{\mathbf{B},\Omega}$. For periodic systems the action and derivations are given by the translations and coordinate derivatives on the Brillouin torus, respectively. For the application of the Sobolev index theorem, one further goes over to the von Neumann algebra $\mathscr{M} = (\mathbb{T}^d_{\mathbf{B},\Omega})'' = L^\infty(\mathscr{M}, \mathscr{T})$ with normal faithful finite trace $\mathscr{T}$. Then given any restriction θ of ρ to an n-parameter subgroup of $\mathbb{T}^d$, there are associated Chern cocycles $\mathrm{C}h_{\mathcal{T},\theta}$ which lead to semi-finite Breuer-Fredholm indices in the von Neumann algebra $\mathscr{M} \rtimes_\theta \mathbb{R}^n$ by the Sobolev index theorem.

To explain the physical motivation that leads to consider non-smooth symbols, let us describe how the projections and unitary elements subject to the index pairings arise. Let be given a self-adjoint Hamiltonian $h = h^*$ in a matrix algebra $M_N(\mathbb{T}^d_{\mathbf{B},\Omega})$ which is smooth w.r.t. the dual action ρ, namely having a rapid decay of the off-diagonal matrix elements. Assume that N is even and h has a chiral symmetry given by

$$JhJ = -h, \; J = \begin{pmatrix} \mathbf{1}_{\frac{N}{2}} & 0 \\ 0 & -\mathbf{1}_{\frac{N}{2}} \end{pmatrix}, \tag{0.3}$$

which is equivalent to h and its phase $\mathrm{sgn}(h) = h|h|^{-1}$ being of the form

$$h = \begin{pmatrix} 0 & a^* \\ a & 0 \end{pmatrix}, \quad \mathrm{sgn}(h) = \begin{pmatrix} 0 & u_F^* \\ u_F & 0 \end{pmatrix}, \tag{0.4}$$

with some operators $a, u_F \in M_{\frac{N}{2}}(\mathscr{M})$. If h is invertible and therefore has a spectral gap around 0, then u_F is called the Fermi unitary. It is then smooth and defines an element $[u_F]_1 \in K_1(\mathbb{T}^d_{\mathbf{B},\Omega})$ so that one can define the numerical index pairings $\mathrm{C}h_{\mathcal{T},\theta}(u_F) = \langle \mathrm{C}h_{\mathcal{T},\theta}, [u_F]_1\rangle$ with Chern cocycles for which θ is generated by an odd number n of generators. Those invariants are called the odd (bulk) Chern numbers of u_F. Likewise, the class of the Fermi projection $p_F = \chi(h \leq 0)$ in $K_0(\mathbb{T}^d_{\mathbf{B},\Omega})$ is used to define pairings with even cocycles which are called even (bulk) Chern numbers. The Chern number with $n = d$ is called the strong Chern number and can be written as an ordinary Fredholm index [33, 45, 46], while those with $n < d$ are called weak Chern numbers and are in general described by semi-finite Breuer-Fredholm indices as above [24, 25]. If the assumption of a spectral gap is dropped, the elements u_F and p_F will in general not be smooth, but in certain cases they satisfy the conditions of the Sobolev index theorem (Theorem 0.0.1) and the Chern numbers continue to be well-defined. In Sect. 5.3 two sufficient conditions are demonstrated. The first is that all Chern numbers of h can be defined if the Fermi energy $E_F = 0$ is in a region of Anderson localization, which describes the regime of strongly disordered topological insulators. The second condition is geared towards topological semimetals, namely if the density of states of h vanishes rapidly enough at the Fermi level, some of the weak Chern numbers continue to be well-defined. Let us, however, emphasize that in the absence of a bulk energy gap the Sobolev index theorem does not imply the invariance of the Chern numbers under perturbations of the Hamiltonian since the dependence of u_F and p_F on h is not norm-continuous, but merely weakly continuous. As the example further below already shows, the Chern numbers can vary continuously with h and take arbitrary real values even for periodic models.

The BBC for general half-planes with normal vector $v_\xi \in \mathbb{S}^{d-1}$ is then based on a smooth Toeplitz extension. The basic idea is to note that the projection P to a half-space can be written as the positive spectral projection $P = \chi(D_\xi \geq 0)$ of the self-adjoint operator $D_\xi = \sum_{i=1}^d (v_\xi)_i X_i$ which is the suitable scalar Dirac operator in this case. Let us for now assume that the components of v are rationally independent, which means that the boundary hypersurface intersects with the lattice $\mathbb{Z}^d$ in exactly one point (for the general case see Sect. 5.2). The adjoint action of $\xi_t = \mathrm{Ad}_{\exp(\imath D_\xi t)}$ then defines a free $\mathbb{R}$-action on $\mathbb{T}^d_{\mathbf{B},\Omega}$ which is used to form a smooth Toeplitz extension:

$$0 \to \mathbb{T}^d_{\mathbf{B},\Omega} \rtimes_\xi \mathbb{R} \hookrightarrow \mathrm{T}(\mathbb{T}^d_{\mathbf{B},\Omega}, \mathbb{R}, \xi) \to \mathbb{T}^d_{\mathbf{B},\Omega} \to 0.$$

This construction can be interpreted as a bulk-boundary exact sequence, namely Sect. 5.2 shows that the algebra $\mathbb{T}^d_{\mathbf{B},\Omega} \rtimes_\xi \mathbb{R}$ can be considered as an algebra of observables which are localized at the hyper-surface with normal vector v, while the smooth Toeplitz extension $\mathrm{T}(\mathbb{T}^d_{\mathbf{B},\Omega}, \mathbb{R}, \xi)$ consists of observables on a half-space that converge to elements of the bulk algebra $\mathbb{T}^d_{\mathbf{B},\Omega}$ at infinity on one side of the hyper-surface and to 0 on the other side. Moreover, the dual trace $\widehat{\mathcal{T}}_\xi$ is shown to admit a description in terms of a trace per unit surface area. All of this is essential for the physical interpretation of the results.

The K-theoretical approach to the BBC presented in Sect. 5.4 is based on this exact sequence. Combined with the duality theorem for smooth Toeplitz extensions, it reproduces and generalizes the BBC of [46] for the Chern numbers of spectrally gapped Hamiltonians. Let us describe the results briefly. When restricting a gapped bulk Hamiltonian $h \in M_N(\mathbb{T}^d_{\mathbf{B},\Omega})$ with non-trivial Chern numbers to a half-space using Dirichlet boundary conditions $\widehat{h} = PhP$ perturbed by an arbitrary local operator $\widehat{k} \in M_N(\mathbb{T}^d_{\mathbf{B},\Omega} \rtimes_\xi \mathbb{R})$ on the boundary, the bulk energy gap is generically filled with additional boundary states to which one can also associate topological invariants, called boundary Chern numbers. The main result (Theorem 5.4.3) is that all boundary Chern numbers can be computed purely in terms of the bulk Chern numbers. In particular, it is shown that the boundary topological invariants have an explicit smooth dependence on the cutting angles of the half-space and are independent of $\widehat{k}$. As a technical improvement over existing results [39, 46], it is also proved that the boundary states associated to non-trivial weak Chern numbers are delocalized (see Sect. 5.5).

Section 5.6 then considers the special case of the weak odd Chern number with a single generator, namely the winding numbers

$$\mathrm{Ch}_{\mathcal{T},\xi}(u) = -\imath\, \mathcal{T}\big(u^*\nabla_\xi u\big) = -\imath \sum_{i=1}^d \big(v_\xi\big)_i \mathcal{T}\big(u^*\nabla_i u\big) \tag{0.5}$$

It turns out that the BBC for this invariant is closely related to the index theory studied in the first part of this work, since the auxiliary von Neumann algebra $\mathcal{M} \rtimes_\xi \mathbb{R}$

with dual trace $\widehat{\mathscr{T}}_\xi$ which allows to write $\mathrm{Ch}_{\mathscr{T},\xi}$ as a semi-finite index coincides precisely with the von Neumann completion of the edge algebra $\mathbb{T}^d_{\mathbf{B},\boldsymbol{\Omega}} \rtimes_\xi \mathbb{R}$ w.r.t. the GNS representation of the dual trace $\widehat{\mathscr{T}}_\xi$. Hence one can reformulate the BBC as a problem concerning Breuer-Fredholm operators. Let $\widehat{h} = PhP + \widehat{k}$ be a chirally symmetric half-space Hamiltonian as above and $\widehat{u} \in \mathscr{M} \rtimes_\xi \mathbb{R}$ the off-diagonal part of its polar decomposition as in (0.4). If h is not spectrally gapped, then $\widehat{h}$ may have a non-trivial kernel and hence $\widehat{u}$ is in general not unitary, but only a partial isometry. Section 5.6 provides conditions under which $\widehat{u}$ is Breuer-Fredholm and a compact perturbation of the Toeplitz operator $Pu_F P$ with symbol given by the Fermi unitary u_F of the bulk Hamiltonian. If the Sobolev index theorem applies to u_F, this allows to strengthen the smooth version of the BBC and make a statement about the kernel of $\widehat{h}$.

Theorem 0.0.3 (Flat bands of surface states). *For a chiral Hamiltonian $h \in M_N(\mathbb{T}^d_{\mathbf{B},\boldsymbol{\Omega}})$ with Fermi unitary u_F and half-space restriction $\widehat{h} = PhP + \widehat{k}$ as described above,*

$$\mathrm{Ch}_{\mathscr{T},\xi}(uF) = \hat{\mathscr{T}_\xi}\Big(J\ \mathrm{Ker}\Big(\hat{h}\Big)\Big), \tag{0.6}$$

whenever one of the following conditions holds:

- *The Hamiltonian h has a bulk gap, i.e. $0 \notin \sigma(h)$.*
- *0 lies in a (Anderson localized) mobility gap of h.*
- *0 is a pseudogap of the density of states with sufficiently high order, namely there exist $\gamma > \frac{3}{2}$ and $C_\gamma < \infty$ such that the spectral projections $\chi(|h| \le \varepsilon)$ satisfy*

$$\mathscr{T}(\chi(|h| \le \varepsilon)) \le C_\gamma \varepsilon^\gamma .$$

This shows that a nontrivial bulk winding number $Ch_{\mathscr{T},\xi}(u_F)$ implies the existence of states in the kernel of the half-space Hamiltonian and that the signed surface density of these zero-energy states is determined by the weak bulk winding numbers. These edge states are said to form a flat band. Condition (i) is already covered by [46]. Part (ii) generalizes the one-dimensional result of [57] to higher dimensional systems, thereby adding to the short list of rigorously proven results on the BBC for mobility gapped topological insulators. The sufficient condition (iii) applies *e.g.* chiral Dirac-semimetals in dimensions larger than one. A particularly vivid example is provided by a standard model of (pure) graphene based on the discrete Laplacian on a hexagonal lattice [60]. Choosing a parametrization of the hexagonal lattice such that a termination in the directions $v_\xi = e_1$ and $v_\xi = e_2$ gives so-called zigzag edges and $v_\xi = 2^{-\frac{1}{2}}(e_2 - e_1)$ an armchair zigzag edges, the two weak Chern numbers (winding numbers) can be computed explicitly to be $-\imath\mathscr{T}(u^*\nabla_i u) = \frac{1}{3}$ (see Sect. 5.7). Therefore Theorem 0.0.3 implies

$$\hat{\mathscr{T}_\xi}\Big(J\ \mathrm{Ker}\Big(\hat{h}\Big)\Big) = \frac{1}{3}\Big(\big(v_\xi\big)_1 + \big(v_\xi\big)_2\Big) \tag{0.7}$$

and thus armchair edges need not have edge states at all, while the signed density of surface states is maximal for zigzag edges. This was known for a long time by an elementary analysis [61, 62], and the formula (0.6) for rationally dependent normal vectors v_ξ follows from a non-rigorous Zak-phase argument [63]. The existence of edge states (but not the connection with the bulk topology) has also been shown for continuum operators with a hexagon symmetry and rational edges [64]. Theorem 0.0.3 also proves the equality (0.6) for irrational angles and shows stability, for example, under adding surface disorder $\tilde{k}$ to the half-space Hamiltonian $\widehat{h} = PhP + \tilde{k}$, hence showing that the actual structure of the surface is not essential. Let us stress that the numerical range of the Chern numbers is not discrete and the value $\frac{1}{3}$ is in this case essentially given by the projected distance between two band-touching points in momentum space, which changes continuously as the bulk model is varied, *e.g.* when other hopping parameters are added to the graphene model, see the model (5.66) in Sect. 5.7. Robust is the relation (0.6), similar as in an extension of Levinson's theorem to surface states where the density of surface states is equal to a time delay density [65]. For higher dimensions one can also write down Hamiltonians which satisfy the conditions of the BBC, for example, by stacking the model above and adding a weak interlayer coupling. A more interesting possibility in $d = 3$ is given by nodal line semimetals where the spectrum at the Fermi level consists of a loop in momentum space. One may again have non-vanishing winding numbers, which in turn lead to flat bands of surface states whose signed density depends linearly on the components of the surface normal vector [66].

This work is organized as follows. Chapter 1 contains preliminaries on C^*- and W^*-crossed products for abelian group actions and semi-finite tracial states on them. This includes Takai and Takesaki duality, Arveson spectra and basic analysis of smoothness of elements w.r.t. the action. Many of the results are taken from the literature without proofs, but a precise formulation is needed in the arguments later on. The experienced reader can rapidly skim through Chap. 1 as it is not the heart of the matter. Chapter 2 presents the construction of Besov spaces for abelian actions on semi-finite von Neumann algebras. The Peller criteria are proved in Chap. 3 and then combined with known index calculations to prove the Sobolev index theorem. This chapter is the mathematical core of this work. Chapter 4 concerns C^*-crossed products with $\mathbb{R}$-actions and various associated exact sequences. The K-theoretic connecting maps are reviewed with care and the proof of the duality theorem is given. This is new, but uses several results from the literature. The long Chap. 5 then presents the applications to solid state systems. Finally the appendices review and extend results on integration in quasi-Banach spaces and non-commutative L^p-spaces, interpolation theory and Breuer-Fredholm semi-finite index theory.

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Acronyms and Notations

$\imath$	imaginary unit $\sqrt{-1}$
$\lvert \cdot \rvert$	absolute value
SOT	strong operator topology
s.n.f.	semi-finite normal and faithful (trace)
$\mathrm{T} \cong [0, 1)$	torus
$G = \mathbb{T}^{n_0} \oplus \mathbb{R}^{n_1}$	abelian group with $n = n_0 + n_1$ parameters
$\hat{G} = \mathbb{T}^{n_0} \oplus \mathbb{R}^{n_1}$	dual group
$\mathscr{S}(\mathbb{R}^n)$	Schwartz functions
E	Banach space
x	elements in Banach space E
β	G-action on Banach space E
$\mathscr{F}$	Fourier transform; Sect 1.1
$FA(\hat{G})$	Fourier algebra $\mathscr{F}L^1(G)$
χ	characteristic function of a set or event
sgn	sign function $\mathrm{sgn}(x) = \chi(x > 0) - \chi(x < 0)$
χ_s	smooth characteristic function of a set from $C_{0,*}(\mathbb{R})$; Eq. (4.2)
$\imath$	imaginary unit $\sqrt{-1}$
γ_i	Clifford generators; Eq. (3.2)
$\mathscr{A}$	C^*-algebra $\mathscr{A}$
a	element of $\mathscr{A}$
$\mathscr{A}^\sim$	unitization of an algebra $\mathscr{A}$
$M_N(\mathscr{A})$	$N \times N$ matrices with entries in $\mathscr{A}$
diag(A, B)	block diagonal matrix built from A and B
Tr	standard trace over Hilbert spaces
$\mathscr{B}(\mathscr{H})$	bounded operators on Hilbert space $\mathscr{H}$
$\mathscr{K}(\mathscr{H})$	compact operators on Hilbert space $\mathscr{H}$
$\mathbf{1}$	identity operator
$(\mathscr{A}, G, \alpha)$	C^*-dynamical system; Sect. 1.1
$\mathscr{A} \rtimes_\alpha G$	C^*-crossed product; Sect. 1.1
(π, U)	left regular representation; Eq. (1.8)

D	generator in left regular representation (π, U); Eq. (1.9)
$(\mathscr{M}, G, \alpha)$	W^*-dynamical system; Sect. 1.2
$\mathscr{N} = \mathscr{M} \rtimes_\alpha G$	W^*-crossed product; Sect. 1.2
$\mathbf{1}_N$	identity in $M_N(\mathbb{C})$ or $M_N(\mathscr{A})$
$\mathscr{T}$	s.n.f. trace; Sect. 1.3
$(\pi_\mathscr{T}, V)$	GNS representation (covariant) of $(\mathscr{M}, G, \alpha)$ on $L^2(\mathscr{M})$; Sect. 1.3
X	generator of V in GNS representation $(\pi_\mathscr{T}, V)$; Eq. (1.14)
$\mathscr{K}_\mathscr{T}$	$\mathscr{T}$-compact operators; Eq. (A.9)
$\mathscr{Q}_\mathscr{T}$	Calkin algebra w.r.t. $\mathscr{T}$; Appendix A.4
$\mathscr{T}$-Ind	Breuer-Fredholm index w.r.t. $\mathscr{T}$; Appendix A.4
$\sigma_\alpha(x)$	Arveson spectrum of x w.r.t. action α; Definition 1.4.1
$\hat{\mathscr{T}}_\alpha$	dual trace; Sect. 1.5
$\hat{\alpha}$	dual action of dual group $\hat{G}$ on crossed product; Sect. 1.6
i_T	Takai duality isomorphism; Sect. 1.6
∇_v	directional derivation of action; Sect. 1.7
$C^m(\mathscr{A}, \alpha)$	m times differentiable elements of $\mathscr{A}$; Sect. 1.7
$\mathscr{A}_{\mathscr{T},\alpha}$	Fréchet algebra of smooth elements; Sect. 1.7
$L^p(\mathscr{M})$	non-commutative L^p-space w.r.t. $\mathscr{T}$; Appendix A.2
$W^m_p(\mathscr{M})$	non-commutative Sobolev spaces; Eq. (1.35)
$\mathscr{M}^C_{\mathscr{T},\alpha}$	space of integrable operators with compact spectrum; Eq. (2.18)
$(W_j)_{j\in\mathbb{N}}$	dyadic decomposition; Eq. (2.1)
$B^s_{p,q}(\mathscr{M})$	scale of Besov spaces w.r.t. a G-action; Eq. (2.7)
$B_n(\mathscr{M})$	short notation for Besov space $B^{\frac{n}{n+1}}_{n+1,n+1}(\mathscr{M})$; Eq. (3.22)
P_I	spectral projections of D on $I \subset \mathbb{R}^n$; Eq. (3.3)
H_a	Hankel operator with symbol a; Definition (3.1.1)
$\hat{H}_a$	two-sided Hankel operator with symbol a; Eq. (3.20)
$\mathrm{Ch}_{\mathscr{T},\alpha}$	Chern cocycle for G-action α; Definition (3.4.2)
ξ	$\mathbb{R}$-action on $\mathscr{M}$; Chap. 4
$\mathrm{Ch}_{\mathscr{T},\theta}$	Chern cocycle for $\mathbb{R}^n$-action θ; Definition 4.3.4
$\mathbf{D}$	Dirac operator associated to action; Eq. (3.1)
$\mathbf{P}$	positive spectral (Hardy) projection of $\mathbf{D}$; Definition (3.1.1)
$\mathrm{T}(\mathscr{A}, G, \xi)$	smooth Toeplitz extension; Definition (4.1.1)
∂^ξ_i	Connes-Thom isomorphism; Sect. 4.2
s_i	suspension maps in K-theory; Sect. 4.2

Acronyms and specific meaning in the applications of Chap. 5

BGH	bulk gap hypothesis; Definition 5.3.1
CH	chiral symmetry hypothesis; Definition 5.3.2
MGR	mobility gap regime; Definition 5.3.4
DOS	density of states; Definition 5.3.7
BBC	bulk-boundary correspondence
$(\Omega, \mathbb{Z}^d, \mathbb{P})$	disorder configuration probability space with $\mathbb{Z}^d$ -action; Sect. 5.1
E_F	Fermi energy
p_F	Fermi projection $\chi(h \leq E_F)$

sgn_ϵ	approximate sign function; Lemma 5.3.6
u_F	Fermi unitary operator for chiral system
J	chiral symmetry operator; Eq. (5.21)
$\mathscr{A} = \mathbb{T}^d_{\mathbf{B},\Omega}$	disordered non-commutative torus, C^*-algebra; Sect. 5.1
π_ω	physical representations of bulk on lattice Hilbert space; Eq. (5.6)
$\mathscr{T}$	trace per unit volume; Eq. (5.4)
$\mathscr{M}$	von Neumann algebra $L^\infty(\mathbb{T}^d_{\mathbf{B},\Omega}, \mathscr{T})$of bulk observables; Sect. 5.1
$\mathscr{E}$	C^*-algebra $\mathbb{T}^d_{\mathbf{B},\Omega} \rtimes_\xi G$ of edge operators; Sect. 5.2
$\hat{\mathscr{A}}$	C^*-algebra $\mathrm{T}(\mathbb{T}^d_{\mathbf{B},\Omega}, G, \xi)$; Sect. 5.2
$\mathscr{N}_\xi = \mathscr{M} \rtimes_\xi G$	von Neumann algebra of half-space observables; Sect. 5.2
$X_\xi = v_\xi \cdot X$	position operator off the surface; Sect. 5.2
ξ	$\mathbb{R}$ -action induced by v_ξ perpendicular on half-space; Eq. (5.8)
ξ	$\mathbb{R}$-action shifting perpendicular to surface; Eq. (5.8)
$\mathscr{A} \rtimes_\xi G$	C^*-algebra of edge operators; Sect. 5.2
P	half-space projection $P = \chi(X_\xi > 0)$; Sect. 5.4
$\mathscr{P}$	soft half-space restriction
h	Hamiltonian from $\mathscr{A}$
$\hat{h}$	half-space Hamiltonian; Proposition 5.4.1 and Eq. (5.42)
ν_h	density of states measure; Definition 5.3.7
θ	$\mathbb{R}^n$-action specifying (weak) invariants; Eq. (5.22)
$\mathrm{Ch}_{\mathscr{T},\theta}(p_F)$	even bulk Chern numbers; Eq. (5.23)
$\mathrm{Ch}_{\mathscr{T},\theta}(u_F)$	odd bulk Chern numbers; Eq. (5.24)
$\hat{\mathscr{T}}_\xi$	averaged trace per surface area; Eq. (5.16)
$\hat{\mathscr{T}}_{\omega,r}$	trace per surface area; Propositions 5.2.8 and 5.2.9

Contents