Applications and Connections between Twisted Equivariant K-theory, Quantum Mechanics and Condensed Matter

by

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Abstract

The present thesis consists of 2 parts. Chapter 1 is about applications of twisted equivariant K-theory to condensed matter. We consider non-interacting electrons on a half-crystal (a crystal with a boundary), with a gapped bulk condition, under quasi-adiabatic evolution. In A. Adem, O. Antolín, G. Semenoff and D. Sheinbaum JHEP, 2016 we found that Fermi surfaces for these systems under quasi-adiabatic evolution are classified by the K^{-1}-group of the surface Brillouin zone $\mathbb{T}^{d-1}$. Systems with time-reversal and particle-hole symmetry were also considered and we obtained different KR-groups for the different cases. In Chapter 1 I rewrite A. Adem, O. Antolín, G. Semenoff and D. Sheinbaum JHEP, 2016 in a more function-analytic language and further solve technical issues to extend it to include crystallographic symmetries on the directions parallel to the boundary. In Chapter 2 I reproduce the relevant parts of my joint work with C. Okay (C. Okay and D. Sheinbaum arXiv:1905.07723). There we explored a connection between twisted equivariant K-theory to contextuality in quantum mechanics. We also reformulated the sheaf-theoretic framework of S. Abramsky and A. Brandenburger New Journal of Physics, 2011 for contextuality and connect it to another one employing a group cohomology approach of C. Okay, S. Roberts, S.D Bartlett, and R. Raussendorf Quantum Information and Computation, 2017. This leads to the construction of a classifying space for contextuality, from which Wigner functions are classes in its twisted K-theory.

Lay Summary

What makes a material conduct electricity? It depends on the existence of a surface (called Fermi surface) inside an abstract space, that comes out from the periodic arrangement of the atoms in a solid. First we study systems which have a boundary and do not have a periodic arrangement in the direction perpendicular to the boundary. There are materials that can only conduct electricity on their surface or not conduct at all. We classify Fermi surfaces of such materials according to whether we can change one into the other as we change a physical property (like the strength of a magnetic field acting on the material or by including extra symmetries). What makes quantum mechanics weird? One of the main contenders is contextuality. In our 2nd chapter we reconcile two different approaches to contextuality by creating another abstract space whose topology (shape) yields many features of quantum mechanics.

Preface

Chapter 1 is based on results published in A. Adem, O. Antolín and G.W. Semenoff and D. Sheinbaum JHEP, 2016. All authors worked equally on the results presented in Sections 1.1 to 1.7. I solely extended the results appearing in Section 1.8. Chapter 2 has been published in very similar form in C. Okay and D. Sheinbaum arXiv:1905.07723. Both authors worked equally on the results presented there. I solely worked in the discussion presented in Chapter 3.

Table of Contents

List of Tables

List of Figures

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Chapter 1

K-theory and Fermi Surfaces

1.1 Introduction

Classification of locally stable Fermi surfaces and topological phases of matter using K-theory was first introduced in the pioneering work of Hořava [3] and Kitaev [4]. This chapter is a presentation and further continuation of [2]. To our knowledge, [2] was the first publication to directly obtain a K-theoretic classification for the global stability of Fermi surfaces without resorting to physically-unjustified mathematical procedures, as had been done previously in the literature. A typical example of a Fermi surface Σ_F of interest for the systems considered here (see section 1.3 and previous ones) is represented in figure 1.1. More generally a Fermi surface is usually a codimension 1 subspace (though there are degenerate cases) inside the surface Brillouin zone, a $d-1$-dimensional torus, where the spectrum of an operator, the fiber single particle Hamiltonian which comes about in 1.2, is equal to a real number known as the Fermi energy $\mathcal{E}_F$. The Fermi surface of a given material determines its physical properties such as whether it is a conductor or an insulator [5], [6].

Once we have a Fermi surface Σ_F for a given Hamiltonian $\mathcal{H}$, we can ask what happens to it as we evolve our Hamiltonian by changing a parameter $\mathcal{H}(s)$. Can we always connect 2 different Fermi surfaces? Classifying Fermi surfaces up to this evolution is the whole point of this work.

Physicist have used the notion of *spectral flow*[7] to describe a physical phenomena known as a chiral anomaly in some condensed matter models [8]. This topological invariant comes out in our construction as well, being the number of crossings of the eigenvalues over an axis with positive slope minus the number of crossings with negative slope. Figure 1.1 is an example of a spectral flow equal to 1 (see section 1.6.1).

Remark 1.1.1. *For readers more familiar with the physics literature and terminology we note that Ryu et al. [9],[10] and Witten [11] among others, have developed a formalism for studying gapped bulk systems by classifying their gapless edge states and the bulk-boundary correspondence, where the*

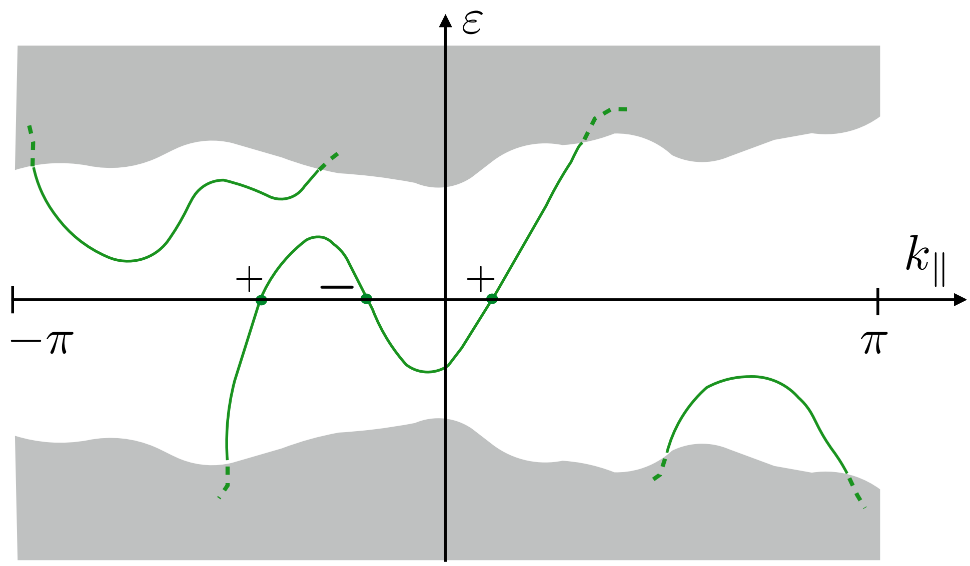

Figure 1.1: $d = 2$ Fermi points. the $\vec{k}_{\|}$-axis represents the surface Brillouin zone from $-\pi$ to π. Solid regions and dashed lines belong to the continuous spectrum (Bulk states and resonance states respectively) Solid lines belong to the discrete spectrum (Surface states). The Fermi points Σ_F are those where the solid lines cross the $\vec{k}_{\|}$-axis. In this example the spectral flow is equal to 2(+) crossings - 1(-) crossing = 1. Figure taken from [2]

.

edge states have an anomaly inflow interpretation [12],[13]. This paradigm is physically similar to that of [2], however these arguments rely upon taking a low-energy limit of a lattice Hamiltonian to obtain an effective relativistic field theory [14] such as Chern-Simons for the IQHE, with a correspondence between topological field theories and symmetry protected topological phases [11],[15]. [2] did not rely on such approximations, but it does have other strong assumptions such as discrete translation-invariance.

We continue the study of systems on a half-solid (see section 1.2). As discrete translation-invariance is broken by the surface $\mathbb{R}^{d-1} \times \{0\}$, only a reduced version of Bloch's theorem holds. Nevertheless this opens up the possibility of having Surface states and so called Bulk states (1.2.2). This, together with a gapped bulk condition (1.3.1) will play the central role in the derivation of the K-theoretic classification of quasi-adiabatically stable Fermi surfaces (section 1.5) shown in theorem 1.6.1. We reproduce the statement of theorem 1.6.1

Quasi-adiabatic equivalence classes of Fermi surfaces Σ_F for non -interacting, gapped bulk Hamiltonians on a d-dimensional half-crystal are in one to one correspondence with the complex K-theory group $K^{-1}(\mathbb{T}^{d-1})$.

Figure 1.1 represents a class in the group $K^{-1}(S^1) \approx \mathbb{Z}$ for $d = 2$ (see section 1.6.1), specifically the class equal to 1. We include the cases with particle-hole symmetry and time-reversal symmetry (and their different variations) in theorems 1.7.2, 1.7.3, 1.7.4, 1.7.5. These results were originally presented in [2]. Finally we extend [2] to half-solids with a surface crystallographic symmetry (section 1.8) in theorem 1.8.3.

Remark 1.1.2. *Issues of aperiodicity, disorder and unitary-antiunitary ambiguities in representations of symmetry operators are considered in a more general framework in [16],[17] for topological phases of non-interacting fermions and are not dealt with in this thesis. However, neither of [16],[17] attempt to classify Fermi surfaces.*

1.2 Systems on a half-solid

Let $\mathscr{H} = L^2(\mathbb{R}^d; W)$ be the *Hilbert space* of equivalence classes of square integrable functions on $\mathbb{R}^d$ valued in W, the standard 2-dimensional representation of the Lie algebra $\mathfrak{su}(2)$.

$\mathcal{H}$ is an unbounded self-adjoint operator with a dense domain $\mathscr{D}(\mathcal{H}) \subset \mathscr{H}$ of the form

$$\mathcal{H} = -\nabla^2 + \mathrm{V}. \tag{1.1}$$

To represent the half-solid, one condition is that our potential V satisfies

$$V(r_\perp, \vec{r}_\parallel) = \begin{cases} \mathrm{W}(r_\perp, \vec{r}_\parallel) & r_\perp \leq 0 \\ 0 & \text{otherwise.} \end{cases} \tag{1.2}$$

where we have split $\mathbb{R}^d = \mathbb{R}_\perp \oplus \mathbb{R}_\parallel^{d-1}$, which will correspond to the directions parallel and perpendicular to the boundary of the solid respectively. Another condition [18],[5] is *periodicity* of V(and hence $\mathcal{H}$) with respect to translations in the direction parallel to the boundary. Let $\Gamma_\parallel \approx \mathbb{Z}^{d-1}$ be a *sublattice* of $\mathbb{R}_\parallel$ and let

$$\mathcal{T} : \Gamma_\parallel \to \mathcal{U}(\mathscr{H}) \tag{1.3}$$

be a unitary representation of $\Gamma_\parallel$. The periodicity condition is given by

$$[\mathcal{H}, \mathcal{T}_{\gamma_\parallel}] = 0 \;\; \forall \gamma_\parallel \in \Gamma_\parallel \tag{1.4}$$

Finally, as in [18] there is a technical condition on the characteristics of the potential V so that $\mathcal{H}$ has empty singular continuous spectrum (see subsection 1.2.1). This condition is that $V \in \mathcal{L}^1_{\mathrm{loc}}(\mathbb{R}^d)$, the space of locally integrable functions on $\mathbb{R}^d$. With this condition we have that the dense domain on which $\mathcal{H}$ is defined is given by

$$D(\mathcal{H}) = D(-\nabla^2) \cap D(V). \tag{1.5}$$

Here $D(-\nabla^2)$ is $\mathscr{C}_0^\infty(\mathbb{R}^d)$, the subspace of infinitely differentiable functions with compact support.

At this point we should also mention that one can include a magnetic field $\vec{B}$ (to break time-reversal symmetry) through a vector potential $\vec{A}$: $\mathbb{R}^d \to \mathbb{R}^d$, $\vec{B} = \nabla \times A$, such that our Hamiltonian is of the form

$$\mathcal{H}_s(\vec{A}) = (i\nabla - \vec{A})^2 + \vec{\sigma} \cdot \vec{B} + V, \tag{1.6}$$

where $\vec{\sigma}$ is the *Pauli-Lubanski* vector, made out of the generators of $\mathfrak{su}(2)$ representing non-relativistic spin [19]. Here one has to be careful since the vector potential $\vec{A}$ may not have the periodicity of the lattice unless some technical conditions are imposed on the magnetic field.

Remark 1.2.1. *There has been an extensive treatment including this technicalities which are relevant when considering disorder, but in what follows here there is no strong loss of generality by assuming implicitly the magnetic field in the notation and we shall only write $\mathcal{H}$.*

Because of the periodicity in the parallel direction our Hilbert space $\mathscr{H}$ and our Hamiltonian $\mathcal{H}$ are unitary equivalent to a *direct integral decomposition* [5],[20]

$$\mathscr{H} \simeq \int_{\mathbb{T}^{d-1}}^{\oplus} \mathscr{H}(\vec{k}_{\|}) d\vec{k}_{\|}\,, \tag{1.7}$$

$$\mathcal{H} \simeq \int_{\mathbb{T}^{d-1}}^{\oplus} \mathcal{H}(\vec{k}_{\|}) d\vec{k}_{\|}\,. \tag{1.8}$$

Let us dissect the different pieces appearing in (1.7) connecting analysis and topology. The integral sign should be thought of as a direct sum of vector spaces, one for each point on the measure space $\mathbb{T}^{d-1}$ but using the measure $d\vec{k}_{\|}$ as $\mathbb{T}^{d-1}$ is uncountable. The measure space $\mathbb{T}^{d-1}$ is in fact the *Pontryagin dual* $\mathrm{Hom}(\Gamma_{\|}, S^1)$ of our lattice $\Gamma_{\|}$, equipped with its *Haar* measure $d\vec{k}_{\|}$, which makes $\mathbb{T}^{d-1}$ a topological group homeomorphic to a $d-1$-dimensional torus. Therefore it is a well-posed problem to ask questions about continuity (or differentiability, analyticity even) of the *spectrum* $\sigma(\mathcal{H}(\vec{k}_{\|}))$ of the *fiber* or *Bloch* Hamiltonian $\mathcal{H}(\vec{k}_{\|})$, as one varies $\vec{k}_{\|}$. $\mathcal{H}(\vec{k}_{\|})$ is an unbounded self-adjoint operator on the fiber Hilbert space $\mathscr{H}(\vec{k}_{\|}) \equiv L^2(\mathbb{R}^d/\Gamma_{\|}; \mathcal{L}_{\{\vec{k}_{\|}\}\times\mathbb{R}^{d-1}/\Gamma_{\|}} \otimes W)$. Here $\mathcal{L}_{\vec{k}_{\|}\times\mathbb{R}^{d-1}/\Gamma_{\|}}$ denotes the fiber at $\vec{k}_{\|}$ of the *Poincaré line bundle* $\mathcal{L} \to \mathbb{R}^d/\Gamma_{\|} \times \mathbb{T}^{d-1}$ given by the quotient under the action of $\Gamma_{\|}$ [16], [21]

$$\begin{aligned}\mathbb{R}^d \times \mathbb{T}^{d-1} \times \mathbb{C} \times \Gamma_{\|} &\to \mathbb{R}^d \times \mathbb{T}^{d-1} \times \mathbb{C}\,,\\ (\vec{r}, \vec{k}_{\|}, z, \gamma_{\|}) &\mapsto (\vec{r} + \gamma_{\|}, \vec{k}_{\|}, z * e^{i\vec{k}_{\|}\cdot\gamma_{\|}})\end{aligned} \tag{1.9}$$

Remark 1.2.2. *To define the above unitary it is useful to first show (see [21] for the construction) $L^2(\mathbb{R}^d; W)$ is unitary equivalent to*

$$L^2_{\mathbb{T}^{d-1}}(\mathbb{T}^{d-1}\times\mathbb{R}^{d-1}; W) = \left\{\psi : \mathbb{T}^{d-1}\times\mathbb{R}^{d-1} | \psi(\vec{k}_{\|}, \vec{r}+\gamma_{\|}) = e^{i\vec{k}_{\|}\cdot\gamma_{\|}}\psi(\vec{k}_{\|}, \vec{r})\, \forall\gamma_{\|} \in \Gamma_{\|}\right\} \tag{1.10}$$

In the physics literature this is known as the *Bloch transform*[6] and $\mathbb{T}^{d-1}$ is known as the *Brillouin zone*. We remark that equation (1.7) means that our Hilbert space is unitarily equivalent to L^2-sections of the *Hilbert* bundle E, where

$$E = \bigcup_{\vec{k}_\parallel \in \mathbb{T}^d} \mathscr{H}(\vec{k}_\parallel), \tag{1.11}$$

which is a Hilbert bundle over the surface Brillouin zone $\mathbb{T}^{d-1}$ [16], [21]. However this bundle turns out to be trivializable, i.e.

$$E = \mathbb{T}^{d-1} \times \mathscr{H}' \tag{1.12}$$

where $\mathscr{H}' = L^2(\mathbb{R}^d/\Gamma_\parallel; \mathbb{C} \otimes W)$. However, it is not equivariantly trivializable as we shall see in section 1.8.

1.2.1 The spectrum of the fiber

Let us briefly remind our selves that the spectrum of an operator $\mathcal{A}$, $\sigma(\mathcal{A})$ is the set of $\lambda \in \mathbb{C}$ such that $\mathcal{A} - \lambda I$ is not invertible [22]. For self-adjoint operators like $\mathcal{H}(\vec{k}_\parallel)$ the spectral theorem implies that their spectrum is real. One can show the spectrum is "closed", it is also bounded for bounded operators and conversely unbounded for unbounded ones. Continuity of the spectrum means viewing σ as a function

$$\sigma : \mathbb{T}^{d-1} \longrightarrow C(\mathbb{R}), \tag{1.13}$$

$$\vec{k}_\parallel \mapsto \sigma(\mathcal{H}(\vec{k}_\parallel)) \tag{1.14}$$

where $C(\mathbb{R})$ is the metric space of closed subsets (the spectrum is always a closed subset of $\mathbb{R}$) under the *Hausdorff* distance.

$$d(C_1, C_2) = \max_{x \in C_1} \min_{y \in C_2} \{d(x, y)\} \tag{1.15}$$

and there are interesting variants of this notion explored in [23]. Since $\mathcal{H}(\vec{k}_\parallel)$ is self-adjoint, by the spectral theorem for unbounded self-adjoint operators, $\sigma(\mathcal{H}(\vec{k}_\parallel))$ is real and the Hilbert space can be decomposed as a direct sum $\mathscr{H}(\vec{k}_\parallel) = \mathscr{H}_{\text{pp}}(\vec{k}_\parallel) \oplus \mathscr{H}_{\text{ac}}(\vec{k}_\parallel) \oplus \mathscr{H}_{\text{sc}}(\vec{k}_\parallel)$ where $\mathscr{H}_{\text{pp}}(\vec{k}_\parallel)$ consists of the span of eigenvectors of $\mathcal{H}(\vec{k}_\parallel)$ whose associated spectral measure on subsets of $\mathbb{R}$ is pure point or atomic, whereas the spectral measure associated to elements of the absolutely continuous and singular continuous subspaces are absolutely continuous and singular continuous with respect to the Lebesgue measure on $\mathbb{R}$. Let us remark that though $\mathscr{H}_{\text{pp}}(\vec{k}_\parallel)$ may be finite, $\mathscr{H}_{ac}(\vec{k}_\parallel)$ and $\mathscr{H}_{\text{sc}}(\vec{k}_\parallel)$ are always infinite dimensional [22]. Thus, the spectrum $\sigma(\mathcal{H}(\vec{k}_\parallel)) = \sigma_{\text{pp}}(\mathcal{H}(\vec{k}_\parallel)) \cup \sigma_{\text{ac}}(\mathcal{H}(\vec{k}_\parallel)) \cup \sigma_{\text{sc}}(\mathcal{H}(\vec{k}_\parallel))$. With the conditions for V stated in 1.2, Davies [18] and Simon show $\sigma_{\text{sc}}(\mathcal{H}(\vec{k}_\parallel)) = \emptyset$.

1.2.2 Surfaces, bulk states and spectral projections

Now that we have introduced more properties of the spectrum of the fiber Hamiltonian, we can use them to partially characterize the solutions to the Schröedinger equation with our choice of V. Here we shall simply follow [18]:

Consider

$$\mathcal{P}_{\mathrm{S}} = \int_{\mathbb{T}^{d-1}}^{\oplus} \mathcal{P}_{\mathrm{pp}}(\mathcal{H}(\vec{k}_{\parallel}))d\vec{k}_{\parallel}\,. \tag{1.16}$$

Here $\mathcal{P}_{pp}(\mathcal{H}(\vec{k}_{\parallel}))$ denotes the projection onto the subspace $\mathscr{H}_{pp}(\mathcal{H}(\vec{k}_{\parallel}))$. It is shown in [18] that under certain restrictions on the potential V, $\eta \in \operatorname{Ran}\mathcal{P}_{\mathrm{S}}$, the rank of $\mathcal{P}_{\mathrm{S}}$ if and only if

$$\lim_{a\to\infty} \sup_{t} \int_{r_{\perp}>a} |e^{-it\mathcal{H}}\eta(\vec{r})|^2 d\vec{r} = 0 \tag{1.17}$$

This means that in a suitable sense η may not be found sufficiently far away from the boundary (surface of the half-solid) for any choice of time t. Therefore as one can guess, the S stands for surface, and any element in $\operatorname{Ran}\mathcal{P}_S \subset L^2(\mathbb{R}^d; W)$ will be called a *Surface state.*
Similarly, we may define

$$\begin{aligned} \mathcal{P}_B &= \int_{\mathbb{T}^{d-1}}^{\oplus} \mathcal{P}_{ac}(\mathcal{H}(\vec{k}_{\parallel}))d\vec{k}_{\parallel} && (1.18)\\ &= I - \mathcal{P}_S. && (1.19) \end{aligned}$$

and elements $\psi \in \operatorname{Ran}\mathcal{P}_{\mathrm{B}}$ are called *Bulk states* since for any t one has a non-zero probability of finding the particle (the integral in the limit) infinitely deep inside the crystal.
We point out that the spectrum of the original Hamiltonian $\sigma(\mathcal{H})$ is absolutely continuous and comes in bands so both $\operatorname{Ran}\mathcal{P}_S$ and $\operatorname{Ran}\mathcal{P}_B$ belong in $\mathscr{H}_{ac}(\mathcal{H})$. A crucial point to make is that though $\mathscr{H}_{\mathrm{pp}}(\vec{k}_{\parallel})$ and $\mathscr{H}_{\mathrm{ac}}(\vec{k}_{\parallel})$ are orthogonal subspaces, $\sigma_{\mathrm{pp}}(\mathcal{H}(\vec{k}_{\parallel})) \cap \sigma_{\mathrm{ac}}(\mathcal{H}(\vec{k}_{\parallel})) \neq \emptyset$. When this occurs we have a *Surface resonance* depicted in 1.2III, together with a Surface 1.2II and Bulk 1.2I state.

Remark. *The continuity explained in the previous section may be represented by having functions $\varepsilon_\alpha : U \subset \mathbb{T}^{d-1} \to \mathbb{R}$, which are continuous. In the literature these are known as bands. Bands consist either of absolutely continuous spectrum (Bulk band) or pure point spectrum (Surface bands).The*

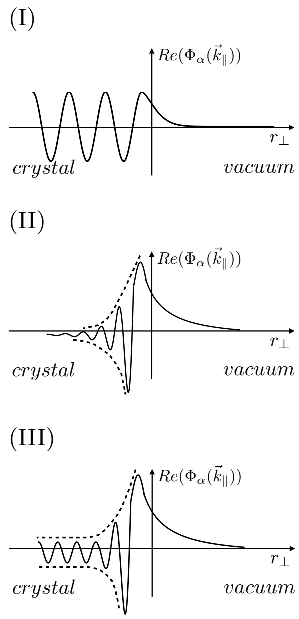

Figure 1.2: Real part of the wave function of the distinct types of states on a half-space as a function of $r_\perp$. All solutions decay exponentially outside the crystal. 1.2I is a bulk state which is periodic inside the crystal. 1.2II Surface state, decays very rapidly away from the boundary. 1.2III Resonance state, the decay eventually stops and the solution is again periodic. Dashed lines represent the *envelope* of the solutions. Figure taken from [2]

index α can be used to denote either of these and we call it band index. The reason why they are defined on an open subset is that Surface bands and Bulk bands may intersect producing a surface resonance.

1.3 Fermi surface

We have thus far only considered the single particle problem moving in the semi-periodic potential of a half-crystal. We now wish to employ this picture together with the Pauli exclusion principle and the non-interacting electron approximation to describe a system in the *thermodynamic limit* (number of particles $N \to \infty$). This conveniently allows us to avoid discussing the Fock space construction $\mathscr{F}_a = \oplus_{n \geq 0} \mathscr{H}^{\wedge n}$, where *wedge* denotes the antisymmetric tensor product and we can very conveniently ignore the so-called *second*

quantization formalism.
The intuitive picture to define the *Fermi energy* $\mathcal{E}_F$ is that each electron (2 electrons if we take into account spin without a magnetic field) occupies a spectral subspace coming from a small ball around a point $\varepsilon(\vec{k}_{\|}) \in \sigma(\mathcal{H}(\vec{k}_{\|}))$ starting at $\min_{\vec{k}_{\|}\in\mathbb{T}^{d-1}} \varepsilon(\vec{k}_{\|}) \in \sigma(\mathcal{H}(\vec{k}_{\|}))$. The reason why it has to be a small ball and not just a single point is due to Heisenberg's uncertainty principle. The above mentioned process continues until one runs out of electrons (in the thermodynamic limit the radius of the balls tends to zero as the volume and number of particles goes to infinity). Surprisingly, it is not that easy to find a proper definition for $\mathcal{E}_F$ in the mathematical literature. To our knowledge the most rigorous one is the following:
Consider the extended Hamiltonian for the *full solid*

$$\mathcal{H} = -\nabla^2 + \tilde{V}(r_\perp, \vec{r}_{\|}), \tag{1.20}$$

with

$$\tilde{V}(r_\perp, \vec{r}_{\|}) = \begin{cases} V(r_\perp, \vec{r}_{\|}) & r_\perp \leq 0 \\ V(-r_\perp, \vec{r}_{\|}) & \text{otherwise.} \end{cases} \tag{1.21}$$

We now have full periodicity $\Gamma \approx \mathbb{Z}^d$, so we can perform a direct integral decomposition over the Pontryagin dual $\mathbb{T}^d$. The difference now is that the fibers $\mathcal{H}(\vec{k})$ are elliptic operators on a compact manifold so their spectrum $\sigma(\mathcal{H}(\vec{k}))$ is pure point and ordered [20]. It therefore allows us to define the density of states (density of levels) measure ρ as [5]

$$\rho(-\infty, E) = \frac{2}{Vol(\mathbb{T}^d)} \sum_n \left\{ \vec{k} \in \mathbb{T}^d \,|\, \varepsilon_n(\vec{k}) = E \right\} \tag{1.22}$$

where the 2 is to take into account spin. We can then define the Fermi energy $\mathcal{E}_F$ as

$$\mathcal{E}_F = \left\{ \inf E \,|\, \rho(-\infty, E) = l \right\} \tag{1.23}$$

where l is the number of atoms in the Wigner-Seitz cell of the lattice Γ. When we truncate the system back into the half-solid this number remains the same (we could have attempted to modify the definition to employ it directly on the half crystal but then we would have to deal with the absolutely continuous spectrum of the fibers) and so, as defined, it has the same physical interpretation.

We can now define the *Fermi surface* Σ_F for the half-solid as

$$\Sigma_F = \left\{ \vec{k}_{\|} \in \mathbb{T}^{d-1} \,|\, \mathcal{E}_F \in \sigma(\mathcal{H}(\vec{k}_{\|})) \right\} \tag{1.24}$$

At this point we mention in passing that an empty Fermi surface represents a material which is an insulator (does not conduct electricity) where as a non-empty one is a metal, with different possible variants of these based on the size of the gap between the highest occupied state and the lowest one unoccupied [6],[5].

1.3.1 Gapped bulk condition and Fredholm operators

When physicists study condensed matter systems (interacting or not) with a boundary, they often impose an extra constraint on their system called the *Gapped Bulk condition*. To present this condition in full generality would derail our attention too much, however we will present a formulation of this constraint for the type of systems consider in this work (non-interacting electrons in a half-solid). If one looks at the graph of the spectrum of the fiber $\sigma(\mathcal{H}(\vec{k}_{\|}))$ vs $\vec{k}_{\|}$ the $d-1$-dimensional hyperplane corresponding to $\sigma(\mathcal{H}(\vec{k}_{\|})) = \mathcal{E}_F$ may intersect the continuous spectrum or not. If

$$\sigma_{\text{ac}}(\mathcal{H}(\vec{k}_{\|})) \cap \{\sigma(\mathcal{H}(\vec{k}_{\|})) = \mathcal{E}_F\} = \emptyset \ \forall \vec{k}_{\|} \tag{1.25}$$

then we say that our system satisfies the gapped bulk condition, which f means that $\mathcal{E}_F$ is between Bulk bands. In physical terms it means that our system only conducts electricity through its surface! (if $\Sigma_F = \emptyset$ then it is simply an insulator). We shall assume from now on that our systems satisfy the gapped bulk condition and see that it is almost equivalent to our fibers being $\mathcal{H}(\vec{k}_{\|})$ in a certain subset of unbounded self-adjoint operators. We must further assume a slightly stronger condition

$$\sigma_{\text{ess}}(\mathcal{H}(\vec{k}_{\|})) \cap \{\sigma(\mathcal{H}(\vec{k}_{\|})) = \mathcal{E}_F\} = \emptyset \ \forall \vec{k}_{\|} \tag{1.26}$$

This is to avoid the unphysical situation of having an infinite number of surface bands intersect at a given point in the surface Brillouin zone.

Here we must start looking at a slightly different family of operators for the following reason: By itself the kernel of $\mathcal{H}(\vec{k}_{\|})$ has no physical meaning. To add a physical meaning to the kernel we must shift the spectrum by an amount that has a physical characteristic of the system. Consider the operator $\mathcal{H} - \mathcal{E}_F I$ and perform the same direct integral decomposition to obtain fibers $\mathcal{H}(\vec{k}_{\|}) - \mathcal{E}_F I_{\vec{k}_{\|}}$, where $I_{\vec{k}_{\|}}$ is the identity operator in the fiber Hilbert space $\mathscr{H}(\vec{k}_{\|})$. Let us enumerate what are the conditions which are satisfied by the fibers $\mathcal{H}(\vec{k}_{\|_{\|}}) - \mathcal{E}_F I_{\vec{k}_{\|}}$:

- dim Ker $\mathcal{H}(\vec{k}) - \mathcal{E}_F I_{\vec{k}_\parallel} < \infty$,
- $\mathcal{H}(\vec{k}) - \mathcal{E}_F I_{\vec{k}_\parallel}$ is *self-adjoint.*

Note that the 2nd condition is the slightly stronger version of the Gapped Bulk condition 1.26 (considering the essential spectrum). Operators satisfying these conditions are known in the literature as unbounded *self-adjoint Fredholm operators*[24]. Let us denote the set of not necessarily bounded self-adjoint Fredholm operators on a Hilbert space $\mathscr{H}'$ by $\mathcal{CF}^{sa}(\mathscr{H}')$. $\mathcal{CF}^{sa}(\mathscr{H}')$ may be decomposed as

$$\mathcal{CF}^{sa}(\mathscr{H}') = \mathcal{CF}^{sa}_{+}(\mathscr{H}') \sqcup \mathcal{CF}^{sa}_{*}(\mathscr{H}') \sqcup \mathcal{CF}^{sa}_{-}(\mathscr{H}'). \tag{1.27}$$

$\mathcal{CF}^{sa}_{+}(\mathscr{H}')$ is the subset of $\mathcal{CF}^{sa}(\mathscr{H}')$ such that there exists a finite codimension subspace $\mathscr{V} \subset \mathscr{H}'$, such that

$$\langle \psi, \mathcal{F}\psi \rangle \geq 0 \ \forall \psi \in \mathscr{V}. \tag{1.28}$$

and operators in $\mathcal{CF}^{sa}_{+}(\mathscr{H}')$ are called *essentially positive.* An analogous definition is employed for $\mathcal{CF}^{sa}_{-}(\mathscr{H}')$, which is called the set of *essentially negative* not necessarily bounded self-adjoint Fredholm operators. $\mathcal{CF}^{sa}_{*}(\mathscr{H}')$ is the complement of these two, that is operators which are neither essentially positive nor essentially negative. Because our fibers have an infinite number of Bulk bands that means that there is absolutely continuous spectrum above and below the kernel of $\mathcal{H}(\vec{k}_\parallel) - \mathcal{E}_F I_{\vec{k}_\parallel}$, therefore the spectrum subspaces associated to that subset of the spectrum are both infinite dimensional by definition of the absolutely continuous spectrum [22]. We may therefore conclude [2]:

$$\mathcal{H}(\vec{k}_\parallel) - \mathcal{E}_F I_{\vec{k}_\parallel} \in \mathcal{CF}^{sa}_{*}(\mathscr{H}(\vec{k}_\parallel)) \ \forall \vec{k}_\parallel \in \mathbb{T}^{d-1}. \tag{1.29}$$

This means that in the special case of a half-solid with no interactions, the slightly stronger version of the gapped bulk condition is equivalent to the fibers being in $\mathcal{CF}^{sa}_{*}$, as stated previously.

1.4 Topology on the fibers and a red herring

So far we have concluded that the fibers $\mathcal{H}(\vec{k}_\parallel) - \mathcal{E}_F I_{\vec{k}_\parallel}$ are in $\mathcal{CF}^{sa}_{*}(\mathscr{H}(\vec{k}_\parallel))$. We have yet to discuss what is the appropriate topology for $\mathcal{CF}^{sa}_{*}(\mathscr{H}(\vec{k}_\parallel))$ that represents the physical properties of the system. Different topologies for $\mathcal{CF}^{sa}_*(\mathscr{H}')$ have been explored in [24]. Nonetheless one could argue that because of the Stone-von Neumann theorem [22] on the isomorphism between differentiable one-parameter family of unitary operators and their self-adjoint generators, the correct topology should be the *strong operator topology* for whatever subset of the set of linear operators $\mathcal{D}(\mathscr{H}')$ the Hamiltonian operator $\mathcal{H}$ belongs to. Indeed this should be the correct topology and it is the position taken in [16]. However, the properties of $\mathcal{CF}^{sa}_*(\mathscr{H}')$ have been hard to explore, mainly because of the unboundedness of the operators. Instead one could take the following perspective: What relevant information to the physical problem would we lose if we described $\mathcal{CF}^{sa}_*$ as if they were *bounded* operators instead? One of the big differences with the strong operator topology and the norm topology is semi-continuity of the spectrum but as we have referred to above, these families of operators have continuous spectrum in either topology. Furthermore as we shall see in the next section we are interested in the quasi-adiabatic character of the physical system [25] (in physical terms the low energy behaviour) and we do not care about the asymptotics of the spectrum as it tends to infinity. Is it possible to treat operators in $\mathcal{CF}^{sa}_*(\mathscr{H}')$ as if they were bounded?

1.4.1 The Riesz metric for unbounded operators

We define the Riesz metric on $\mathcal{CF}^{sa}(\mathscr{H}')$ as

$$\begin{aligned} L : \mathcal{CF}^{sa} &\to \mathcal{F}^{sa}\,, \\ \mathcal{H} &\mapsto \mathcal{H}(I + \mathcal{H}^{\dagger}\mathcal{H})^{-\frac{1}{2}}\,, \\ d_R : \mathcal{CF}^{sa} \times \mathcal{CF}^{sa} &\to \mathbb{R}^{\geq 0}\,, \\ d_R(\mathcal{H}_1, \mathcal{H}_2) &\mapsto \|L(\mathcal{H}_1) - L(\mathcal{H}_2)\|, \end{aligned} \tag{1.30}$$

where $\|\,.\,\|$ denotes the standard operator norm and L is known as the Riesz transform [24]. The topology on $\mathcal{CF}^{sa}$ induced by d_R is known as the *Riesz* topology and the natural inclusion of *bounded* self-adjoint Fredholm operators $\mathcal{F}^{sa}(\mathscr{H}') \hookrightarrow \mathcal{CF}^{sa}$ with the norm topology is a *homotopy equivalence.* This fact will be very important to us in later sections. With this topology the disjoint subsets of $\mathcal{CF}^{sa}(\mathscr{H}')$ have three path-components $\mathcal{CF}^{sa}_*(\mathscr{H}')$ and each component is homotopic to the corresponding bounded component of $\mathcal{F}^{sa}(\mathscr{H}')$ [24]. One technical issue with this choice of topology is that it is generally hard to determine whether a family of operators in $\mathcal{CF}^{sa}$ is continuous [24]. However, as is shown in [20],[5],[18] $\mathcal{H}(\vec{k}_{\parallel})$ with $V(\vec{r})$ bounded has a *fixed domain* for all $\vec{k}_{\parallel}$ in the Brillouin zone and as explained in [26], families of operators with a fixed domain are continuous in the Riesz topology.

An other issue that may arise is if we want to consider more symmetries. In that case we will view the direct integral decomposition of our Hilbert space $\mathscr{H}$ as a Hilbert bundle (1.11) over the Brillouin zone $\mathbb{T}^{d-1}$ with an action of a group G on the fibers, i.e.

$$\mathcal{U}(g) : \mathscr{H}(\vec{k}_{\|}) \to \mathscr{H}(g\vec{k}_{\|}) \ \forall g \in G. \tag{1.31}$$

For compact Lie groups this action is not continuous in the norm topology in general. However since the groups of interest for these physical systems are always *discrete* (they come from crystallographic groups or actions of a single operator in the case of time-reversal symmetry) then the action is indeed trivially continuous. We may also comment that the structure group on Projective Hilbert bundles is $\mathcal{PU}(\mathscr{H})$ and one might worry that its topological character is different with the norm topology or the strong operator topology but due to Kuiper's contractibility theorem [27] of $\mathcal{U}(\mathscr{H})$ for infinite dimensional separable $\mathscr{H}$ in both the strong and norm topology $\mathcal{PU}(\mathscr{H})_{norm}$ and $\mathcal{PU}(\mathscr{H})_{strong}$ are homotopic.

Since for any of the physical systems considered we have none of the technical issues mentioned above due to their characteristics (such as only having actions from discrete groups) it would seem that the issue of the choice of topology for the space of our fibers is a *Red Herring*. It may well be that $\mathcal{CF}_*^{sa}(\mathscr{H}^{'})$ in the Riesz topology or strong topology are homotopically equivalent or if not, it may be due to the asymptotic character of the spectrum as it tends to infinity but it certainly does not seem relevant for the problem at hand. Therefore we shall endow $\mathcal{CF}_*^{sa}(\mathscr{H}^{'})$ with the Riesz topology from now on. Furthermore to simplify notation we shall set $\mathcal{E}_F = 0$ and simply write $\mathcal{H}(\vec{k}_{\|})$.

1.5 Adiabatic and quasi-adiabatic evolution

From previous sections we arrived at studying a half-crystal which may or may not have a Fermi surface but must satisfy the gapped bulk condition. We further wish to study what happens to our system as we vary a parameter such as the strength of the magnetic field $\vec{B}$ or change the potential $V(\vec{r})$ through doping or other means. Since physically we mean changing any of those parameter with respect to time we can view each of them as parametrized by t , i.e. $\vec{B}(t)$, etc. In general this is represented by assuming that we now have a family of single particle Hamiltonians $\mathcal{H}(s)$ that often depends differentiably on our parameter $s = t/\tau$, s being is *rescaled* time and τ represents the time scale of the physical problem. We will now proceed to sketch briefly the notion of adiabatic evolution defined in [25] for any given quantum mechanical system.

Let $\mathcal{H}(s)$ be a smooth family of self-adjoint operators. Consider the spectral projection $\mathcal{P}(s)$ onto a spectral subspace. We can define the adiabatic evolution generator as

$$\mathcal{H}_{ad}(s;\mathcal{P}) = \mathcal{H}(s) + i\tau[\mathcal{P}(s), \mathcal{P}'(s)] \tag{1.32}$$

where $\mathcal{P}'(s)$ is the derivative of $\mathcal{P}(s)$. This generator has been defined so as to decouple $\operatorname{Ran} P(s)$ from its complement $1 - \mathcal{P}(s)$ from the evolution. This decoupling has been forced, however what one is actually really interested in is whether the actual physical evolution by $\mathcal{H}(s)$ approximates the evolution by $\mathcal{H}_{ad}(s;\mathcal{P})$ in a suitable sense. Let $\mathcal{U}(s)$ be the one-parameter family of unitary operators with generator $\mathcal{H}(s)$ and $\mathcal{U}_{ad}(s;\mathcal{P})$ with generator $\mathcal{H}_{ad}(s;\mathcal{P})$ respectively. Let $\mathcal{P}_0 = \mathcal{P}(0)$. Then we say the evolution by $\mathcal{U}(s)$ is adiabatic if there exists $\gamma \geq 0$ such that

$$\|\big(\mathcal{U}(s) - \mathcal{U}_{ad}(s)\big)\mathcal{P}_0\| \leq O(\tau^{-\gamma}). \tag{1.33}$$

Where the γ depends on different criteria of differentiability and $O()$ as usual means terms up to said order in τ. In physical jargon we are looking at how close the ground state of the evolved Hamiltonian $\mathcal{H}(s)$ is to the state corresponding to the evolved ground state of the initial Hamiltonian $\mathcal{H}(0)$. For systems on a complete solid satisfying a *gapped condition* where the Fermi energy $\mathcal{E}_F$ is not in any of the spectrums of the fibers $\sigma(\mathcal{H}(\vec{k}))$, so that we have an insulator, then for the choice of $\mathcal{P}_0$ the projection onto the spectral subspace separated by the gap the evolution can be considered adiabatic [25].

However, the systems we are interested in are half-solids that only satisfy a gapped bulk condition and there is no spectral gap formally separating the spectral subspaces. Therefore there is, to our knowledge, no known adiabatic theorem for this class of Hamiltonians and spectral subspaces (those below the Fermi energy). There may not even be one. However in real experiments crystals have a boundary and furthermore it would seem that the systems of interest often only satisfy the gapped bulk condition and not the gapped condition (through the so-called *bulk-boundary* correspondence).

Adiabatic evolution is for our purposes a model of what is actually occurring in the laboratory, where experiments have shown that something like adiabatic evolution is satisfied if we restrict the amount of energy that is injected into the system because of the bulk gap. The concept of *quasi-adiabatic evolution* has been defined with the intent to model what occurs experimentally in systems with only a gapped bulk condition. To do this we first reinterpret adiabatic evolution as looking at paths on the space of Hamiltonians satisfying a gapped condition, that is to interpret adiabatic evolution $\mathcal{H}(s)$ as a homotopy

$$\mathcal{H} : [0,1] \to Gapped(L^2(\mathbb{R}^d; W)), \tag{1.34}$$

between two Hamiltonians $\mathcal{H}(0)$ and $\mathcal{H}(1)$, where for each s, $\mathcal{H}(s)$ satisfies the gapped condition. If the above is satisfied then we have that for sufficiently smooth paths (1.33) is satisfied. We can extend this to define quasi-adiabatic evolution to say that a quasi-adiabatic evolution is a homotopy $\mathcal{H}(s)$ between $\mathcal{H}(0)$ and $\mathcal{H}(1)$, where each $\mathcal{H}(s)$ satisfies the gapped bulk condition.

$$\mathcal{H} : [0,1] \to Gapped - Bulk(L^2(\mathbb{R}^d; W)). \tag{1.35}$$

What is still missing (to our knowledge) in the mathematical physics literature, specially on the one focused on the analytical side, is an analogue of (1.33). We leave this to future analysts and content ourselves with a topological interpretation of quasi-adiabatic evolution that seems to model correctly what occurs in many experiments.

1.6 Quasi-adiabatic equivalence relation of Fermi surfaces and K-theory

Consider a Fermi surface $\Sigma_{F,0}$ associated to $\mathcal{H}_0$ and $\Sigma_{F,1}$ associated to $\mathcal{H}_1$, both satisfying the gapped bulk condition. We say that these two are in the same *quasi-adiabatic equivalence relation* if there exists a map

$\mathcal{H} : [0,1] \to Gapped - Bulk(L^2(\mathbb{R}^d; W))$

satisfying

$$\begin{aligned} \mathcal{H}(0) &= \mathcal{H}_0 & (1.36)\\ \mathcal{H}(1) &= \mathcal{H}_1. & (1.37) \end{aligned}$$

We write $\Sigma_{F,0} \sim_{qa} \Sigma_{F,1}$ in this case. Therefore quasi-adiabatic equivalence classes of Fermi surfaces for bulk-gapped Hamiltonains is by definition the set of path-components of gapped-bulk Hamiltonians $\pi_0(Gapped - Bulk(L^2(\mathbb{R}^d; W))$. We are at last finally ready to present the *main result* of this chapter, originally published in [2].

Theorem 1.6.1. *Quasi-adiabatic equivalence classes of Fermi surfaces Σ_F for non-interacting, gapped bulk Hamiltonians on a d-dimensional half-crystal are in one to one correspondence with the complex K-theory group $K^{-1}(\mathbb{T}^{d-1})$.*

Proof. As shown before, the gapped-bulk condition on $\mathcal{H}$ is equivalent to saying the fibers $\mathcal{H}(\vec{k}_{\|}) \in \mathcal{F}_*^{sa}(\mathscr{H}(\vec{k}_{\|}))$. Using the direct integral decomposition and definition 1.11 we can view any d-dimensional half-crystal Hamiltoninan as a continuous section on the self-adjoint Fredholm bundle $\mathcal{F}_*^{sa}(E)$, i.e.

$$\mathcal{H} : \mathbb{T}^{d-1} \to \mathcal{F}_*^{sa}(E), \tag{1.38}$$

Therefore $\pi_0(\text{Gapped-Bulk}(L^2(\mathbb{R}^d; W)) \approx [\mathbb{T}^{d-1}, \mathcal{F}_*^{sa}(E)]$, where $[,]$ means *homotopy classes of sections*, that is equivalence classes of sections $\mathcal{H} : \mathbb{T}^{d-1} \to \mathcal{F}_*^{sa}(E)$ where two sections $\mathcal{H}_0, \mathcal{H}_1$ are equivalent if there exists a continuous section $\mathcal{H} : \mathbb{T}^{d-1} \times [0,1] \to \mathcal{F}_*^{sa}(E)$ such that $\mathcal{H}(0) = \mathcal{H}_0$ and $\mathcal{H}(1) = \mathcal{H}_1$ [28]. Because the Hilbert bundle E (defined in 1.2) is trivial, that is, $E = \mathbb{T}^{d-1} \times \mathscr{H}'$, this is equivalent to homotopy classes of *maps* $[\mathbb{T}^{d-1}, \mathcal{F}_*^{sa}(\mathscr{H}')]$ We now employ a theorem of Atiyah and Singer [29] that shows $\mathcal{F}_*^{sa}(\mathscr{H}')$ is a *classifying space* for the K^{-1}-functor. Hence

$$\begin{aligned} \pi_0(Gapped - Bulk(L^2(\mathbb{R}^d; W)) &\approx [\mathbb{T}^{d-1}, \mathcal{F}_*^{sa}(\mathscr{H}')]\,, \\ &\approx K^{-1}(\mathbb{T}^{d-1}). \end{aligned} \tag{1.39}$$

□

Remark. *Systems considered here may have more symmetry than discrete translation invariance in $\vec{r}_{\|}$, but this symmetry may not be preserved under quasi-adiabatic evolution. In later sections we will include paths which preserve more symmetries.*

Here, $K^{-1}(X) \equiv \tilde{K}^0(\Sigma X_+)$, where $\tilde{K}^0(\Sigma X_+)$ denotes the *Grothendieck completion* of the monoid of stably equivalent complex vector bundles over ΣX_+, the reduced suspension on the space X_+, which is the topological space X with a disjoint point attached [30].

1.6.1 Spectral flow

The most famous example is the case for $d = 2$, called the *spectral flow* [7]. Let us compute

$$\begin{aligned} K^{-1}(S^1) &\approx \tilde{K}(\Sigma S^1_+) \\ &\approx \tilde{K}^0(S^2 \vee S^1), \\ &\approx \tilde{K}^0(S^2) \oplus \tilde{K}^0(S^1), \\ &\approx \mathbb{Z} \oplus 0 \\ &\approx \mathbb{Z} \end{aligned} \tag{1.40}$$

were $\approx$ means isomorphism of groups. We have used our theorem 1.6.1 and the above computation to deduce that there is an infinite number of quasi-adiabatic equivalence classes of Fermi surfaces for $d = 2$ from pure algebra. Atiyah gave an interpretation of this invariant which is the number of times $\sigma_{\text{pp}}(\mathcal{H}(\vec{k}_{\|}))$ crosses the $\mathcal{E} = \mathcal{E}_F = 0$ axis with a positive slope minus the number of times it crosses with a negative slope. A non-trivial state is shown in subfigure 1.4I

For $d \geq 2$ one can employ James's splitting [28]

$$\Sigma(X \times Y) \simeq \Sigma X \vee \Sigma Y \vee \Sigma(X \wedge Y) \tag{1.41}$$

to obtain a recursive formula

$$\Sigma\mathbb{T}^{d-1} \simeq S^2 \vee \Sigma\mathbb{T}^{d-2} \vee \Sigma^2\mathbb{T}^{d-2}. \tag{1.42}$$

Using this formula we further compute the case $d = 3$

$$\begin{aligned} K^{-1}(\mathbb{T}^2) &\approx \tilde{K}(\Sigma\mathbb{T}^2_+) \\ &\approx \tilde{K}^0(\Sigma\mathbb{T}^2 \vee S^1), \\ &\approx \tilde{K}^0(\Sigma\mathbb{T}^2) \oplus \tilde{K}^0(S^1), \\ &\approx \tilde{K}^0(\Sigma\mathbb{T}^2) \\ &\approx \tilde{K}^0(S^2 \vee S^2 \vee S^3) \\ &\approx \mathbb{Z}^2 \end{aligned} \tag{1.43}$$

Note that for $d = 1$ (half-line solid) $\mathbb{T}^{1-1} = *$, a point. Therefore

$$\begin{aligned} K^{-1}(*) &\approx \tilde{K}(\Sigma S^0) \\ &\approx \tilde{K}^0(S^1), \\ &\approx 0 \end{aligned} \tag{1.44}$$

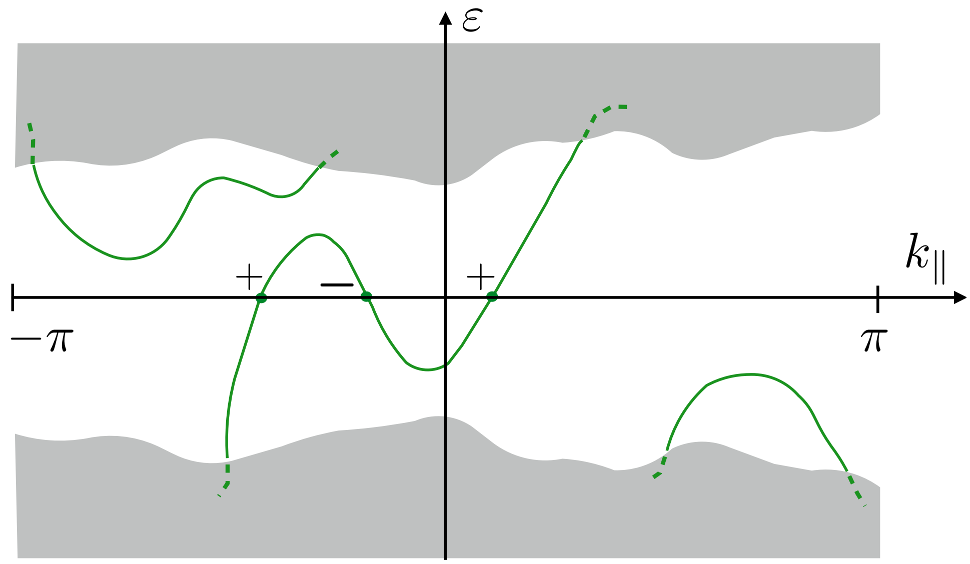

Figure 1.3: $d = 2$ Topologically stable Fermi points. Solid regions and dashed lines belong to the continuous spectrum $\sigma_{\rm ac}(\mathcal{H}(\vec{k}_{\|}))$ (bulk states and resonance states respectively). Solid lines to $\sigma_{\rm pp}(\mathcal{H}(\vec{k}_{\|}))$ (surface state). + (−) signs label the sign of the slope at crossings. 1.4I corresponds to class A (IQHE) with a net spectral flow = 1. Figure taken from [2]

.

1.6.2 Local stability of Fermi surfaces

To put 1.6.1 in context, we now present an adaptation of Hořava's work [3] on a classification of locally stable Fermi surfaces, that is, pieces of the Fermi surfaces which are robust to small perturbations near a given $\vec{k}_0$ on the Fermi surface. Consider a fully periodic system with Brillouin zone $\mathbb{T}^d$ with a non-empty Fermi surface. Let us denote one of the path-components of the Fermi surfaces by Ω and let $\dim \Omega = d - p - 1$. We now look at the $p+1$-transverse directions to Ω in $\mathbb{T}^d$ around a chosen point $\vec{k}_0 \in \Omega$. Hořava's stability analysis is to consider the boundary of a $p + 1$- dimensional ball $\partial B_{r_0}(\vec{k}_0) \subset \mathbb{T}^d$, which does not intersect Ω. The boundary is topologically a sphere S^p of dimension p, whose radius $r_0 \equiv r_0(\vec{k}_0)$ depends on the choice of $\vec{k}_0 \in \Omega$. We can once again consider quasi-adiabatic evolution of the system $\mathcal{H}(\vec{k}, s)$. As long as we assume that the quasi-adiabatic evolution of the system does not generate a new point of the Fermi surface on the boundary, i.e. with $\vec{k} \in \mathrm{S}^p$, we have that $\mathcal{H}(\vec{k}, s)$ satisfies the gap condition for all $\vec{k} \in \mathrm{S}^p$ and for all s. Operators satisfying the gapped condition, which we denote $\mathcal{TP}(\mathscr{H}')$ have been widely studied [16],[17],[31],[32] and they are (under the Riesz topology) homotopy equivalent to the colimit of infinite dimensional Grassmannians $Gr_n(\mathbb{C}^\infty)$. This can be easily seen by taking the spectral subspace for each $\mathcal{H}(\vec{k}, s)$ under $\mathcal{E}_F$, which is finite dimensional because of the full periodicity, and because of the global gapped condition the dimension of this subspace is constant in S^p. If we consider all possible dimensions n for this spectral subspace we get our colimit. Therefore the different quasi-adiabatic equivalence classes of this component Fermi surface Ω with "sufficiently small" perturbations are given by

$$[S^p, \mathcal{TP}(\mathscr{H}')] \quad \approx \quad Vect_{\mathbb{C}}(S^p). \tag{1.45}$$

$Vect_{\mathbb{C}}(S^p)$ is the monoid of isomorphism classes of complex *vector bundles* with base space S^p [30]. Note that to derive Equation (1.45) we simply repeated the analysis in [16], section 10. The arguments presented in [16] follow through, except that in our case, we must restrict the parameter space for our families of Bloch Hamiltonians to $\partial B_{r_0}(\vec{k}_0) \approx S^p$ instead of the whole Brillouin zone $\mathbb{T}^d$. Hořava then performs a mathematical operation, which is not warranted by any physical property of the system and also loses information. Hořava *stabilizes*, i.e. sets two vector bundles to be in the same equivalence class if adding a trivial vector bundle produces the same (to the original) isomorphism class of vector bundles [30]. One hence obtains the reduced K-theory group

$$\tilde{K}(S^p) = \begin{cases} \mathbb{Z} & p \text{ even} \\ 0 & \text{otherwise.} \end{cases} \tag{1.46}$$

Here again $\tilde{K}(S^p)$ denotes the *reduced* Grothendieck completion of $Vect_{\mathbb{C}}(S^p)$, the monoid of isomorphism classes of complex vector bundles with base space S^p [30].

Limitations of local stability

To perform Hořava's analysis we had to impose the strong condition of gapped fibers at the boundary of a ball $\partial B_{r_0}(\vec{k}_0)$. There is no universal way to tell whether during a more general quasi-adiabatic evolution the fiber will produce a new Fermi point on the boundary or not. Thus, we would have to look at the particularities of each chosen point $\vec{k}_0 \in \Omega$ to define an adequate S^p and relative to that what would be a "small" perturbation. In particular this construction is not well suited for modeling globally stable gapless edge modes observed at the boundaries of topological phases of matter. That being said, because of the role of $\mathcal{TP}(\mathscr{H}')$ in Hořava's analysis, under the right codimension $d-p-1$, the local analysis imitates several aspects of the global analysis of gapped (not bulk gapped) topological phases.

1.6.3 K-theory or vector bundles?

Hořava's analysis allowed us to introduce indirectly what has been done in the literature for the classification of so-called fermionic gapped topological phases for non-interacting systems. These constructions often arrive at an equivalence between a phase and an isomorphism classes of n-dimensional vector bundles over the d-dimensional Brillouin zone $\mathbb{T}^d$ for fully periodic systems, $Vect^n_{\mathbb{C}}(\mathbb{T}^d)$. In general, passing from $Vect^n_{\mathbb{C}}(\mathbb{T}^d)$ to K-theory involves a series of steps. First we must allow addition of isomorphism classes $[E_1] \oplus [E_2] = [E_1 \oplus E_2]$ and adding 1-dimensional vector bundles (i.e. single bands), which forces us to consider isomorphism classes of vector bundles of any dimension over $\mathbb{T}^d$, arriving then at the semigroup $Vect_{\mathbb{C}}(\mathbb{T}^d)$. Then, we have 2 options available to us to produce K-theory, either impose the *stabilization equivalence relation* [30], as we did in subsection 1.6.2 to obtain the reduced $\tilde{K}(\mathbb{T}^d)$ group or we can define another equivalence relation, defined on pairs $([E_1],[E_2]),([E'_1],[E'_2])$ of isomorphism classes, turning $Vect_{\mathbb{C}}(\mathbb{T}^d)$ into the abelian group $K(\mathbb{T}^d)$ [30]. The latter process is called a Grothendieck completion or Grothendieck construction and is usually ignored in the physics literature, where most works compute the unreduced $K^0(\mathbb{T}^d)$ group directly to classify fermionic gapped phases, without justifying the transition to K-theory. As a matter of fact they often prefer to look at so-called strong phases in which they replace the torus $\mathbb{T}^d$ by a d-dimensional sphere [9] without any rigorous justification to our knowledge (although it does make computing the K-theory a little bit simpler). Note that though related by the inclusion of a point to the space X being considered, the computations of K^0 and $\tilde{K}^0$ yield different results. As adequately put by Thiang [17], this has produced a *conflation* between the full $K^0(\mathbb{T}^d)$ groups and their reduced versions $\tilde{K}^0(\mathbb{T}^d)$.

The mathematical literature on the other hand addresses the issue in different ways. As examples we can consider the work of De Nittis and Gomi [31],[32], which uses n-dimensional vector bundles and their characteristic classes to classify fermionic phases, without appealing to K-theory. In a different vein Freed and Moore [16] employ a process equivalent to a Grothendieck completion but emphasize that they are not aware of an a priori good physical motivation for its use. There are also examples in the C^*-algebraic approach of Prodan and Schulz-Baldes [33] together with references therein. Prodan and Schulz-Baldes motivate the use of K-theory for lattice Hamiltonians in the so called *tight-binding* approximation [6], through its applications in the bulk-boundary correspondence when combined with *cyclic cohomology*. Though a classification using K-theory is not a direct logical consequence of their formalism, its use in their approach is certainly well motivated and it employs K-theory of C^*-algebras for both surface states and bulk states, with similar results as ours for the surface states in symmetry class A, employing the functor K^{-1} but on a *real space* algebra of surface observables.

After publishing [2] we became aware of further work by Thiang [34] where a physical interpretation to elements in $K^0(\mathbb{T}^d)$ is given to relative phases (as a difference between 2 topological phases where there is a boundary) although his analysis is more general and includes disorder in the C^*-algebraic framework. From the physical point of view we believe this interpretation to be unsatisfactory. When systems have a boundary the surface Brillouin zone is a torus of one lower dimension, thus the moment we put an interface we lose the periodicity and the C^*-algebra involved would have to include said interface in its construction. Therefore we hold that the construction for systems on a half-crystal [2] was the first one for which K-theory arises naturally from the simple mathematical representations of quasi-adiabatic evolution and a gapped bulk spectrum for surface Bloch Hamiltonians on half-crystal. We also do not restrict to Hamiltonians in the tight-binding approximation nor lattice systems. In the opposite direction note that our construction has the rather strong assumption of discrete translation-invariance on directions parallel to the boundary. It also has the more common assumption of a gapped bulk spectrum. Both of these restrictions are better handled in [33],[17].

1.7 Adding global symmetries

Thus far, we have only considered half-crystals whose only symmetry is discrete translation invariance of the surface lattice $\Gamma_{\parallel}$. Thus our systems don't even need to respect time-reversal symmetry, since they may include a magnetic field, which in fact is what allows for the spectral flow to be non-zero. We now wish to extend the above analysis to include two different possible symmetries, which are independent of the crystallographic structure. Therefore, we will only study systems on half-crystals for which the boundary conditions preserve these symmetries. Thus, both the absolutely continuous and pure point spectrum of our Hamiltonians $\sigma_{\text{pp}}(\mathcal{H}(\vec{k}_{\parallel}))$, $\sigma_{\text{ac}}(\mathcal{H}(\vec{k}_{\parallel}))$ respectively, inherit the same structure when a symmetry is implemented.

1.7.1 Real and quaternionic structure on a complex vector space

We must first digress and introduce the following mathematical definitions taken from [35]. A *real* structure on a complex vector space V is an *anti-linear* operator K, such that $K^2 = I$. In this case V $\approx$ W $\otimes_{\mathbb{R}} \mathbb{C}$, where W is vector space over $\mathbb{R}$. A *quaternionic* structure on a complex vector space V is an *anti-linear* operator K, such that $K^2 = -I$. The operators I, K, iI and $J = iK$ satisfy the quaternion relations. As will be shown below our symmetry operators defined below can be considered as either real or quaternionic structures on our Hilbert space. This will modify the complex K-theory that appears in our classification to a different (but related) extraordinary cohomology theory [28]. We will use this modified theory to compute the distinct classes of globally topologically stable Fermi surfaces in a given symmetry class. Note that adding symmetries to the above analysis is one of the main extensions done in [2], lacking in [36] among other important differences.

1.7.2 Particle-hole symmetry

The first symmetry we consider is the so called *particle-hole* symmetry. This symmetry as normally implemented, cannot be realized by non-relativistic condensed matter systems, however we could slightly modify its implementation to make it correct and we shall describe this modification. Systems with only particle-hole symmetry and discrete translation-invariance are denoted as symmetry classes C and D in the physicist's Altland-Zirnbauer classification [1]. The operator representing said symmetry is traditionally denoted by Ξ. There are different choices of implementations of Ξ one can make, such as whether it is a unitary or antiunitary operator [16],[17] and each one of them represents systems in condensed matter with different physical properties. Our choice of implementation is the one most commonly used throughout the physics literature [4],[37] [38], where our symmetry operator Ξ acts on the fiber Hamiltonians in the following way [16]

$$\begin{aligned} \Xi\mathcal{H}(\vec{k}_{\parallel}) &= -\mathcal{H}(-\vec{k}_{\parallel})\Xi\,, && (1.47)\\ \Xi i &= -i\Xi\,. && (1.48) \end{aligned}$$

This implies that for each band index α of $\mathcal{H}(\vec{k}_{\parallel})$, there exists a band index β of $\mathcal{H}(-\vec{k}_{\parallel})$, such that

$$\begin{aligned} \Xi\phi_{\alpha}(\vec{k}_{\parallel}) &= \phi_{\beta}(-\vec{k}_{\parallel})\,, && (1.49)\\ \varepsilon_{\alpha}(\vec{k}_{\parallel}) &= -\varepsilon_{\beta}(-\vec{k}_{\parallel})\,, && (1.50) \end{aligned}$$

where $\phi_{\alpha}(\vec{k}_{\parallel})$ lives in the spectral subspace associated to the band index α (which may be finite dimensional if $\varepsilon_{\alpha}(\vec{k}_{\parallel}) \in \sigma_{\mathrm{pp}}(\mathcal{H}(\vec{k}_{\parallel}))$ or infinite dimensional if $\varepsilon_{\alpha}(\vec{k}_{\parallel}) \in \sigma_{\mathrm{ac}}(\mathcal{H}(\vec{k}_{\parallel}))$). Our surface Brillouin zone always had a canonical *involution* $\tau : \mathbb{T}^{d-1} \to \mathbb{T}^{d-1}$, $\tau(\vec{k}_{\parallel}) = -\vec{k}_{\parallel}$, making $\mathbb{T}^{d-1}$ a *real* space in the sense of [39]. However, up until now, because our fibers did not need to satisfy a symmetry condition, this real structure was irrelevant for our classification. This however will drastically change once we include symmetries. We shall denote $(\mathbb{T}^{d-1}, \tau)$ by X_s to remind ourselves we are always taking into account its real structure. In general $\beta \neq \alpha$ to respect the symmetry, however if $\varepsilon_{\alpha}(\vec{k}_{\parallel}) \in \sigma_{\mathrm{pp}}(\mathcal{H}(\vec{k}_{\parallel}))$ passes through an involution fixed-point $\vec{k}_{\parallel} = -\vec{k}_{\parallel}$, then β may equal α. This is a subtle but non-trivial point as it permits the existence of some topologically non-trivial Fermi surfaces for all symmetry classes considered here (see subfigures 1.4II, 1.4III). At this point, looking at 1.50, the keen reader will note an inconsistency with previous established facts about $\sigma(\mathcal{H}(\vec{k}_{\|}))$. We had mentioned earlier that $\sigma(\mathcal{H}(\vec{k}_{\|}))$ is bounded from below and unbounded from above [20]. This is clearly inconsistent with 1.50. This is an other instance where the unboundedness of the Hamiltonian is more of a technical difficulty than a truely qualitative constraint. We could surmount this difficulty by instead setting

$$\Xi\mathcal{H}(\vec{k}_{\|})\mathcal{P}_E(\vec{k}_{\|}) \quad = \quad -\mathcal{H}(\vec{k}_{\|})\mathcal{P}_E(-\vec{k}_{\|})\Xi \tag{1.51}$$

Where $\mathcal{P}_E(\vec{k}_{\|})$ would be the projection onto the spectral subspace corresponding to $\sigma_{\leq E}(\mathcal{H}(\vec{k}_{\|}))$ of elements of the spectrum of the fiber which are smaller than a *cutoff* E. Note that E should be independent of $\vec{k}_{\|}$. From a physical point of view, as with quasi-adiabatic evolution and our choice of the Riesz topology in section 1.4, we are not interested in modelling the high energy asymptotics of the system. Therefore we will simply continue to work with 1.47 and treat $\mathcal{H}(\vec{k}_{\|})$ as if it were bounded above as well.

1.7.3 Real vector bundles and KR-theory

We must make another digression in order to introduce some concepts which may not be that well known to topologists nor physicists. Given a space X with an involution τ, one can define a *Real* vector bundle over (X, τ) as a complex vector bundle E that is also a real space and satisfies the following conditions [39]

- The projection $P : E \to X$ commutes with the involution
- The map $E_x \to E_{\tau(x)}$ is anti-linear

$$\begin{array}{ccc} \mathbb{C} \times E_x & \longrightarrow & E_x \\ \downarrow & & \downarrow \\ \mathbb{C} \times E_{\tau(x)} & \longrightarrow & E_{\tau(x)} \end{array}$$

  where the horizontal maps $(z, v) \mapsto zv$ and the vertical maps are involutions, where the involution on $\mathbb{C}$ is the standard complex conjugation.

This anti-linearity property is the main difference with normal $\mathbb{Z}/2\mathbb{Z}$-equivariant vector bundles (see 1.7.4), where the structure maps must be unitary.

One can define the Grothendieck ring of Real bundles over X, $KR(X)$. Naturally there is a topological suspension with an involution Σ_τ together with the usual suspension Σ on Real spaces to get a bi-graded cohomology theory $KR^{p,q}(X)$ (see [39] for more details). The number p counts the number of involution suspensions one performs on X and q the number of normal suspensions. However Atiyah proves in [39] that there is an isomorphism

$$KR^{p,q}(X) \approx KR^{0,q-p}(X) \equiv KR^{q-p}(X). \tag{1.52}$$

He further showed there is an isomorphism

$$KR(X) \approx KR^{-8}(X), \tag{1.53}$$

which is another instance of Bott periodicity. Dupont [40] was the first to generalize this construction to *symplectic* vector bundles E, which have the same definition as above except their involution is of order 4 (the involution on the base X still being order 2), that is when $E_x \to E_{\tau(x)}, \tau^2 = -I$. Analogously, one defines $KH(X)$. Gukov shows in [41] the isomorphism

$$KH^{-n}(X) \approx KR^{-n-4}(X). \tag{1.54}$$

To compute examples we will use the fact that KR^j is a functor from the category (see [42] for the basics of category theory) of spaces with an involution to abelian groups, the inclusion of the fixed point $i : \{x_0\} \to X$ is a morphism (τ-equivariant maps) in that category and furthermore, there is another one, $r : X \to \{x_0\}$, such that the composition $r \circ i$ is the identity. Hence we have

$$KR^n(x_0) \xrightarrow{r^*} KR^n(\mathrm{X}) \xrightarrow{i^*} KR^n(x_0), \qquad i^* \circ r^* = I \tag{1.55}$$

Meaning that the long exact sequence of the pair (X, x_0)

$$\begin{gathered} KR^{n-1}(\mathrm{X}) \xrightarrow{i^*} KR^{n-1}(x_0) \xrightarrow{0} KR^n(\mathrm{X}, \mathrm{x}_0) \longrightarrow \\ KR^n(\mathrm{X}) \xrightarrow{r^*} KR^n(x_0) \xrightarrow{0} KR^{n+1}(\mathrm{X}, x_0) \end{gathered} \tag{1.56}$$

splits and we have an isomorphism

$$KR^n(\mathrm{X}) \approx KR^n(\mathrm{X}, x_0) \oplus KR^n(x_0). \tag{1.57}$$

We can generalize this to the pair $(\mathrm{X}\times\mathrm{Y},\{x_0\}\times\mathrm{Y})$

$$KR^{n-1}(\mathrm{X}\times\mathrm{Y}) \xrightarrow{i^*} KR^{n-1}(\{x_0\}\times\mathrm{Y}) \xrightarrow{0} KR^{n}(\mathrm{X}\times\mathrm{Y}/\{\mathrm{x}_0\}\times\mathrm{Y}) \longrightarrow \tag{1.58}$$

$$KR^{n}(\mathrm{X}\times\mathrm{Y}) \xrightarrow{r^*} KR^{n}(Y) \xrightarrow{0} KR^{n+1}(\mathrm{X}\times\mathrm{Y}/\{x_0\}\times\mathrm{Y})$$

to obtain

$$KR^{n}(\mathrm{X}\times\mathrm{Y}) \approx \tilde{KR}^{n}(\mathrm{X}\times\mathrm{Y}/\{x_0\}\times\mathrm{Y}) \oplus KR^{n}(\mathrm{Y}). \tag{1.59}$$

Equation 1.59 will be a fundamental tool in computing examples. We must make a last comment before we move to equivariant homotopy theory. If one considers vector bundles, where the fibers are vector spaces over $\mathbb{R}$ instead of being vector spaces over $\mathbb{C}$, these are called real vector bundles. One can repeat the above process and define the group $KO(X)$ of real vector bundles. There is an equivalence between Real subbundles over the fixed points under the involution τ and real bundles over these fixed points. Therefore $KR^n(x_0) \approx KO^n(x_0)$ and this is useful because we can use real *Bott periodicity* [30].

1.7.4 A splash of equivariant homotopy theory

An action of a group G on a space X is a continuous map

$$\rho : G \times X \to X \tag{1.60}$$

such that

$$\rho(g_1, \rho(g_2, x)) = \rho(g_1 g_2, x) \tag{1.61}$$

The action is usually left implicit implicit in the notation by writing gx instead of $rho(x, g)$. Given spaces X, Y with a G-action, one can define maps that are equivariant, i.e.

$$f : X \to Y \tag{1.62}$$

$$f(gx) = gf(x) \tag{1.63}$$

And so one can construct a homotopy theory of equivariant maps [43] and study homotopy classes of equivariant maps $[\,,\,]_G$. The subject is not just a trivial extension of ordinary homotopy theory and it gets quite complicated. For example, up until this point the results presented only cared about the homotopy type of our spaces but did not put any other restrictions (i.e. compact,connected, Hausdorff nor CW-structure). In contrast, results in equivariant homotopy theory often require our G-spaces to be G-CW complexes (see [43] for a definition). Here we present a theorem which is an equivariant version of Whitehead's theorem of weak homotopy equivalences between two G-CW complexes.

Theorem 1.7.1. *(Whitehead) An equivariant map $f : X \to Y$ of G-CW complexes is a G-homotopy equivalence if and only if $f^H : X^H \to Y^H$ is a weak homotopy equivalence for all H-fixed points X^H, Y^H and all closed subgroups $H \subseteq G$.*

We will make extensive use of this theorem in the next sections.

1.7.5 Class D

Systems in class D are defined by the condition

$$\Xi^2 = I\,. \tag{1.64}$$

Thus, Ξ represents a *real* structure on our complex fiber Hilbert space $\mathscr{H}'$, as defined above, which we denote as $\mathscr{H}'_R$. We extend our previous analysis on quasi-adiabatic stability of Fermi surfaces by employing equivariant homotopy theory, where the above implementation of the symmetry naturally induces the action $\mathcal{H}(\vec{k}_\parallel) \mapsto -\Xi\mathcal{H}(-\vec{k}_\parallel)\Xi$. We wish to use a slightly different action, defined in [44] (so that we can use the results in there). To do so we pass to the skew-adjoint operator $i\mathcal{H}(\vec{k}_\parallel)$, with the action

$$i\mathcal{H}(\vec{k}_\parallel) \mapsto \Xi i\mathcal{H}(-\vec{k}_\parallel)\Xi. \tag{1.65}$$

This leads to the following result:

Theorem 1.7.2. *([2]-Class D) Systems on a half-crystal with gapped bulk and particle-hole symmetry in class D are given by $KR^{-1}(X_s)$.*

Proof. Quasi-adiabatic equivalence classes of Fermi surfaces in symmetry class D are defined as $[\mathrm{X}_s, \hat{\mathcal{F}}(\mathscr{H}'_R)]_{C_2}$. We can employ a result of Matumoto [44]

$$[\mathrm{X}_s, \mathcal{F}(\mathscr{H}'_R)]_{C_2} \approx KR(\mathrm{X}_s)\,. \tag{1.66}$$

where $\mathcal{F}(\mathscr{H}'_R)$ are Fredholm operators that anti-commute with the involution on $\mathscr{H}'_R$ and C_2 denotes the cyclic group of order 2 and also denotes the choice of the action defined above (1.65). Using Whitehead's equivalence (theorem 1.7.1) it suffices to have plain homotopy equivalence on the fixed-points of the subgroups of C_2 to have the full equivariant equivalence. The original result of Atiyah and Singer [45] gives the equivalence when $H = e$ is the trivial subgroup. For the full group C_2, (1.66) gives an equivariant homotopy equivalence between $\mathcal{F}(\mathscr{H}'_R)$ and the classifying space associated to the functor KR. Thus, Matumoto's result trivially implies $(\Omega\mathcal{F}(\mathscr{H}'_R))^{C_2}$ is equivalent to the fixed points of the loop space of the classifying space of KR $(\omega\mathcal{F}(\mathscr{H}'_R)^{C_2} \simeq (\omega KR)^{C_2})$. Since the Atiyah-Singer map is equivariant this means that there is an equivalence $\hat{\mathcal{F}}(\mathscr{H}'_R)^{C_2} \simeq (\Omega\mathcal{F}(\mathscr{H}'_R))^{C_2}$, where $\hat{\mathcal{F}}$ denotes *skew-adjoint* Fredholm operators [45]. Using the triviality of our Hilbert bundle E we conclude

$$[\mathrm{X}_s, \hat{\mathcal{F}}(\mathscr{H}'_R)]_{C_2} \approx KR^{-1}(\mathrm{X}_s)\,. \tag{1.67}$$

□

Class C

Now we move on to the case where

$$\Xi^2 = -I \tag{1.68}$$

also known as symmetry class C. For this case, the particle-hole symmetry operator induces a *quaternionic* structure on $\mathscr{H}$, $i\Xi$ being the third generator. Let us denote this quaternionic structure by $\mathscr{H}'_Q$. Again we employ the same strategy as above, passing to skew-adjoint operators. Following [44] we denote by D_2 the cyclic group of order 2 but with a different action on $\mathcal{F}(\mathscr{H}'_Q)$

$$i\mathcal{H}(\vec{k}_{\|}) \mapsto -\Xi i\mathcal{H}(-\vec{k}_{\|})\Xi\,. \tag{1.69}$$

Matumoto also proved the equivalence

$$[\mathrm{X}_s, \mathcal{F}(\mathscr{H}'_Q)]_{D_2} \approx KH(\mathrm{X}_s)\,. \tag{1.70}$$

We have the following analogous result:

Theorem 1.7.3. *([2]-Class C) Systems on a half-crystal with gapped bulk and particle-hole symmetry in class C are given by $KH^{-1}(X_s)$.*

Proof. Repeating the fixed-point argument as above we have that stable isomorphism classes of Fermi surfaces in class C are given by

$$[\mathrm{X}_s, \hat{\mathcal{F}}(\mathscr{H}'_Q)]_{D_2} \approx KH^{-1}(\mathrm{X}_s)\,. \tag{1.71}$$

□

1.7.6 Time-reversal symmetry

The other symmetry we will study is far more ubiquitous in quantum mechanics and is that of *time-reversal symmetry* through an operator Θ [4],[38]

$$\begin{aligned} \Theta\mathcal{H}(\vec{k}_{\|}) &= \mathcal{H}(-\vec{k}_{\|})\Theta\,, &(1.72)\\ \Theta i &= -i\Theta\,. &(1.73)\end{aligned}$$

Similarly to particle-hole symmetry, this implies that for each band index α of $\mathcal{H}(\vec{k}_{\|})$, there exists a spectrum index β of $\mathcal{H}(-\vec{k}_{\|})$, such that

$$\begin{aligned} \Theta\phi_{\alpha}(\vec{k}_{\|}) &= \phi_{\beta}(-\vec{k}_{\|})\,, &(1.74)\\ \varepsilon_{\alpha}(\vec{k}_{\|}) &= \varepsilon_{\beta}(-\vec{k}_{\|})\,. &(1.75)\end{aligned}$$

Unlike particle-hole symmetry, time-reversal symmetry is always implemented by an anti-unitary operator and the issues of upper unboundedness of $\sigma(\mathcal{H}(\vec{k}_{\|}))$ with (1.50) do not arise with (1.75). There are two classes in the Altland-Zirnbauer classification that correspond to systems with only discrete translation-invariance and time-reversal symmetry, namely classes AI and AII, whose properties we describe below.

Class AI

Systems in class AI must obey

$$\Theta^2 = I\,. \tag{1.76}$$

We now have the appropriate action directly on self-adjoint operators since

$$\mathcal{H}(\vec{k}_{\|}) \mapsto \Theta\mathcal{H}(-\vec{k}_{\|})\Theta\,. \tag{1.77}$$

Theorem 1.7.4. *([2]-Class AI) Systems on a half-crystal with gapped bulk and time-reversal symmetry in class AI are given by* $KR^{-7}(X_s)$.

Proof. These are $[\mathrm{X}_s, \mathcal{F}_*^{sa}(\mathscr{H}_R)]_{C_2}$. The main difference with the above theorems is that the fixed points are homotopic to the fixed points of the *seventh loop space*. Looking again at the fixed-points of the subgroups of C_2 using Bott periodicity

$$\mathcal{F}_*^{sa}(\mathscr{H}_R)^{C_2} \simeq \Omega^7\mathcal{F}(\mathscr{H}'') \tag{1.78}$$

proven in [45], which holds for the fixed-points of all subgroups of C_2 and where $\mathscr{H}''$ is a $*$-representation of the Real $\mathcal{C}_6$ Clifford algebra. This equivalence is equivariant with respect to (1.77), hence, together with the trivial fact that

$$\mathcal{F}_*^{sa}(\mathscr{H}) \simeq \Omega^7\mathcal{F}(\mathscr{H}) \tag{1.79}$$

due to Bott periodicity, the same argument with (1.66) runs through and

$$[\mathrm{X}_s, \mathcal{F}_*^{sa}(\mathscr{H}_R)]_{C_2} \approx KR^{-7}(\mathrm{X}_s)\,, \tag{1.80}$$

□

Class AII

Finally, for stable Fermi surfaces in symmetry class AII, we must assume

$$\Theta^2 = -I\,. \tag{1.81}$$

By repeating the same process for self-adjoint operators as we did for skew-adjoint operators in class C, since

$$\mathcal{H}(\vec{k}_{\|}) \mapsto -\Theta\mathcal{H}(-\vec{k}_{\|})\Theta \tag{1.82}$$

and we obtain

Theorem 1.7.5. *([2]-Class AII) Systems on a half-crystal with gapped bulk and time-reversal symmetry in class AII are given by* $KH^{-7}(X_s)$*.*

Proof. Repeating same arguments as in theorem 1.7.4 with 1.82 we can conclude

$$[\mathrm{X}_s, \mathcal{F}_*^{sa}(\mathscr{H}_Q)]_{D_2} \approx KH^{-7}(\mathrm{X}_s)\,. \tag{1.83}$$

□

We remark that both Ξ and Θ are either real or quaternionic structures on the fiber Hilbert space and that the difference between them lies in the set of fixed-points under (1.65), (1.69), (1.77), (1.82) in the space of Hamiltonian operators $\mathcal{F}_*^{sa}(\mathscr{H}'_R)$, $\mathcal{F}_*^{sa}(\mathscr{H}'_Q)$ or their action-induced skew-adjoint counterparts. We also note that this does not contain all of the Altland-Zirnbauer classification appearing in other classifications [16],[17] as we are missing the cases with *chiral* symmetry (classes BDI, DIII, CI, CII). For these classes there is instead a unitary operator which is assumed in general to be $\mathcal{S} = \Theta\Xi$ (see [16] for the general case) and they will not be considered in this thesis.

1.7.7 Examples

We should now compute a few examples. Let $d = 2$, then $X_s = S^{1,1}$, the unit circle in the complex plane, where the involution is given by complex conjugation [39], [46]. In general $S^{p,q}$ is the $(p+q-1)$-dimensional sphere embedded in $\mathbb{R}^{p,q} = i\mathbb{R}^p \oplus \mathbb{R}^q$.

$$KR^j(S^{1,1}) \approx KR^j(S^{1,1}, \{x_0\}) \oplus KO^j \tag{1.84}$$

where KO^j denotes the real (trivial involution) j-th K-group of a point. Now by definition

$$\begin{aligned} KR^j(S^{1,1}, \{x_0\}) &\equiv \tilde{KR}^j(S^{1,1}), \\ &\approx \tilde{KR}^{j+1}(S^{0,1}), \\ &\approx \tilde{KO}^{j+1}(S^0), \\ &\approx KO^{j+1}. \end{aligned} \tag{1.85}$$

We hence obtain

$$KR^j(S^{1,1}) \approx KO^j \oplus KO^{j+1}. \tag{1.86}$$

For class D, $j = -1$ [46]

$$KR^{-1}(S^{1,1}) \approx KO^{-1} \oplus KO^0 \approx \mathbb{Z} \oplus \mathbb{Z}/2. \tag{1.87}$$

The $\mathbb{Z}$-factor again corresponds to a spectral flow of surface states similar to class A, but now $\forall\ \varepsilon_\alpha(\vec{k}_\parallel) \in \sigma(\mathcal{H}(\vec{k}_\parallel))$, there exists $\varepsilon_\beta(-\vec{k}_\parallel) \in \sigma(\mathcal{H}(-\vec{k}_\parallel))$ such that $\varepsilon_\beta(-\vec{k}_\parallel) = -\varepsilon_\alpha(\vec{k}_\parallel)$. Thus for each zero mode at $\vec{k}_\parallel$, there must also be one at $-\vec{k}_\parallel$, as shown in subfigure 1.4II. Hence the parity of the spectral flow in class D depends on the existence of an odd number of zero modes at one of the involution fixed-points.

We first choose one of the involution fixed-points. If there is an even/odd number of zero modes at the chosen point, we can determine if there is an even/odd number of zero modes at the other fixed-point by computing the parity of the spectral flow. In subfigure 1.4III we represent a state with no net spectral flow that has two zero modes one at each fixed-point. This is the non-trivial $0 \oplus 1$ state in $\mathbb{Z} \oplus \mathbb{Z}/2$. Let us remark that there is no canonical way of defining this invariant and a choice of a fixed-point must be taken. We also comment that the stability of this class depends on 1) respecting particle-hole symmetry and 2) the existence of 2 fixed-points on X_s.

Examples of systems with a non-trivial class on the $\mathbb{Z}$-factor are spinless p-wave superconductors [38], where Bogoliubov surface zero modes at one of the involution fixed-points $\{-1, 1\}$, satisfy an analogous reality condition to that of *Majorana* fermions, hence they are called *Majorana zero modes*. Bogoliubov quasi-particles are effectively charge-less, thus, our zero modes only contribute to the thermal current. Such a current could be induced by a thermal gradient on our system, similar to the electric field for class A [47]. This spectral flow has an analogy with an anomaly inflow interpretation, where the anomaly would be a gravitational one (thermal energy) [47].

For symmetry class C, using eqs. (1.54), (1.86) we have

$$\begin{aligned} KH^{-1}(S^{1,1}) &\approx KO^{-5} \oplus KO^{-4} \\ &\approx \mathbb{Z}\,. \end{aligned} \tag{1.88}$$

Since now $\Xi^2 = -I$, Fermi points at the involution fixed-points must be doubly degenerate and the $mod\,2$ invariant must always vanish. Thus the spectral flow must come in pairs because of the symmetry. There is the same gravitational anomaly inflow physical interpretation as in symmetry class D (subfigure 1.4II) for the Bogoliubov zero modes. Condensed matter systems with $\Xi^2 = -I$ in $d = 2$ correspond to so-called d-wave superconductors [38].

For symmetry classes AI and AII the spectral flow must vanish because of the symmetry of the spectrum $\varepsilon_\beta(-\vec{k}_\parallel) = \varepsilon_\alpha(\vec{k}_\parallel)$ for some α, β. By computing class AI, $d = 2$

$$\begin{aligned} KR^{-7}(S^{1,1}) &\approx KO^{-7} \oplus KO^{-6} \\ &= 0\,. \end{aligned} \tag{1.89}$$

We see there is only the trivial class of Fermi points, i.e. all Fermi points are quasi-adiabatically gappable in class AI, $d = 2$. For symmetry class AII, $d = 2$ we obtain

$$\begin{aligned} KH^{-7}(S^{1,1}) &\approx KO^{-3} \oplus KO^{-2} \\ &\approx \mathbb{Z}/2\,. \end{aligned} \tag{1.90}$$

Due to Kramers theorem, if Fermi points arise at the involution fixed-points $\{1, -1\}$ of X_s, they must be doubly degenerate, and thus the invariant is the number of double-crossed Fermi points $mod\,2$ [38]. Such double-crossed Fermi points have a $U(1)$-*spin* anomaly inflow interpretation [10] and are

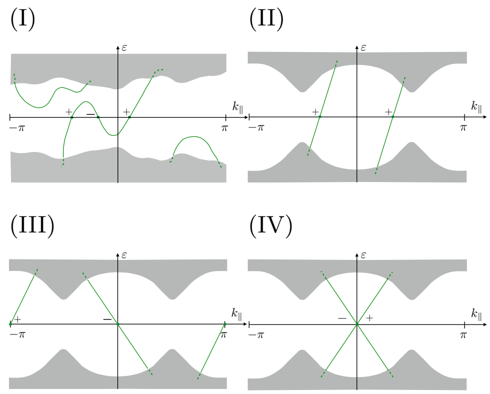

Figure 1.4: $d = 2$ Topologically stable Fermi points. Solid regions and dashed lines belong to the absolutely continuous spectrum $\sigma_{\mathrm{ac}}(\mathcal{H}(\vec{k}_\parallel))$ (bulk states and resonance states respectively). Solid lines to $\sigma_{\mathrm{pp}}(\mathcal{H}(\vec{k}_\parallel))$ (surface state). $+$ $(-)$ signs label the sign of the slope at crossings. 1.4I corresponds to class A (IQHE) with a net spectral flow $= 1$. 1.4II corresponds to a spectral flow of 2, that may occur for both classes C and D at non fixed-points in $S^{1,1}$. 1.4III represents two Majorana zero modes in class D. 1.4IV represents a helical Dirac fermion edge mode (SQHE). Figure taken from [2].

often called helical Dirac zero modes because of the analogous role to the helicity of relativistic Dirac fermions played by spin-orbit coupling. A physical example is the quantum spin Hall effect (QSHE) [38].

1.7.8 Higher dimensional cases and weak topological phases

For $d = 3$ $\mathrm{X}_s = S^{1,1} \times S^{1,1}$, we will use 1.59, taking $\mathrm{X} = \mathrm{Y} = S^{1,1}$ and obtain

$$KR^j(S^{1,1} \times S^{1,1}) \approx \tilde{KR}^j(S^{1,1} \times S^{1,1}/\{x_0\} \times S^{1,1}) \oplus KR^j(S^{1,1}). \quad (1.91)$$

The latter term we have already computed for any j. To compute $\tilde{KR}^j(S^{1,1} \times S^{1,1}/\{x_0\} \times S^{1,1})$ we note that $X \times Y/(\{x_0\} \times Y) \simeq X \wedge Y_+$ and $X \wedge Y_+ \equiv X \times Y_+/X \vee Y_+$ since we are collapsing $X \times \{+\}$ to a point. This is τ-equivariant as the involution is the product of the involutions and the spaces we are collapsing are τ-invariant.

Thus

$$\begin{aligned}
\tilde{KR}^j(S^{1,1} \times S^{1,1}/\{x_0\} \times S^{1,1}), &\approx \tilde{KR}^j(S^{1,1} \wedge S^{1,1}_+), \\
&\approx \tilde{KR}^j(\Sigma_\tau S^{1,1}_+), \\
&\approx \tilde{KR}^{j+1}(S^{1,1}_+), \\
&\approx KR^{j+1}(S^{1,1}). \qquad (1.92)
\end{aligned}$$

Hence we conclude

$$KR^j(S^{1,1} \times S^{1,1}) \approx KO^j \oplus KO^{j+1} \oplus KO^{j+1} \oplus KO^{j+2} \qquad (1.93)$$

We summarize the results for all symmetry classes and for $d = 1, 2, 3$ on Table 1.1.

	Symmetry			d	
AZ	Θ	Ξ	1	2	3
A	0	0	0	$\mathbb{Z}$	$\mathbb{Z}^2$
AI	I	0	0	0	0
AII	$-I$	0	0	$\mathbb{Z}/2$	$(\mathbb{Z}/2)^3$
D	0	I	$\mathbb{Z}/2$	$\mathbb{Z} \oplus \mathbb{Z}/2$	$\mathbb{Z}^2 \oplus \mathbb{Z}/2$
C	0	$-I$	0	$\mathbb{Z}$	$\mathbb{Z}^2$

Table 1.1: Classes of topologically stable Fermi surfaces for half-space systems with a gapped bulk in dimension $d = 1, 2$ and 3. Θ is the time-reversal operator and Ξ is the particle-hole symmetry operator. We use the names given in [1] (AZ). 0 on the right-side denotes the trivial group. 0 on the left-side indicates absence of said symmetry. When $\Theta = \Xi = 0$ the surface Brillouin zone X_s is a regular torus $\mathbb{T}^{d-1}$ and for either $\Theta^2 = \pm I$ or $\Xi^2 = \pm I$ it is a torus with involution $\bar{\mathbb{T}}^{d-1}$. Higher-dimensional classes relate to weak bulk topological phases. Table taken from [2].

Unfortunately we do not have as of yet a picture of these topological invariants in terms of the spectrum of the fiber Hamiltonians, though one can speculate that it will be analogous and one must look at codim one subspaces such as intervals and circles but we leave this for future work.

1.8 Extending to crystallographic groups

We shall now extend the work presented in [2] to include *spatial* symmetries for our Hamiltonian. These symmetries correspond to crystals of one lower dimension as it is only on the direction parallel to the boundary that these are preserved. We shall follow [16] and [21] up to a point. For their construction, equivariant vector bundles over the Brillouin zone trivially yield equivariant K-theory after Grothendieck completion. In our case we have to see whether sections of our Fredholm bundle over our particular Hilbert bundle E, with an action of the group is equivalent to equivariant K-theory.

A d-dimensional crystallographic group G is defined via the group extension

$$0 \longrightarrow \Gamma_{\|} \xrightarrow{i} G \xrightarrow{\pi} P \longrightarrow 0 \tag{1.94}$$

where $P \subset O(d-1)$ is known as the *point group*, the group of extra symmetries besides discrete translations, the latter are given by the subgroup $\Gamma_{\|} \approx \mathbb{Z}^{d-1}$. There are two types of crystallographic groups, those which are simply a semi-direct product $\Gamma_{\|} \rtimes P$ are known as *Symmorphic* and those which aren't are known as *Non-symmorphic*. The twistings that will appear later are those arising when the symmetry group of our Hamiltonian is non-symmorphic [21]. Since the Brillouin zone is the Pontryagin dual $\mathrm{Hom}(\Gamma_{\|}, U(1))$, there is an action of P on $\mathrm{Hom}(\Gamma_{\|}, U(1))$ given by

$$p\vec{k}_{\|}(m_1, \cdots, m_{d-1}) = \vec{k}_{\|}(\pi(\tilde{p}^{-1}(\tilde{m}_1, \cdots, \tilde{m}_{d-1}))), \tag{1.95}$$

where $(\tilde{m}_1, \cdots, \tilde{m}_{d-1})$ is the inclusion of $(m_1, \cdots, m_{d-1}) \in \Gamma_{\|}$ in G and $\tilde{p} \in \pi^{-1}(p)$ where π is the projection of G onto P in (1.94). Note that the choice of $\tilde{p}$ is not unique but the outcome is independent of it.

While we have described the action of the point group P on the base, we need to also describe the map induced by P on sections of our Hilbert bundle E. Any wave function $\psi(\vec{k}_{\|}, \vec{r})$ in $L^2_{\mathbb{T}^{d-1}}(\mathbb{T}^{d-1} \times \mathbb{R}^d; W)$ (see (1.2.2)) can be viewed as section $\psi \in L^2(\mathbb{T}^{d-1}; E)$ in the following way

$$\begin{aligned} \psi(\vec{k}_{\|}) : \mathbb{R}^d/\Gamma_{\|} &\to E|_{\vec{k}_{\|}}, \\ [\vec{r}] &\mapsto [\vec{k}_{\|}, \vec{r}, \psi(\vec{k}_{\|}, \vec{r})]. \end{aligned} \tag{1.96}$$

This facilitates the understanding of the induced action of P on E as the action of P on $L^2_{\mathbb{T}^{d-1}}(\mathbb{T}^{d-1} \times \mathbb{R}^d; W)$ is given by

$$\begin{aligned}(p\hat{\psi})(\vec{k}_\parallel, \vec{r}) &= U(p)\psi(p^{-1}\vec{k}_\parallel, p^{-1}\vec{r} + a_{p^{-1}})\,, \\ &= U(p)e^{i\vec{k}_\parallel \cdot a_{p^{-1}}}\psi(p^{-1}\vec{k}_\parallel, p^{-1}\vec{r}) \end{aligned} \tag{1.97}$$

where $U(p) : W \to W$ and (p, a_p) is a representation of $P \subset G \subset \mathbb{R}^{d-1} \rtimes O(d-1)$. Here it is very important to remark that the phase $e^{i\vec{k}_\parallel \cdot a_{p^{-1}}}$ will be the source of the "twist" in the non-symmorphic case.
Thus we have

$$p : E|_{\vec{k}_\parallel} \to E|_{p\vec{k}_\parallel}\,,$$

$$\{[\vec{r}] \mapsto [\vec{k}_\parallel, \vec{r}, \psi(\vec{k}_\parallel, \vec{r})]\} \mapsto \{[\vec{r}] \mapsto [p\vec{k}_\parallel, \vec{r}, U(p)e^{i\vec{k}_\parallel \cdot a_{p^{-1}}}\psi(\vec{k}_\parallel, p^{-1}\vec{r})]\} \tag{1.98}$$

And finally we get a Hilbert bundle map that covers the action on $\mathbb{T}^{d-1}$:

$$\begin{array}{ccc} E & \xrightarrow{p} & E \\ \downarrow & & \downarrow \\ \mathbb{T}^{d-1} & \xrightarrow{p} & \mathbb{T}^{d-1} \end{array}$$ and therefore an associated Fredholm bundle map:

$$\begin{array}{ccc} \mathcal{F}^{sa}_*(E) & \xrightarrow{p} & \mathcal{F}^{sa}_*(E) \\ \downarrow & & \downarrow \\ \mathbb{T}^{d-1} & \xrightarrow{p} & \mathbb{T}^{d-1} \end{array}$$

Notice that this map is not in general an action since from (1.97) we see that

$$(p_2(p_1\psi)(\vec{k}_\parallel, \vec{r}) = U(p_2)U(p_1)\psi(p_2^{-1}p_1^{-1}\vec{k}_\parallel, p_2^{-1}p_1^{-1}\vec{r} + p_2^{-1}a_{p_1^{-1}} + a_{p_2}) \tag{1.99}$$

But

$$(p_2p_1\psi)(\vec{k}_\parallel, \vec{r}) = U(p_2p_1)\psi((p_2p_1)^{-1}\vec{k}_\parallel, (p_2p_1)^{-1}\vec{r} + a_{p_2p_1}). \tag{1.100}$$

and these are equal if and only if

$$p_2^{-1}a_{p_1^{-1}} + a_{p_2^{-1}} - a_{(p_2p_1)^{-1}} = 0 \tag{1.101}$$

which is true for symmorphic crystallographic groups and not for non-symmorphic. Since the action of P leaves $\Gamma_{\|} \subset \mathbb{R}^d$ we can in fact view the above equation as a group 2-cocycle

$$\nu : P \times P \to \Gamma_{\|}\,, \tag{1.102}$$

$$(p_1, p_2) \mapsto a_{p_1} + p_1 a_{p_2} - a_{p_1 p_2} \tag{1.103}$$

so that fiberwise we have the *twisted* action

$$p_1(p_2\psi(\vec{k}_{\|})) = \tau(p_1, p_2, \vec{k}_{\|}) p_1 p_2 \psi(\vec{k}_{\|}) \tag{1.104}$$

with

$$\tau(p_1, p_2, \vec{k}_{\|}) = e^{i\vec{k}_{\|}\cdot\nu(p_2^{-1}, p_1^{-1})}. \tag{1.105}$$

All twists coming from projective Hilbert bundles with P-equivariant fibers over $\mathbb{T}^{d-1}$ are elements of the equivariant cohomology group $H^3_P(\mathbb{T}^{d-1};\mathbb{Z})$ since $B\mathcal{PU}(\mathscr{H})$ is the Eilenberg-Maclane space $K(3,\mathbb{Z})$ [16],[48]. Gomi [21] clarified using the arguments presented above that the twist τ belongs to a subgroup and in fact $\tau \in H^2(P; C^0(\mathrm{Hom}(\Gamma_{\|}, U(1))))$, where $H^2(P; C^0(\mathrm{Hom}(\Gamma_{\|}, U(1))))$ denotes the *group cohomology* [48] of P with coefficients in $C^0(\mathrm{Hom}(\Gamma_{\|}, U(1)))$. Note that $\nu(p_1, p_2) = a_{p_1} + p_1 a_{p_2} - a_{p_1 p_2}$, $\nu \in H^2(P; \Gamma_{\|})$ that precisely classifies extensions of the form (1.94).

We will now use that $E|_{\vec{k}_{\|}} \equiv \mathscr{H}(\vec{k}_{\|}) = L^2(\mathbb{R}^d/\Gamma_{\|}; \mathcal{L}_{\{\vec{k}_{\|}\}\times\mathbb{R}^d/\Gamma_{\|}} \otimes W)$. But first we must make a few restrictions on the action: Let P be a discrete group acting on a a topological measure space (X, μ) such that $L^2(X; d\mu)$ is well defined and $\mu(pU)) = \mu(U)\,\forall p \in P$. Furthermore we ask that X/P is also a measure space with measure μ_P, the one inherited from (X, μ). Define

$$X_P^{free} = \{x \in X | px \neq x \;\forall p \neq e \in P\} \tag{1.106}$$

That is, X_P^{free} are the points which are neither fixed nor periodic. Then we have the following Lemma

Lemma 1.8.1. *If the P-action on X satisfies $\mu(X - X_P^{free}) = 0$ then there is an equivalence between $L^2(X; d\mu)$ and $L^2(P; d\mu_{count}) \otimes L^2(X/P; d\mu_P)$ as P-representations.*

Proof. There exists a non-canonical injective map $q_P : X_P^{free}/P \times P \to X$ that sends $([x], e)$ to any one of the representatives of $[x]$, and then define $q_P([x], p) = p q_P([x], e)$ and this is injective because $q_P([x], e) \in X_P^{free}$.

Let $U : L^2(X/P \times P; d\mu_P \times d\mu_{count}) \to L^2(X; d\mu)$ that sends f in an equivalence class in $L^2(X/P \times P; d\mu_P \times d\mu_{count})$ (μ_{count} being the counting measure of a set) to

$$U(f)(x) = \begin{cases} f(q_P^{-1}(x)) & \text{if } x \in X_P^{free} \\ 0 & \text{if } x \text{ not in } X_P^{free} \end{cases} \tag{1.107}$$

and let $U^* : L^2(X; d\mu) \to L^2(X_P^{free}/P \times P; d\mu_P \times d\mu_{count})$ that sends f in an equivalence class in $L^2(X; d\mu)$ to

$$U * (f)([x], p) = f(q_P([x], p)) \tag{1.108}$$

Since $\mu(X - X_P^{free}) = 0$, $U(U^*(f))$ is in the same class as f and the same for $U^*(U(f))$, thus U, U^* is a unitary equivalence that commutes with the action of P on $L^2(X; d\mu)$ and on $L^2(X_P^{free}/P \times P; d\mu_P \times d\mu_{count})$, therefore, as representations of P, they are equivalent. □

The above lemma has probably been proven before (or something stronger) but we were unable to find such a statement in the literature.

Remark 1.8.2. *In general, crystallographic groups where P is non-trivial combinations of rotations, reflections and translations satisfy 1.8.1. However there are exceptions like $G = \mathbb{Z} \times \mathbb{Z}_4$, with the action of the generator of $\mathbb{Z}_4$ being $\vec{r} \mapsto -\vec{r}$. Hence at this point we have to check each case individually.*

Let us now employ this result. Whenever the action of P satisfies 1.8.1, we can rewrite the fiber of our Hilbert bundle $E|_{\vec{k}_\parallel} = L^2(\mathbb{R}^d/\Gamma_\parallel; \mathcal{L}_{\{\vec{k}_\parallel\} \times \mathbb{R}^d/\Gamma_\parallel} \otimes W)$, as the equivalent G-representation

$$E|_{\vec{k}_\parallel} \approx L^2(P; L^2((\mathbb{R}^d/\Gamma_\parallel)_P^{free}/P;\, \mathcal{L}_{\{\vec{k}_\parallel\} \times \mathbb{R}^d/\Gamma_\parallel} \otimes W)) \tag{1.109}$$

Then we can apply a result in the appendix *A.4* of Freed, Hopkins and Teleman [49] to prove

Theorem 1.8.3. *Quasi-adiabatic equivalence classes of Fermi surfaces on a half-crystal with point group P and total symmetry group G, satisfying $0 \to \Gamma_\parallel \to G \to P \to 0$ and the P-action on $\mathbb{R}^d/\Gamma_\parallel$ as in 1.8.1 are in one to one correspondence with the twisted P-equivariant K-group $K_P^{\tau-1}(\mathbb{T}^{d-1})$, τ as in (1.105).*

Proof. Since the fiber $E|_{\vec{k}_\parallel}$ is of the form $L^2(P;l^2)$, then E is a *locally universal* Hilbert bundle (see [49] for the properties of universal Hilbert bundles), and furthermore, using 1.7.1 and [45] on the fixed points proves that $\mathcal{F}_*^{sa}(E)$ is a classifying space for $K_P^{\tau-1}$. Quasi-adiabatic equivalence classes of Fermi surfaces with symmetry group G are given by $[\mathbb{T}^{d-1}, \mathcal{F}_*^{sa}(E)]_P \approx K_P^{\tau-1}(\mathbb{T}^{d-1})$ □

Remark 1.8.4. *In [50] a similar result was stated without proof.*

It is straightforward to combine 1.8.3 to include time-reversal symmetry or particle-hole symmetry when these do not interact with the point group P since we also have equivariant Bott peridocity. We obtain the groups

$$KR_P^{\tau-1}(X_s)\,,\ \ \Xi^2 = I\,, \tag{1.110}$$
$$KR_P^{\tau-5}(X_s)\,,\ \ \Xi^2 = -I\,, \tag{1.111}$$
$$KR_P^{\tau-7}(X_s)\,,\ \ \Theta^2 = I\,, \tag{1.112}$$
$$KR_P^{\tau-3}(X_s)\,,\ \ \Theta^2 = -I\,. \tag{1.113}$$

When there is a non-trivial relation between point group and time-reversal symmetry one has the magnetic point group satisfying

$$0 \to P \to \hat{P} \to \mathbb{Z}/2 \to 0 \tag{1.114}$$

and this has been formalized in [16],[21] and [51] as a new type of K-theory that combines KR-theory and equivariant K-theory through twists but we shall leave that for future work.

Chapter 2

K-theory and Contextuality

2.1 Introduction

In quantum mechanics only mutually commuting observables can be simultaneously measured to reveal their joint outcome. Such a set of commuting observables is called a context. It is a fundamental property of quantum mechanics that its predictions cannot be reproduced by assuming predetermined context independent outcomes—a phenomenon called contextuality [52, 53]. This special feature of quantum systems is expected to play an important role in any computation scheme relying on quantum principals. Indeed, in quantum computation contextuality is established as a resource to achieve universal quantum computation and quantum speed-up can only be attained if contextuality is present [54–58]. To better characterize contextuality from the quantum computation perspective different frameworks have been developed such as [59–63]. Here we extend the topological approach of [63] and makes a connection to the sheaf-theoretic approach of [62].

Classifying spaces are fundamental objects in algebraic topology that play a prominent role in the classification of principal bundles [64]. These geometric objects appear in gauge theories in the standard model [65]. Motivated by questions arising from gauge theory [66, 67], Adem et al. [68, 69] introduced the notion of a classifying space for commutativity in Lie groups. Here we introduce the classifying space for contextuality, which is a variant of this construction tailored for applications to contextuality. Not only is it a unifying object for contextual interpretations, it is an interesting mathematical object in its own right because of its rich homotopy-theoretic structure. The classifying space for commutativity of extraspecial groups studied in [70–72] demonstrates such an interesting behavior. There is a close connection to quantum computation since the basic observables called the Pauli observables constitute a finite group which is an extraspecial group. Our goal here is to make this connection precise by showing how traditional quantities relevant to contextuality (such as Wigner functions) can be viewed as elements in algebro-topological groups coming from our classifying space.

A context specifies a set of observables that can be measured simultaneously. In more mathematical terms for us a context in quantum computation refers to an abelian subgroup of the Pauli group. Given a collection $\mathcal{I}$ of contexts we construct a topological space $B_{\text{cx}}(\mathcal{I})$, called the classifying space for contextuality, and identify two classes:

- a cohomology class in the second cohomology group with mod-p coefficients
$$[\beta] \in H^2(B_{\text{cx}}\mathcal{I})$$
- a K-theory class, that depends on a quantum state ρ, in the β-twisted K-group
$$[W_\rho] \in \mathbb{R} \otimes K^\beta(B_{\text{cx}}\mathcal{I}).$$

The cohomology class $[\beta]$ is introduced in [63] using chain complexes obtained from a cover of contexts. The chain complex of $B_{\text{cx}}\mathcal{I}$ specializes to the construction given there for small dimensions. But the space itself is infinite dimensional analogous to the case of classifying spaces of finite groups. This class captures contextuality in the strong sense measuring only the failure of assigning pre-determined measurement outcomes. The full formulation of contextuality involves probability distributions on outcomes over contexts and can be formalized using sheaf theory [62]. Given a quantum state ρ the empirical model e_ρ provides a description as a probability distribution on measurement outcomes over each context. If the empirical model can not be described using a deterministic hidden-variable model then it is called contextual. When this approach is transferred to our topological language the empirical model e_ρ can equivalently be described as the class $[W_\rho]$ which lives in the twisted K-group of $B_{\text{cx}}\mathcal{I}$. This class is essentially the discrete Wigner function [73] of the quantum state.

We have the following structure for this chapter. In §2.2 we start with the sheaf-theoretic definition of contextuality, and restrict this framework to Pauli observables [63]. This is summarized in Corollary 2.2.8. Section 2.3 uses twisted representations to describe the space of empirical models. Theorem 2.3.9 explains the relationship between the empirical model e_ρ and the class $[W_\rho]$ corresponding to the Wigner function. The classifying space for contextuality is introduced in §2.4. We study its cohomology and explain the distinction between the even and odd prime cases. We refer to the quantum computation literature to point out the consequences of these observations. Representation theoretic approach of §2.3 and the topological approach of §2.4 come together in §2.5. In this section we compute the β-

twisted K-theory of $B_{\mathrm{cx}}\mathcal{I}$ in Theorem 2.5.4 whose proof mostly follows the computation in [70] for the untwisted version.

2.2 Contextuality for Pauli observables

In this section we introduce the basic ingredients of quantum computation. We define contextuality in the sheaf-theoretic language of [62]. Then we specialize to the Pauli group, the basic observables of quantum computation. Our description makes a connection to the topological framework of [63]. For basics of quantum computation we refer to [74].

2.2.1 Contexts in quantum mechanics

In quantum mechanics the state of a system is specified by a density matrix ρ acting on a Hilbert space $\mathcal{H}$. A density matrix is a Hermitian matrix that is positive and has trace $\mathrm{Tr}(\rho) = 1$. We will denote the space of density matrices by $\mathrm{Den}(\mathcal{H})$. An observable is a Hermitian matrix acting on the Hilbert space. In quantum computation the Hilbert space is finite dimensional. Here we will only consider the case when the dimension is a power of a prime p.

Remark 2.2.1. When $p = 2$ the observables are Hermitian matrices as usual, but for $p > 2$ the type of observables we will consider are unitary matrices that are not necessarily Hermitian. In fact, the results here can be applied to the more general observables introduced in [63]. But we restrict to Pauli observables since for this case the topology of the classifying space for contextuality is well-understood, and independently studied (see Theorem 2.4.6).

An observable A can be measured on a system at state ρ. The measurement result is specified by an eigenvalue λ_A of the observable. Born's rule says that the probability of a measurement result λ_A occurs is given by the trace $\mathrm{Tr}(\rho P_{\lambda_A})$ where P_{λ_A} is the projector onto the eigenspace corresponding to the eigenvalue λ_A. This can be generalized to a set of pairwise commuting observables, also known as a *context*. Let C be a context and λ be a function that assigns an eigenvalue to each observable in the context. The probability of obtaining λ_A as a measurement result for each observable $A \in C$ is given by $\mathrm{Tr}(\rho P_\lambda)$ where P_λ projects onto the simultaneous eigenspace of the observables in C.

2.2.2 Sheaf-theoretic description of contextuality

Abramsky and Brandenburger introduced a sheaf theoretic approach in [62] to study probability distributions for measurements over various contexts. The general framework consists of

- a set X of measurements,
- a set O of outcomes,
- a collection $\mathcal{M}$ of contexts such that

$$X = \bigcup_{C \in \mathcal{M}} C.$$

The collection $\mathcal{M}$ is sometimes referred to as a *cover of contexts*. We will assume that $\mathcal{M}$ is closed under intersections and regard it as a partially ordered set ordered under inclusion. Given this data one can construct a *sheaf of events*

$$\mathcal{E} : \mathcal{M}^{\mathrm{op}} \to \mathbf{Set}$$

which assigns the set O^C of all functions $C \to O$ to a given context C. For a set U let $D(U)$ denote the set of probability distributions over U with finite support. This gives a functor

$$D : \mathbf{Set} \to \mathbf{Set}$$

where for a function $f : U \to U'$ the corresponding function $D(f) : D(U) \to D(U')$ is defined by

$$D(f)(d) : U' \to \mathbb{R}_{\geq 0}, \quad u' \mapsto \sum_{u \in f^{-1}(u')} d(u).$$

We are interested in the inverse limit of the composite functor $D\mathcal{E} : \mathcal{M}^{\mathrm{op}} \to \mathbf{Set}$. An element d of the inverse limit is a collection of distributions $\{ d \mid_C \mid C \in \mathcal{M} \}$, where $d|_C$ means restriction to C, such that further restriction to pairwise intersections coincide: $(d|_C)|_{C \cap C'} = (d|_{C'})|_{C' \cap C}$. Thus the inverse limit is a subset of the product

$$\lim_{\leftarrow} D\mathcal{E} \subset \prod_{C \in \mathcal{M}} D\mathcal{E}(C).$$

In physics literature an element of the inverse limit is called an *empirical model*.

An important example comes from quantum mechanics. Given a state ρ we can define an element e_ρ of the inverse limit. Let us denote this assignment by a map

$$e : \mathrm{Den}(\mathcal{H}) \to \lim_{\leftarrow} D\mathcal{E}, \quad \rho \mapsto e_\rho$$

where $e_\rho|_C$ is defined on $\lambda : C \to O$ by the quantum mechanical probability

$$e_\rho|_C(\lambda) = \mathrm{Tr}(\rho P_\lambda) \in \mathbb{R}_{\geq 0}.$$

Let $S(\rho)$ denote the set of functions $s \in \mathcal{E}(X) \equiv O^X$ such that the restriction of the empirical model satisfies $e_\rho|_C(s|_C) \neq 0$ for all $C \in \mathcal{M}$.

Definition 2.2.2. A state ρ is called *non-contextual* if there exists a distribution $d \in D\mathcal{E}(X)$ such that $d|_C = e_\rho|_C$ for all $C \in \mathcal{M}$, otherwise, it is called *contextual* (with respect to $\mathcal{M}$). A state ρ is called *strongly contextual* if the set $S(\rho)$ is empty.

In sheaf theory language we can summarize this definition by the statement that a state ρ is contextual if e_ρ does not comes from a global section, also known as a deterministic hidden-variable model.

2.2.3 Pauli group

In quantum computation there is a distinguished set of observables called the Pauli observables acting on a Hilbert space $\mathcal{H}$ of dimension d. More precisely, $\mathcal{H}$ is the complex group ring $\mathbb{C}[\mathbb{Z}/d]$ of the additive group $\mathbb{Z}/d$ of integers modulo d. Pauli observables acting on $\mathcal{H}$ can be defined by the unitary representation

$$Z \langle a| = \omega^a \langle a| \quad X \langle a| = \langle a+1|$$

where $a \in \mathbb{Z}/d$ and ω is the d-th root of unity $e^{2\pi i/d}$. We are using the quantum mechanical notation $\langle a|$ to denote the basis elements of the Hilbert space. This representation is usually called a 1-qudit, or more popularly a 1-qubit when $d = 2$. Here we will only consider the case where d is a prime p.

Qudits can be composed to obtain larger systems. An n-qudit has the Hilbert space

$$\mathcal{H}_n = \underbrace{\mathcal{H} \otimes \cdots \otimes \mathcal{H}}_{n}$$

which can be identified with the complex group ring $\mathbb{C}[(\mathbb{Z}/p)^n]$. Let us set $V = (\mathbb{Z}/p)^n \times (\mathbb{Z}/p)^n$. For an element $(a, b) \in V$ the corresponding Pauli operators are defined as the tensor powers

$$Z(a) = Z^{a_1} \otimes \cdots \otimes Z^{a_n} \quad X(b) = X^{b_1} \otimes \cdots \otimes X^{b_n}.$$

When it comes to define the Pauli group, or the group of Pauli observables, there is a distinction between the cases $p = 2$ and $p > 2$. Let us set

$$\mu = \begin{cases} \sqrt{\omega} & \text{if } p = 2 \\ \omega & \text{if } p > 2. \end{cases}$$

The Pauli group of an n-qudit system is defined by

$$P_n = \langle \mu I, Z(a), X(b) | \; (a, b) \in V \rangle \tag{2.1}$$

as a subgroup of the unitary group $U(p^n)$.

Example 2.2.3. The Hilbert space of a 1-qubit system is given by $\mathcal{H} = \mathbb{C}[\mathbb{Z}/2]$. Pauli observables constitute a subgroup of the unitary group $U(2)$ generated by the Pauli matrices

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

together with iI.

2.2.4 Extension class

As an abstract group P_n is an extraspecial p-group.A p-group is group G such that to each element g, there is a power $n(g)$ so that $g^{p^{n(g)}} = 1$. A finite group is a p-group if its order is a power of p. A finite p-group G is extraspecial if its center, $Z(G)$ is cyclic of order p and $G/Z(G)$ is abelian of order p. When $p = 2$ it is of complex type, and for $p > 2$ it has exponent p.

The subgroup $\langle \mu I \rangle \subset P_n$ is isomorphic to the additive group

$$Z_\mu = \begin{cases} \mathbb{Z}/4 & p = 2 \\ \mathbb{Z}/p & p > 2 \end{cases}$$

under the canonical homomorphism $I \mapsto \mu$. Under this identification the Pauli group can be written as a central extension

$$0 \to Z_\mu \to P_n \xrightarrow{\pi} V \to 0 \tag{2.2}$$

since up to an element of $\langle \mu I \rangle$ a Pauli operator is specified by an element of V. Given a function $\gamma : V \to Z_\mu$ we can write down a set theoretic section

$$\eta_\gamma(v) = \mu^{\gamma(v)} Z(v_z) X(v_x)$$

of the projection homomorphism and the extension cocycle can be computed from the formula $\beta(v, v') = \eta(v)\eta(v')\eta(v + v')^{-1}$. The cohomology class $[\beta] \in H^2(V, Z_\mu)$ of the extension is independent of the choice of the section.

Let η_0 denote the section corresponding to the zero function $\gamma = 0$, then the corresponding cocycle can be computed as

$$\beta_0(v, v') = \begin{cases} v_x \cdot v'_z & p > 2 \\ 2\, v_x \cdot v'_z & p = 2 \end{cases} \tag{2.3}$$

where the notation $v \cdot w$ stands for the standard inner product. For any other choice of γ we have that $\beta_\gamma = \beta_0 + d\gamma$ where $d\gamma(v, v') = \gamma(v) - \gamma(v+v') + \gamma(v')$.

2.2.5 Isotropic subspaces

Commutation properties of Pauli operators are determined by a symplectic form $\mathfrak{b} : V \times V \to \mathbb{Z}/p$ defined by

$$\mathfrak{b}(v, v') = v_x \cdot v'_z - v'_x \cdot v_z. \tag{2.4}$$

This fact about Pauli operators can be seen from the commutator $[\eta(v), \eta(v')]$ and the expression $\mathfrak{b}(v, v') = \beta(v, v') - \beta(v', v)$ (for $p = 2$, $\mu = \sqrt{\omega}$ and we can identify $2(\mathbb{Z}/4)$ with $\mathbb{Z}/2$) that relates the symplectic form to the extension cocycle. We can choose a symplectic basis $\{ z_1, \cdots, z_n, x_1, \cdots, x_n \}$ for V where x_i and z_i are the symplectic pairs satisfying $\mathfrak{b}(z_i, x_i) = 1$. The suitable choice compatible with the representation of P_n is to take z_i the canonical basis for the first factor of $V = (\mathbb{Z}/p)^n \times (\mathbb{Z}/p)^n$ and x_i the basis for the second factor.

Definition 2.2.4. A subspace $I \subset V$ is called *isotropic* if $\mathfrak{b}|_I = 0$ i.e. $\mathfrak{b}(v, v') = 0$ for all $v, v' \in I$. We write $\mathcal{I}(V)$ for the collection of all isotropic subspaces in V.

We will derive a property of β restricted onto an isotropic subspace. For this purpose we make a canonical choice for the extension cocycle:

$$\beta = \beta_0 + d\mathfrak{q}/2 \tag{2.5}$$

where $\mathfrak{q} : V \to Z_\mu$ denotes the function

$$\mathfrak{q}(v) = \begin{cases} 2v_x \cdot v_z & p = 2 \\ v_x \cdot v_z & p > 2. \end{cases}$$

The motivation for this choice is provided by the following result.

Proposition 2.2.5. *For any isotropic subspace I the restricted cocycle satisfies $2\beta|_I = 0$. Moreover, for $p > 2$ we have that $2\beta = \mathfrak{b}$.*

Proof. For $p = 2$ as a consequence of 2.3 we have that $2\beta = d\mathfrak{q} = 2\mathfrak{b}$ since $2\mathfrak{q}$ can be thought of a quadratic form on $2(\mathbb{Z}/4) \cong \mathbb{Z}/2$. Thus 2β restricted to I vanishes. In the case of $p > 2$ one can calculate to obtain $\beta = \mathfrak{b}/2$. □

2.2.6 Contextuality for Pauli observables

The observables that are used in quantum computation have eigenvalues given by the set $\{1, \omega, \cdots, \omega^{p-1}\}$. These observables are precisely the elements of order p in the Pauli group.

In the sheaf theoretic description of contextuality for Pauli observables we consider the triple $(\Sigma, \mathcal{I}, \mathbb{Z}/p)$ where

- the collection $\mathcal{I}$ of contexts is given by a subcollection of $\mathcal{I}(V)$ satisfying the property that if $I, I' \in \mathcal{I}$ then $I \cap I' \in \mathcal{I}$
- the set of measurements is $\{\eta(a) \mid a \in \Sigma(\mathcal{I})\}$ where
$$\Sigma(\mathcal{I}) = \bigcup_{I \in \mathcal{I}} I$$
- the set of outcomes is $\mathbb{Z}/p$.

Remark 2.2.6. As a consequence of Proposition 2.2.5 the cocycle $\beta|_I$ is the zero function when $p > 2$, and is divisible by 2 when $p = 2$. For the $p = 2$ case we identify $2(\mathbb{Z}/4)$ with $\mathbb{Z}/2$ and regard $\beta|_I$ as a function $I \times I \to \mathbb{Z}/2$.

Next we introduce a modified version of the event sheaf. In the Pauli case we will use the set of functions

$$\mathcal{E}_\beta(I) = \{ s : I \to \mathbb{Z}/p \mid \beta|_I = ds \}$$

which as an assignment gives a functor

$$\mathcal{E}_\beta : \mathcal{I}^{\text{op}} \to \mathbf{Set}.$$

Note that this is a subfunctor of the sheaf of events: $\mathcal{E}_\beta \subset \mathcal{E}$ (as a subcategory of the image). The motivation for this definition is the following observation in quantum mechanics.

Proposition 2.2.7. *If a function $s : I \to \mathbb{Z}/p$ does not belong to $\mathcal{E}_\beta(I)$ then $e_\rho|_I(s) = 0$.*

Proof. If $e_\rho|_I(s) \neq 0$ then there is a common eigenstate $\langle s|$ with eigenvalue $\omega^{s(a)}$ for the observable $\eta(a)$. Thus we can write

$$\omega^{s(a)+s(b)} \langle s| = \eta(a)\eta(b) \langle s| = \omega^{\beta(a,b)}\eta(a+b) \langle s| = \omega^{\beta(a,b)+s(a+b)} \langle s|$$

which implies that $s \in \mathcal{E}_\beta(I)$. □

This means that the distribution $e_\rho|_I \in D\mathcal{E}(I)$ can be regarded as an element of $D\mathcal{E}_\beta(I)$ for each $I \in \mathcal{I}$. As a consequence the empirical model e_ρ associated to a state ρ gives a function

$$e : \mathrm{Den}(\mathcal{H}) \to \underset{\leftarrow}{\lim}\, D\mathcal{E}_\beta.$$

Proposition 2.2.7 has another implication. To demonstrate this we introduce the set

$$\mathcal{E}_\beta(\mathcal{I}) = \underset{\leftarrow}{\lim}\, \mathcal{E}_\beta$$

as the inverse limit of the functor $\mathcal{E}_\beta : \mathcal{I}^{\mathrm{op}} \to \mathbf{Set}$. More explicitly, this set consists of functions that are obtained by"gluing" functions $\mathcal{E}_\beta(I)$ over contexts. By naturality of the inverse limit we have a commutative diagram

$$\begin{array}{ccccc} \mathrm{Den}(\mathcal{H}) & \xrightarrow{e} & \underset{\leftarrow}{\lim}\, D\mathcal{E}_\beta & \xleftarrow{\theta} & D\mathcal{E}_\beta(\mathcal{I}) \\ & \searrow & \downarrow & & \downarrow \\ & & \underset{\leftarrow}{\lim}\, D\mathcal{E} & \longleftarrow & D\mathcal{E}(\Sigma) \end{array} \tag{2.6}$$

where the union of all contexts is denoted by $\Sigma = \Sigma(\mathcal{I})$.

Corollary 2.2.8. *Let ρ be a state and $\mathcal{I}$ be a cover of contexts.*

1. *ρ is strongly contextual if $\mathcal{E}_\beta(\mathcal{I}) = \emptyset$.*

2. *ρ is contextual if and only if $e_\rho \notin Im(\theta)$.*

Proof. Recall from Definition 2.2.2 that ρ is strongly contextual if $S(\rho)$ is empty. By definition $s \in \mathcal{E}(\Sigma)$ belongs to this set if $e_\rho|_I(s|_I) \neq 0$ for all $I \in \mathcal{I}$. By Proposition 2.2.7 the restriction $e_\rho|_I$ belongs to $\mathcal{E}_\beta(I)$ for each I.

This implies that $s|_I$ is in $\mathcal{E}_\beta(I)$. But this suffices to conclude that s belongs to $\mathcal{E}_\beta(\mathcal{I})$, since it is obtained by patching the local functions.

For the second statement observe that if e_ρ can be written as $\theta(d')$ for some $d' \in D\mathcal{E}_\beta(\mathcal{I})$ then regarding d' as an element of $D\mathcal{E}(\Sigma)$ in the obvious way implies that ρ is non-contextual. Conversely, it suffices to check that if $e_\rho = \theta(d)$ for some $d \in D\mathcal{E}(\Sigma)$ then d belongs to $DS(\rho)$, which is a subset of $D\mathcal{E}_\beta(\mathcal{I})$ by the previous paragraph. Observe that if $d(s) \neq 0$ then $e_\rho|_I(s|_I) = \theta(d)|_I(s|_I) \neq 0$ for all I, and thus s belongs to $S(\rho)$. $\square$

2.3 Wigner function as a global section

The purpose of this section is to interpret empirical models described in the previous section in representation theoretic terms. The approach taken here is to extend probability distributions over $\mathbb{R}_{\geq 0}$ to the whole field of real numbers. After extending the coefficients the empirical model map becomes

$$e : \mathrm{Den}(\mathcal{H}) \to \lim_{\leftarrow} \mathbb{R} \otimes \mathcal{E}_\beta.$$

Our main result is proposition (2.3.5) that gives an identification of the inverse limit as the representation ring $\mathbb{R} \otimes R(V)$. Under this identification the empirical model e_ρ corresponds to the Wigner function W_ρ of the state ρ. In general W_ρ is not a probability distribution and may assume negative values. An important application to contextuality, for $p > 2$, says that W_ρ is a probability distribution if and only if ρ is non-contextual. This result displays a distinct feature of the odd prime case as first demonstrated in [54, 55].

2.3.1 Twisted representations

Let $\iota : \mathbb{Z}/p \to U(1)$ denote the embedding $\iota(1) = \omega$ where ω is the p-th root of unity $e^{2\pi i/p}$. Under this identification the cohomology class $\beta|_I$ corresponds to a class in $H^2(I, U(1))$, also denoted by the same symbol. Such a class can be used to define a twisted representation [75].

In general, for a finite group G and a cohomology class $\alpha \in H^2(G, U(1))$ an α-twisted representation can be thought of as a linear representation of the extension $\tilde{G}$ corresponding to α. Therefore most of the properties of linear representations can be transferred to twisted representations. There is a Grothendieck group of twisted representations [76], denoted by $R_\alpha(G)$.

Proposition 2.3.1. *The embedding $\iota : \mathbb{Z}/p \to U(1)$ induces a natural isomorphism of $\mathbb{R}$-vector spaces*

$$\iota_* : \mathbb{R}\mathcal{E}_\beta(I) \to \mathbb{R} \otimes R_\beta(I).$$

Remark 2.3.2. Note that when $p > 2$ the twisted representation group coincides with the ordinary representation group $R(I)$ as a consequence of Proposition 2.2.5.

The benefit of passing to representations is the character map [77]:

$$\mathrm{ch} : R_\alpha(G) \to \mathrm{Cl}_\alpha(G) \tag{2.7}$$

where $\mathrm{Cl}_\alpha(G)$ denotes the $\mathbb{C}$-vector space of α-class functions. A function $f : G \to \mathbb{C}$ is an *α-class function* if it satisfies the formula

$$f(hgh^{-1}) = \frac{\alpha(h, h^{-1})}{\alpha(h, gh^{-1})\alpha(g, h^{-1})} f(g) \tag{2.8}$$

for all $g, h \in G$.

Lemma 2.3.3. *Let $I \subset V$ be an isotropic subspace. Then $Cl_\beta(I)$ coincides with the $\mathbb{C}$-vector space $\mathbb{C}^I$ of complex valued functions on I.*

Proof. The $p > 2$ case follows from Remark 2.3.2. For $p = 2$ we check that

$$\frac{\omega^{\beta(w,-w)}}{\omega^{\beta(w,v-w)}\omega^{\beta(v,-w)}} = \frac{\eta(w)\eta(w)\eta(0)}{\eta(w)\eta(v+w)\eta(v)\,\eta(v)\eta(w)\eta(v+w)} = 1$$

for all $v, w \in I$. Recall that each $\eta(v)$ squares to the identity matrix, $\eta(0) = I$, and $[\eta(v), \eta(w)] = I$ since v, w belong to an isotropic subspace. $\square$

2.3.2 Computing the inverse limit

Let $\mathcal{I} \subset \mathcal{I}(V)$ be a cover of contexts. We are interested in the inverse limit of the functor $\mathbb{R}\mathcal{E}_\beta : \mathcal{I}^{\mathrm{op}} \to \mathbf{Set}$. We will compute it using the character map 2.7. The first step is to extend the scalars to complex numbers.

Lemma 2.3.4. *There is a natural isomorphism of $\mathbb{C}$-vector spaces*

$$\mathbb{C} \otimes (\varprojlim \mathbb{R}\mathcal{E}_\beta) \cong \mathbb{C}^\Sigma.$$

Proof. Up to isomorphism we can consider the functor $\mathbb{R} \otimes R_\beta$ instead (Proposition 2.3.1). Since the character map 2.7 is natural it gives a natural transformation $\mathrm{ch} : \mathbb{R} \otimes R_\beta \to \mathrm{Cl}_\beta$, where Cl_β is regarded as a functor on $\mathcal{I}^{\mathrm{op}}$. Tensoring $\mathbb{R} \otimes R_\beta$ with $\mathbb{C}$ the character map becomes an isomorphism of $\mathbb{C}$-vector spaces. We denote the resulting natural isomorphism by $\mathrm{ch} : \mathbb{C} \otimes R_\beta \to \mathrm{Cl}_\beta$. Since taking inverse limit commutes with tensoring with $\mathbb{C}$ we have

$$\mathbb{C} \otimes (\varprojlim \mathbb{R} \otimes R_\beta) \cong \varprojlim \mathbb{C} \otimes R_\beta \cong \varprojlim \mathrm{Cl}_\beta.$$

Using Lemma 2.3.3 we can compute the inverse limit of Cl_β. The functor Cl_β is isomorphic to the functor $\mathbb{C}^-$ which sends I to the set $\mathbb{C}^I$ of complex valued functions. Inverse limit of $\mathbb{C}^-$ is simply the set of functions from the union $\Sigma = \Sigma(\mathcal{I})$ to complex numbers. $\square$

Next step is to identify the inverse limit over $\mathbb{R}$. We take $\mathcal{I} = \mathcal{I}(V)$ and $\Sigma = V$ since smaller sets of measurements can be dealt with by naturality, i.e. restricting from $\mathcal{I}(V)$. The analysis depends on the prime p. Let us define a map

$$\phi_p : \mathbb{R} \otimes R(V) \to \varprojlim \mathbb{R} \otimes R_\beta$$

as follows:

- $p = 2$: A β-twisted representation is a linear representation (compatible with the embedding ι) of the extension

  $$0 \to \mathbb{Z}/2 \to \tilde{I} \to I \to 0$$

  corresponding to the cocycle β. By definition of β (2.5) every element of the group $\tilde{I}$ has order at most 2. Therefore the class function of a representation takes values in $\mathbb{R}$. This means that the character map 2.7 factors through the isomorphism

  $$\mathrm{ch}_{\mathbb{R}} : \mathbb{R} \otimes R_\beta(I) \to \mathbb{R}^I.$$

  A similar observation is true for $\mathbb{R} \otimes R(V)$, i.e. the character map induces an isomorphism to $\mathbb{R}^V$. Using these identifications we can define

  $$\phi_2 : \mathbb{R} \otimes R(V) \to \varprojlim \mathbb{R} \otimes R_\beta$$

  by sending a representation to the restriction of the associated character to each isotropic subspace. More explicitly, we have a commutative diagram

$$\begin{array}{ccc}
\mathbb{R}\otimes R(V) & \xrightarrow{\phi_2} & \lim\limits_{\leftarrow} \mathbb{R}\otimes R_\beta \\
\Big\downarrow \mathrm{ch}_{\mathbb{R}} & & \Big\downarrow \mathrm{ch}_{\mathbb{R}} \\
\mathbb{R}^V & \xrightarrow{\cong} & \lim\limits_{\leftarrow} \mathbb{R}^-
\end{array}$$

where $\mathbb{R}^-$ is the functor $I \mapsto \mathbb{R}^I$. The lower horizontal map is an isomorphism by an analogous argument given in the proof of Lemma 2.3.4. The point is that for $p = 2$ extending coefficients to real numbers is sufficient.

- $p > 2$: We have seen that a β-twisted representation is the same as an ordinary representation. Therefore for each isotropic subspace we have a restriction map $R(V) \to R(I)$. These maps induce a map to the inverse limit

  $$\phi_p : \mathbb{R}\otimes R(V) \to \lim_{\leftarrow} \mathbb{R}\otimes R_\beta$$

  and again this map turns out to be an isomorphism as in the $p = 2$ case. This can be seen by extending the scalars to complex numbers and using Lemma 2.3.4. Indeed, tensoring ϕ_p with $\mathbb{C}$ gives an isomorphism since we obtain a commutative diagram

  $$\begin{array}{ccc}
  \mathbb{C}\otimes R(V) & \xrightarrow{\phi_p} & \mathbb{C}\otimes (\lim\limits_{\leftarrow} \mathbb{R}\otimes R_\beta) \\
  \Big\downarrow \mathrm{ch} & & \Big\downarrow \mathrm{ch} \\
  \mathbb{C}^V & \xrightarrow{\cong} & \lim\limits_{\leftarrow} \mathbb{C}^-
  \end{array}$$

  Here left-vertical map is an isomorphism by definition of class functions and right-vertical arrow is an isomorphism by Lemma 2.3.4.

Both diagrams imply that ϕ_p is an isomorphism, and under the identification of Proposition 2.3.1 we obtain:

Proposition 2.3.5. *There is a natural isomorphism*

$$\phi_p : \mathbb{R}\otimes R(V) \to \lim_{\substack{\leftarrow \\ \mathcal{I}(V)}} \mathbb{R}\mathcal{E}_\beta \qquad \textit{for any prime } p.$$

Remark 2.3.6. Note that the inverse limit of R_β is a subgroup of the product $\prod_{I \in \mathcal{I}(V)} R_\beta(I)$. In particular, it is a torsion-free abelian group. Therefore Proposition 2.3.5 shows that the inverse limit of R_β is isomorphic to $\mathbb{Z}^{|V|}$—the free abelian group of rank $|V| = p^{2n}$.

2.3.3 Wigner functions

Density matrices map to the inverse limit of $\mathbb{R}\mathcal{E}_\beta$ by the assignment $\rho \mapsto e_\rho$. As a consequence of the isomorphism ϕ_p of Proposition 2.3.5 there must be a map W that fits in the commutative diagram

$$\begin{array}{ccc} \mathrm{Den}(\mathcal{H}) & \xrightarrow{W} & \mathbb{R} \otimes R(V) \\ & \searrow^{e} & \downarrow \phi_p \\ & & \varprojlim \mathbb{R}\mathcal{E}_\beta \end{array} \tag{2.9}$$

We write $\rho \mapsto W_\rho$ for this assignment. It turns out that W_ρ, an element of the representation group, is in fact the (discrete) Wigner function of ρ. Wigner functions are introduced to the quantum computation literature in the work of Gross [73].

Let us introduce the Wigner function of a density matrix. First we define the point operators

$$A_v = |V|^{-1/2} \sum_{u \in V} b_u(v) \eta(u)$$

where b_u is the representation $V \to U(1)$ defined by $b_u(v) = \omega^{\mathfrak{b}(v,u)}$ ($\mathfrak{b}$ is the symplectic form in 2.4).

Definition 2.3.7. *Wigner function* of ρ is the function $W_\rho : V \to \mathbb{R}$ defined by the equation

$$W_\rho(v) = |V|^{-1/2} \mathrm{Tr}(\rho A_v).$$

We construct an element of the representation group

$$W_\rho = \sum_{v \in V} W_\rho(v) b_v \ \in \mathbb{R} \otimes R(V)$$

by regarding the values $W_\rho(v)$ as coefficients of the representations b_v. The set $\{ A_v \mid v \in V \}$ is an orthonormal basis for the $p^n \times p^n$ matrices over $\mathbb{C}$ with respect to the inner product $(A, B) = |V|^{-1/2} \mathrm{Tr}(A^\dagger B)$, where $(-)^\dagger$ stands for the conjugate transpose. Therefore we can write

$$\rho = \sum_{v \in V} W_\rho(v) A_v.$$

Note that the Pauli observables $\{ \eta(v) \mid v \in V \}$ is also an orthonormal basis with respect to the same inner product.

The operator inner product introduced above is related to the inner product of characters. The set of irreducible α-twisted representations of a finite group G constitutes an orthonormal basis of $\mathrm{Cl}_\alpha(G)$ with respect to the inner product

$$(\phi, \psi) = \frac{1}{|G|} \sum_{g \in G} \phi(g)\bar{\psi}(g).$$

Let $\chi_s \in R_\beta(I)$ denote the twisted representation corresponding to $s \in \mathcal{E}_\beta(I)$ under the isomorphism of Proposition 2.3.1. The projector onto the common eigenspace of $\{ \eta(u) \mid u \in I \}$ corresponding to the eigenvalues specified by s can be written as

$$P_s = \frac{1}{|I|} \sum_{u \in I} \bar{\chi}_s(u)\eta(u).$$

Using this we can show the following.

Lemma 2.3.8. *We have*

$$e_\rho|_I(s) = Tr(\rho P_s) = \sum_{t \in V} (b_t|_I, \chi_s) W_\rho(t).$$

Proof. This follows from the formula for P_s and the calculation

$$\mathrm{Tr}(\rho\, \eta(u)) = \sum_{t \in V} W_\rho(t) b_t(u).$$

□

The main result of this section is the identification of the empirical model e_ρ as an element of the representation group. We will write $W_\rho|_I$ for the restriction of $\phi_p(W_\rho)$ to an isotropic subspace I.

Theorem 2.3.9. *(OS 2019) Sending a density matrix ρ to the element W_ρ in $\mathbb{R} \otimes R(V)$ defines a map*

$$W : Den(\mathcal{H}) \to \mathbb{R} \otimes R(V) \tag{2.10}$$

that makes the diagram 2.9 commute.

Proof. The interpretation of $W_\rho|_I$ depends on the prime p since the map ϕ_p does as well.

- $p > 2$: In this case ϕ_p is induced by the restriction maps $R(V) \to R(I)$. Lemma 2.3.8 implies that

$$e_\rho|_I(s) = (W_\rho|_I, \chi_s)$$

which is what we want to prove.

- $p = 2$: The interpretation in this case is through the character map. The restriction is induced by the restriction maps $\mathbb{R}^V \to \mathbb{R}^I$. The representations b_t are regarded as functions $\mathbb{R}^V$. Again Lemma 2.3.8 finishes the proof.

□

Remark 2.3.10. As an immediate corollary of this theorem and the fact that a state is uniquely determined by its Wigner function we observe that the map W is injective. Extending the coefficients to $\mathbb{R}$ in the domain of 2.10 the map W becomes an isomorphism of $\mathbb{R}$-vector spaces. Commutativity of diagram 2.9 implies that the map e is injective. A subtle point is that W_ρ is not necessarily a probability distribution as it may assume negative values. In quantum mechanics the negativity of the Wigner function indicates a divergence from the classical behavior and this is related to contextuality as we will see next.

2.3.4 Contextuality

As we emphasized in Remark 2.3.10 the coefficients $W_\rho(v)$ can take negative values. We write $W_\rho \geq 0$ when $W_\rho(v) \geq 0$ for all $v \in V$, and say that the Wigner function is non-negative. Recall that a state ρ is contextual if e_ρ is not in the image of the map

$$\theta : D\mathcal{E}_\beta(\mathcal{I}) \to \lim_{\leftarrow} D\mathcal{E}_\beta.$$

We will look at the odd prime and $p = 2$ cases separately.

- $p > 2$: The odd prime case is nicer since β-twisted representations coincide with ordinary representations. We can consider $D\mathcal{E}_\beta(V)$ as a subset of $\mathbb{R} \otimes R(V)$, and θ is the restriction of ϕ_p to this subset. The Wigner function, regarded as an element of $\mathbb{R} \otimes R(V)$, can be used as a distribution when $W_\rho \geq 0$. Thus it lies in $D\mathcal{E}_\beta(V)$ and furthermore satisfies $\theta(W_\rho) = e_\rho$ by Theorem 2.3.9. Conversely, if ρ is non-contextual, i.e. there exits d with $\theta(d) = e_\rho$, that means $W_\rho \geq 0$ since $d = W_\rho$ because ϕ_p is an isomorphism. Thus we obtain a proof of the following result, which is first proved in [54] for $n = 1$ and generalized to all n in [55].

Corollary 2.3.11. *Assume that $p > 2$. Then $W_\rho \geq 0$ if and only if ρ is non-contextual.*

- $p = 2$: This case is much trickier and the Wigner function does not determine contextuality as in $p > 2$. There are partial results in the physics literature, for example see [56, 78]. For some $\mathcal{I}$ the set $\mathcal{E}_\beta(\mathcal{I})$ turns out to be empty, thus for such a cover of contexts any state ρ is strongly contextual. For example, this happens if $\mathcal{I}$ contains one of the Mermin square $\mathcal{I}_\square$ or Mermin star $\mathcal{I}_\star$ cover of contexts.

Remark 2.3.12. The notion of non-contextuality we use relies on the existence of deterministic value assignments for measurement outcomes, also known as deterministic hidden-variable models. There is a different approach that uses ontological models and a more flexible notion of contextuality, see [61]. For $p = 2$ although the characters b_t do not correspond to possible outcome assignments (Proposition 2.2.7) a non-negative W_ρ can be regarded as a distribution over the "ontic space" $\{ b_t \mid t \in V \}$.

2.4 Classifying space for contextuality

In [63] a topological approach is introduced to study contextuality in quantum mechanics. The essential ideal is that contexts can be regarded as geometric simplices, and glued to each other to form a topological space. Strong contextuality is shown to be detected by the cohomology class $[\beta]$ that lives in the second cohomology group of a certain chain complex. Here we can introduce a space, called the classifying space for contextuality, which realizes this chain complex. The name "classifying space" stems from the fact that the resulting space classifies principal bundles whose transition functions, whenever simultaneously defined, are given by contexts.

In this section we give the construction of the classifying space $B_{\text{cx}}\mathcal{I}$ for a given cover $\mathcal{I}$ of contexts and prove its basic properties. Homotopy theoretic properties of this space are independently studied in [72]. We recall these properties and show how to use them in contextuality. A crucial feature of $B_{\text{cx}}\mathcal{I}$ is that the higher homotopy groups are non-trivial in contrast to the usual classifying space of a finite group. In the next section we will interpret the results of the previous section (§2.3) on Wigner functions in terms of the (twisted) topological K-theory of $B_{\mathrm{cx}}\mathcal{I}$.

2.4.1 Construction of the space

Let $\mathcal{I} \subset \mathcal{I}(V)$ be a cover of contexts. We will construct a space out of this cover. For this the language of simplicial sets, a generalization of simplicial complexes, is most suitable. A simplicial set consists of a sequence of sets $X_0, X_1, \cdots$ indexed by natural numbers together with face and degeneracy maps, see [79]. Each set X_n is referred to as the set of n-simplices. Face maps reduce the dimension $d_i : X_n \to X_{n-1}$, whereas the degeneracy maps increase the dimension $s_j : X_n \to X_{n+1}$. This structure is enough to obtain a topological space, and the procedure is called the geometric realization

$$|X_\bullet| = \coprod_{n\geq 0} X_n \times \Delta^n / \sim$$

where the identification $\sim$ is generated by the face and the degeneracy maps. In effect, each combinatorial n-simplex is replaced by the topological simplex

$$\Delta^n = \{\, (t_0, \cdots, t_n) \in \mathbb{R}^{n+1} \mid \sum_{i=0}^{n} t_i = 1, \;\; t_i \geq 0 \,\}$$

and glued to each other using the face and the degeneracy maps.

The standard example of a simplicial set is the nerve of a category. A (small) category comes with a set of objects and a set of morphisms. Let $\mathbf{C}$ be a category. The nerve of $\mathbf{C}$ is the simplicial set whose set of n-simplices consists of composable arrows of the form

$$A_0 \to \cdots \to A_n.$$

We denote the nerve by $N(\mathbf{C})$. Face maps correspond to composing two adjacent morphisms, and degeneracy maps are given by inserting an identity morphism.

Definition 2.4.1. The classifying space for contextuality, denoted by $B_{\mathrm{cx}}(\mathcal{I})$, is the geometric realization of the simplicial set $B_{\mathrm{cx}}(\mathcal{I})_\bullet$ whose set of n-simplices is given by

$$B_{\mathrm{cx}}(\mathcal{I})_n = \{\, (v_1, v_2, \cdots, v_n) \mid \; v_i \in I, \; 1 \leq i \leq n, \; \text{for some } I \in \mathcal{I} \,\}$$

with the simplicial structure maps

$$d_i(v_1, \cdots, v_n) = \begin{cases} (v_2, \cdots, v_n) & i = 0 \\ ((v_1, \cdots, v_i + v_{i+1}, \cdots, v_n)) & 0 < i < n \\ (v_1, \cdots, v_{n-1}) & i = n \end{cases}$$

and $s_i(v_1, \cdots, v_n) = (v_1, \cdots, v_{i-1}, 0, v_i, \cdots, v_n)$ for $0 \leq i \leq n$.

Remark 2.4.2. This construction is analogous to a construction introduced in [68]. For a group G one can construct a classifying space $B_{\text{com}}(G)$ for commutativity. When G is abelian the construction recovers the usual classifying space BG. A similar definition works for an arbitrary collection $\mathcal{F}$ of subgroups of G which is closed under taking intersections. We can define a space from the set of n-tuple of elements which belong to a subgroup in $\mathcal{F}$. Taking $\mathcal{F}$ to be the collection of all abelian subgroups of G gives $B_{\text{com}}(G)$. Homotopy theoretic properties of these spaces are studied in [70–72].

Note that the construction is a variation of the standard construction of a classifying space for a group. The set of n-simplices of $B_{\text{cx}}(\mathcal{I})$ are contained in the set of n-simplices, which is given by the n-fold direct product V^n, of the classifying space BV. The simplicial structure of BV is defined similarly. We denote the inclusion map by

$$\iota : B_{\text{cx}}(\mathcal{I}) \to BV.$$

Remark 2.4.3. The name "classifying space" refers to the fact that BG classifies principal G-bundles [80]. More precisely, given a CW-complex X the set $[X, BG]$ of homotopy classes of maps is in one-to-one correspondence with the set of isomorphism classes of principal G-bundles over X. Similarly $B_{\text{com}}G$ is a classifying space for certain types of principal bundles. These bundles have the property that the transition functions commute whenever simultaneously defined [69]. A similar conclusion can be made for $B_{\text{cx}}\mathcal{I}$. This space classifies principal V-bundles whose transition functions, whenever simultaneously defined, specifies a context. We denote the equivalence classes of such bundles by $\text{Prin}_{\text{cx}}^V(X)$.

2.4.2 Homotopy theory

The space $B_{\text{cx}}\mathcal{I}$ is studied in [72]. Formally, there is a structural similarity to the space $B_{\text{com}}G$ (see 2.4.2), which has been studied in [70, 71], and most of the tools developed there also applies to $B_{\text{cx}}\mathcal{I}$. We sketch the relevant homotopical properties whose proofs can be found in these papers.

By construction $B_{\mathrm{cx}}(\mathcal{I})$ can be expressed as the union of classifying spaces

$$B_{\mathrm{cx}}(\mathcal{I}) = \bigcup_{I \in \mathcal{I}} BI.$$

This can be seen from the description of n-simplices. We can also think of the union as a colimit in the category of spaces. To study homotopy theoretic properties the union is usually replaced by a homotopy colimit [81]—a gluing process that has nice homotopical properties. We can define a functor $B : \mathcal{I} \to \mathbf{Top}$ that sends I to the classifying space BI. There is a natural map

$$\operatorname*{hocolim}_{\mathcal{I}} B \to B_{\mathrm{cx}}(\mathcal{I})$$

which turns out to be a homotopy equivalence, see [70]. This approach also helps us to compute cohomology of the space by using a spectral sequence. Cohomology (or even generalized cohomology) of a homotopy colimit can be computed using a spectral sequence.

Another benefit that we gain by switching to homotopy colimits is a formula for the fundamental group

$$\pi_1(B_{\mathrm{cx}}\mathcal{I}) = \langle e_v,\ v \in \Sigma |\ e_v e_{v'} = e_{v+v'} \ \text{ if } \{ v, v' \} \subset I \text{ for some } I \in \mathcal{I} \rangle. \tag{2.11}$$

We will denote the fundamental group by $\pi(\mathcal{I})$, or just by π if the context is understood. Note that each isotropic subspace $I \in \mathcal{I}$ can be regarded as a subgroup of π by sending an element u to the corresponding generator e_u. Indeed, there is a set map $\Sigma \to \pi$. Moreover, this map induces a map of spaces

$$\varphi : B_{\mathrm{cx}}\mathcal{I} \to B\pi$$

that is defined by sending an n-simplex $(v_1, \cdots, v_n)$ to the tuple $(e_{v_1}, \cdots, e_{v_n})$. It is an interesting fact that φ is not a homotopy equivalence in general. In other words, the higher homotopy groups $\pi_i(B_{\mathrm{cx}}\mathcal{I})$, $i \geq 2$, can be non-trivial in contrast to $B\pi$ whose homotopy groups are zero except $\pi_1(B\pi) = \pi$.

Example 2.4.4. Let us explain the simplest case of $n = 1$. Let $X \vee Y$ denote the wedge sum of the spaces X and Y at a specified basepoint. The homotopy colimit decomposition for $n = 1$ is simply given by

$$B_{\mathrm{cx}}\mathcal{I}(V) \simeq \bigvee^{r_p} B\mathbb{Z}/p.$$

where $r_p = (p^{2n} - 1)/(p - 1)$ is the number of maximal isotropic subspaces.

From the homotopical point of view all the information about the higher homotopy groups is hidden in the homotopy fiber of φ. It turns out that the homotopy fiber has a very concrete description in terms of a combinatorial object called the coset poset.

2.4.3 Coset poset

We introduce this space for an arbitrary group G.

Definition 2.4.5. For a collection of subgroups $\mathcal{F}$ of G we define the poset

$$C_G(\mathcal{F}) = \{\, gA \mid \ A \in \mathcal{F}, \ \ g \in G\,\}$$

ordered by the inclusion relation.

We usually identify the poset with the associated space given by the geometric realization of its nerve. Our convention for the morphisms of the category associated to a poset $\mathcal{P}$ is that we write $A \to B$ if $A \leq B$. The associated space has n-simplices given by composable morphisms $A_1 \to \cdots \to A_n$.

Given this construction and the fundamental group $\pi(\mathcal{I})$ of $B_{\mathrm{cx}}(\mathcal{I})$ we can describe the homotopy fiber of φ. Each subspace in the context $\mathcal{I}$ can be regarded as subgroup of π thus we can construct the coset poset $C_\pi(\mathcal{I})$.

Theorem 2.4.6. *[72] (OS 2019) Consider $\mathcal{I} = \mathcal{I}(V)$ where $V = (\mathbb{Z}/p)^{2n}$ and $n \geq 2$. The fundamental group $\pi_1(B_{cx}\mathcal{I})$ is given by the central extension associated to the cocycle $\mathfrak{b}$*

$$\pi \cong V \times_{\mathfrak{b}} \mathbb{Z}/p$$

and the higher homotopy groups are given by

$$\pi_i(B_{cx}\mathcal{I}) \cong \pi_i\Big(\bigvee^{d(p,n)} S^n\Big)$$

for all $i \geq 2$, where the number of spheres is given by the formula

$$d(p,n) = (-1)^{r+1} + p^{2r+1+r^2} + \sum_{j=1}^{r} (-1)^j p^{2r+1-j+(r-j)^2} \left(\prod_{t=0}^{j-1} \frac{p^{2r-t} - p^t}{p^j - p^t} \right)$$

Remark 2.4.7. We will see some applications of this result. However, we do not know of an interpretation for the numbers $d(p,n)$. This number gives information about the global structure of the classifying space for contextuality. Interpreted in terms of principal bundles we have

$$\mathrm{Prin}^V_{\mathrm{cx}}(S^n) = \mathbb{Z}^{d(p,n)}$$

where we used the notation of Remark 2.4.3. On the other hand, The set $\mathrm{Prin}^V(S^n)$ of equivalence classes of ordinary principal bundles over the n-sphere, $n \geq 2$, has a single element given by the trivial bundle.

Remark 2.4.8. A better way to rephrase Theorem 2.4.6 is to say that for $n \geq 2$ there is a fibration sequence

$$\bigvee^{d(p,n)} S^n \to B_{\mathrm{cx}}(\mathcal{I}) \xrightarrow{\varphi} B\pi. \tag{2.12}$$

To see that the fiber is a wedge of spheres we refer the readers to the general methodology of [70],[72]. Moreover, the group π turns out to be

$$V \times_{\mathfrak{b}} \mathbb{Z}/p \cong \begin{cases} V \times \mathbb{Z}/2 & p = 2 \\ P_n & p > 2 \end{cases}$$

as a consequence of the presentation given in 2.11.

2.4.4 Cohomology revisited

Having the homotopical description of $B_{\mathrm{cx}}(\mathcal{I})$ we can improve our statements about cohomology. The first application is to determine the extra factor in $H^1(B_{\mathrm{cx}}\mathcal{I})$ when $p = 2$.

Corollary 2.4.9. *Assume $n \geq 2$. There is an isomorphism*

$$H^1(B_{cx}\mathcal{I}) \cong \begin{cases} (V \times \mathbb{Z}/2)^* & p = 2 \\ V^* & p > 2 \end{cases}$$

where $(-)^*$ stands for the dual vector space.

Proof. This follows form the description of the fundamental group π, and the standard fact that for a connected space X the first homology group is the abelianization of the fundamental group [82]. □

The Serre spectral sequence [82] of the fibration 2.12 gives us an isomorphism

$$\varphi^* : H^i(B\pi) \to H^i(B_{\mathrm{cx}}\mathcal{I})$$

in degrees $i \leq n-1$ and an injection in degree $i = n$. When $p = 2$ we have $\pi = V \times \mathbb{Z}/2$ as observed in Remark 2.4.8, so its cohomology is easy to describe. Fixing the basis $\{ x_i, z_i \mid 1 \leq i \leq n \} \cup \{ x_0 \}$ for $V \times \mathbb{Z}/2$ the cohomology ring is given by the polynomial ring

$$H^*(B\pi) = \mathbb{F}_2[x_0^*, x_1^*, \cdots, x_n^*, z_1^*, \cdots, z_n^*].$$

Let us define a homomorphism

$$q : \pi \to V \times \mathbb{Z}/2 \quad (v, t) \mapsto (v, t + \mathfrak{q}(v))$$

which turns out to be an isomorphism of groups. Now consider the composite map of spaces

$$\hat{q} : B_{\text{cx}}\mathcal{I} \xrightarrow{\varphi} B\pi \xrightarrow{Bq} B(V \times \mathbb{Z}/2)$$

As a consequence Corollary (2.4.9) we have:

Corollary 2.4.10. *The cohomology class* $[\beta] \in H^2(B_{cx}\mathcal{I})$ *is the image of*

$$Q = x_0^* + \sum_{i=1}^{n} x_i^* \cup z_i^* \quad \in H^2(B(V \times \mathbb{Z}/2))$$

under the map $H^*(B(V \times \mathbb{Z}/2)) \to H^*(B_{cx}\mathcal{I})$ *induced by* $\hat{q}$.

2.5 Contextuality and twisted K-theory

The goal of this section is to compute the β-twisted K-theory of $B_{\text{cx}}\mathcal{I}$. The idea follows the computation of the topological K-theory of $B_{\text{com}}G$ given in [70]. We refer to this paper for the details of the constructions involved. Another reference that is useful for the homotopical properties of this space is [72]. The computation will bridge a connection to the representation theoretic description of the Wigner function given in §2.3. This will allow us to interpret the Wigner function as a class $[W_\rho]$ in the β-twisted K-theory of $B_{\text{cx}}\mathcal{I}(V)$ after extending the coefficients to $\mathbb{R}$.

Remark 2.5.1. Another form of K-theory, namely operator K-theory, has been used in the study of contextuality by De Silva and Barbosa [83]. Therein the authors relate operator K-theory to topological K-theory via the Gelfand spectrum. However, there seems to be no direct connection to the way K-theory appears in the present work.

2.5.1 Sketch of the computation

Before embarking in the details, let us first summarize the idea of the proof. As an element of the inverse limit of $\mathbb{R} \otimes R_\beta$ the Wigner function is a sum

$$W_\rho = \sum_{v \in V} W_\rho(v)\, b_v$$

of 1-dimensional irreducible representations of the group V. Such a sum is usually referred to as a "virtual" sum when the coefficients assume negative values. In this section we will explain a chain of ideas, due to Atiyah and Segal, that will allow us to pass from twisted representations to twisted K-theory. This is given by the "completion" of the representation group in the sense that Cauchy sequences are convergent in the resulting completed module. In the space level the completion process corresponds to a construction known as the Borel construction. Let G be a group and let $EG \to BG$ denote the universal principal G-bundle [48, Chapter II]. For a space X with an action of G the Borel construction is defined to be the space

$$EG \times_G X = (EG \times X)/G$$

obtained as the quotient under the diagonal action. The Atiyah–Segal completion theorem [84] says that the topological K-theory group $K(EG \times_G X)$ is the completion of the equivariant K-theory group $K_G(X)$. The equivariant K-theory group is a generalization of the representation group. When X is a point with the trivial G-action then $K_G(X) = R(G)$. All of this is also true in the twisted setting [85]. We are only interested in twisting by the cocycle β.

In our case we take X to be the coset poset $\mathcal{C}_\pi\mathcal{I}$ with the action of π given by left multiplication on the cosets. The Borel construction gives us $B_{\mathrm{cx}}\mathcal{I}$, as shown in [72]. Therefore by the Atiyah–Segal completion theorem twisted K-theory of $B_{\mathrm{cx}}\mathcal{I}$ is the completion of the twisted equivariant K-theory of the coset poset. There are two steps of the computation

- After extending the coefficients to $\mathbb{R}$ we show that $K_\pi^\beta(\mathcal{C}_\pi\mathcal{I})$ is equal to the inverse limit of $\mathbb{R} \otimes R_\beta$. Thus W_ρ belongs to the β-twisted equivariant K-theory group.

- Completing $K_\pi^\beta(\mathcal{C}_\pi\mathcal{I})$ we obtain $K^\beta(B_{\mathrm{cx}}\mathcal{I})$ and after extending coefficients to $\mathbb{R}$ we conclude that the Wigner function can be regarded as a class $[W_\rho]$ in the β-twisted K-theory group.

2.5.2 Twisted equivariant K-theory

We can twist the equivariant K-theory groups by the cohomology class $[\beta] \in H^2(B_{\text{cx}}\mathcal{I}(V))$. Recall that $[\beta] = 0$ when p is odd. Thus in this case the twisting disappears. For $p = 2$ we observed in Corollary 2.4.10 that $[\beta]$ comes from a class in $H^2(B\pi, \mathbb{Z}/2)$. We will treat the two cases in a uniform way. Therefore we think of $[\beta]$ as living in $H^2(B\pi, \mathbb{Z}/p)$ given by the class Q when $p = 2$, and understood to be zero when $p > 2$. We assume $n \geq 2$ so that π is a finite group (Remark 2.4.8). The case $n = 1$ can be computed directly, and we defer this case to the proof of Theorem 2.5.4.

As observed in [76] twisted equivariant K-group can be obtained from the untwisted version. To see this let us consider the group extension

$$0 \to \mathbb{Z}/p \to \pi_\beta \to \pi \to 0$$

corresponding to $[\beta]$. Note that the coset poset $C_\pi \mathcal{I}$ can be regarded as a π_β-space via the quotient homomorphism $\pi_\beta \to \pi$. Irreducible represention of $\mathbb{Z}/p$ consist of the homomorphisms $\omega^j : \mathbb{Z}/p \to U(1)$ sending the additive generator 1 to the element ω^j where $0 \leq j \leq p-1$. Then we have

$$K^*_{\pi_\beta}(C_\pi \mathcal{I}) = \bigoplus_{j=0}^{p-1} K^*_{\pi_\beta}(C_\pi \mathcal{I})(\omega^j) \tag{2.13}$$

where the factors correspond to equivariant bundles on which $\mathbb{Z}/p$ acts by the specified representation. We can identify the twisted equivariant groups $K_\pi^{\beta+*}(C_\pi \mathcal{I})$ with the factor corresponding to the $j = 1$ representation:

$$K_\pi^{\beta+*}(C_\pi \mathcal{I}) = K^*_{\pi_\beta}(C_\pi \mathcal{I})(\omega).$$

Note that this representation corresponds to the usual embedding $\mathbb{Z}/p \subset U(1)$.

Equivariant K-theory of the coset poset can be computed using the methods of [70]. The main tool is a spectral sequence that can be applied to homotopy colimit decompositions. As shown in [72] the coset poset is the homotopy colimit of the functor $\pi/- : \mathcal{I} \to \mathbf{Top}$ which sends I to the coset π/I regarded as a discrete space. Furthermore, as a consequence of 2.13 the spectral sequence decomposes and we can use it to compute the twisted equivariant K-groups. Therefore the results for the twisted version are essentially obtained in the same way as the untwisted case.

Before discussing the spectral sequence we need a construction that extends the construction of the inverse limit of a functor. Let $F : \mathcal{I}^{\text{op}} \to \mathbf{Ab}$

be a functor that takes values in the category of abelian groups. One can construct a cochain complex $C^*(\mathcal{I}, F)$ which is indexed over the n-simplices of the nerve of the poset $\mathcal{I}$:

$$C^n(\mathcal{I}, F) = \bigoplus_{A_1 \to \cdots \to A_n} F(A_1)$$

and the boundary map comes from the simplicial structure of the nerve of $\mathcal{I}$. The cohomology group $H^i(\mathcal{I}, F)$ gives the i-th derived functor of the inverse limit of F. Note that $H^0(\mathcal{I}, F)$ is canonically isomorphic to the inverse limit of F. We can also think of the groups $H^i(\mathcal{I}, F)$ as the Čech cohomology groups of the presheaf F with respect to the cover $\mathcal{I}$.

For homotopy colimits we can use the (equivariant) Bousfield-Kan spectral sequence—the spectral sequence used in [70] for the untwisted case. As a consequence of the direct sum decomposition in 2.13 the spectral sequence decomposes:

$$E_2^{i,j} = H^i(\mathcal{I}, K_\pi^{\beta+j}(\pi/-)) \Longrightarrow K_\pi^{\beta+*}(C_\pi \mathcal{I}).$$

The functor $K_\pi^{\beta+j}(\pi/-)$ can be identified with the β-twisted representation group functor $R_\beta : \mathcal{I}^{\mathrm{op}} \to \mathbf{Ab}$ for j even and it is zero otherwise. This is the key connection to §2.3.

Remark 2.5.2. We would like to remind that $[\beta] = 0$ for the odd prime case (Remark 2.3.2). Therefore the twisting disappears in this case, and we are dealing with untwisted K-groups.

We are interested in understanding the spectral sequence after tensoring with $\mathbb{R}$. The following serves to this purpose.

Lemma 2.5.3. *The derived limit functor $H^i(\mathcal{I}, R_\beta)$ is torsion for $i > 0$.*

Proof. This follows from [70, Theorem 4.7] once we show R_β is a pre-Mackey functor. Restriction and induction of twisted characters provide the necessary structure [76, Theorem 4.2]. □

As a consequence of this result our spectral sequence collapses after tensoring with $\mathbb{R}$. Here we are also using the fact that the spectral sequence is bounded in the i-direction—all the terms vanish for sufficiently large i. For $i > 0$ the terms $\mathbb{R} \otimes E_2^{i,j}$ are zero since $E_2^{i,j}$ are torsion as proved above. When $i = 0$ and j even we have $\mathbb{R} \otimes E_2^{0,j} = H^0(\mathcal{I}, \mathbb{R} \otimes R_\beta)$, and for j odd $\mathbb{R} \otimes E_2^{0,j} = 0$. Recall that $H^0(\mathcal{I}, \mathbb{R} \otimes R_\beta)$ can be identified with the inverse limit of the functor $\mathbb{R} \otimes R_\beta$. For $\mathcal{I} = \mathcal{I}(V)$ we have computed this inverse limit in Proposition 2.3.5. Thus we obtain

$$\mathbb{R} \otimes K_\pi^{\beta+i}(C_\pi \mathcal{I}) \cong \begin{cases} \mathbb{R} \otimes R(V) & i = 0 \\ 0 & i = 1. \end{cases} \tag{2.14}$$

Therefore we can take the target of the function W in 2.10, that sends a state ρ to the Wigner function W_ρ, to be the twisted equivariant K-theory group:

$$W : \mathrm{Den}(\mathcal{H}) \to \mathbb{R} \otimes K_\pi^\beta(C_\pi \mathcal{I}(V)). \tag{2.15}$$

We can express this by saying that a state ρ can be interpreted as a probabilistic combination of π-equivariant β-twisted vector bundles over $C_\pi \mathcal{I}$. Our next goal is to relate this to the twisted K-theory of the classifying space for contextuality.

2.5.3 Twisted K-theory

The twisted version [85] of Atiyah-Segal completion theorem gives an isomorphism

$$K^{\beta+*}(B_{\mathrm{cx}}\mathcal{I}) \cong K_\pi^{\beta+*}(C_\pi \mathcal{I})^\wedge$$

where $(-)^\wedge$ means completion with respect to the augmentation ideal $I(\pi)$. The augmentation ideal is defined to be the kernel of the homomorphism $R(\pi) \to \mathbb{Z}$ which sends a representation to its dimension.

Let us explain the completion process. First of all $K_\pi^{\beta+*}(C_\pi \mathcal{I})$ is a module over the representation ring $R(\pi)$. This is the case since $K_{\pi_\beta}^*(C_\pi \mathcal{I})$ is a module over the ring $R(\pi_\beta)$ via the map $C_\pi \mathcal{I} \to *$ which contracts the coset poset to a point, and using the ring map $R(\pi) \to R(\pi_\beta)$ induced by the quotient homomorphism we see that the β-twisted K-group is a module over $R(\pi)$. Then the completion can be computed by tensoring with the completion of $R(\pi)$:

$$K_\pi^{\beta+*}(C_\pi \mathcal{I})^\wedge \cong K_\pi^{\beta+*}(C_\pi \mathcal{I}) \otimes_{R(\pi)} R(\pi)^\wedge.$$

Therefore it suffices to understand the completion of $R(\pi)$. Recall from Remark 2.4.8 that π is a p-group. It is well-known that for p-groups completion of the representation ring turns out to be essentially tensoring with the p-adic numbers $\mathbb{Z}_p$:

$$R(\pi)^\wedge \cong \mathbb{Z} \oplus (\mathbb{Z}_p \otimes I(\pi)).$$

Theorem 2.5.4. *(OS 2019) There is an isomorphism*

$$\mathbb{R} \otimes K^{\beta+i}(B_{cx}\mathcal{I}(V)) \cong \begin{cases} \mathbb{R} \oplus \left(\mathbb{R} \otimes \mathbb{Z}_p^{|V|-1}\right) & i = 0 \\ 0 & i = 1. \end{cases}$$

Proof. The proof follows the proof of the untwisted version in [70, Theorem 5.2]. For $n = 1$ the result is a direct consequence of the decomposition in Example 2.4.4. Assume $n \geq 2$. The order of completion and tensoring with $\mathbb{R}$ matters. We first complete then tensor with $\mathbb{R}$. Lemma 2.5.3 says that for $i > 0$ the groups $E_2^{i,j}$ are torsion. Under the completion process, which is essentially tensoring with $\mathbb{Z}_p$, these groups do not change. After tensoring with $\mathbb{R}$ they disappear. Therefore we focus on $i = 0$ part. Completion of $H^0(\mathcal{I}, R_\beta)$ gives us $\mathbb{Z} \oplus \mathbb{Z}_p^{|V|-1}$ (see Remark 2.3.6). Finally tensoring with $\mathbb{R}$ gives the desired result. □

As a consequence of this result we can think of the W map as landing inside twisted K-theory

$$W : \mathrm{Den}(\mathcal{H}) \to \mathbb{R} \otimes K^\beta(B_{\mathrm{cx}}\mathcal{I}(V)).$$

Note that the completion map

$$K_\pi^\beta(C_\pi\mathcal{I}(V)) \to K^\beta(B_{\mathrm{cx}}\mathcal{I}(V))$$

is injective since tensoring with $\mathbb{Z}_p$ is. This means that we do not lose any information during the completion process and can identify the Wigner function W_ρ as a class in the β-twisted K-group.

Chapter 3

Conclusions

3.0.1 On K-theory and Fermi surfaces

For chapter 1 we have rewritten [2] and clarified points, particularly of analysis, such as what was meant by Bulk and Surface states in terms of projections and employed the correct terminology of quasi-adiabatic evolution equivalence relation. We have also argued that the choice of topology for unbounded self-adjoint Fredholm operators which was discussed in [16] to be a red harring. Furthermore we have extended our results to the twisted equivariant case for most crystallographic groups. What remains to be done in future work on the crystallographic side is the computation of these groups $K_P^{\tau-1}(\mathbb{T}^{d-1})$ using an equivariant version of the Atiyah-Hirzebruch spectral sequence and multiplying in there by the class of the twist to take it into account. We also need to extend to the case of non-trivial magnetic point group. On the global symmetry side we must include all the classes in the Altland-Zirnbauer classification that we are missing, which are those with chiral symmetry (classes BDI, CI, CII, DIII). On the analytical side a proper analytical formulation of quasi-adiabaticity, when the systems in question posses a gapped bulk would be an interesting task for analysts.

3.0.2 On K-theory and contextuality

On chapter 2 we have presented the essential parts of [86] to show that adapting the formulation of Abramsky et al [62], which is designed for general resource theories, to the formalism of [63], that is specific to finite dimensional quantum mechanics and observables for quantum computation, leads to reinterpreting any density matrix as a class in the twisted K-group $K^{\beta}(B_{\mathrm{cx}}\mathcal{I}) \otimes \mathbb{R}$. Motivated by this connection to physics we computed it for the case $\mathcal{I} = \mathcal{I}(V)$. Though there is a natural interpretation that relates the algebraic topology of $B_{\mathrm{cx}}\mathcal{I}$ to state-independent contextuality and Wigner functions, we do not as of yet have employed the K-theory interpretation to address a specific physical problem such as state-dependent contextuality. It is vital to continue the search for such an application to consolidate the mathematical relevance of $B_{\mathrm{cx}}\mathcal{I}$ as a unifying object in contextuality for quantum mechanics. Nonetheless from a mathematical point of view, these spaces are interesting as they posses non-trivial higher homotopy, unlike the classifying space which is an Eilenberg-Maclane space. Furthermore one might use this mathematical richness as a motivation to look for new physical phenomena related to these groups. From a mathematical perspective it would be interesting to compute more examples when $\mathcal{I} \neq \mathcal{I}(V)$.

3.0.3 Connections between the two topics

Both chapters employ twisted equivariant K-theory to reinterpret aspects in quantum mechanics (Fermi surfaces on a half crystal and density matrices on finite dimensional Hilbert spaces). However it seems so far that these arise in a very different manner. In the former the context is infinite dimensional Hilbert spaces and it is through the dynamics (the Hamiltonian) which is an unbounded operator and its spectral decomposition, that one arrives at K-theory, without any reference to contexts. On the latter it is through finite dimensional representation theory and the higher dimensional torsion of a spectral sequence that one can reinterpret density matrices as classes in a K-theory group, and no connection to analysis was made nor any reference to dynamics. However a generalization to non-interacting Fermionic topological phases are so called SPT phases [15], [87], [88] these are supposed to be generalizations of topological phases that include short range entanglement. Though a topological theory for them has been presented [87], [88] in terms of invertible topological quantum field theories, these rely on a relativistic field interpretation, which from the physical point of view seems unwarranted given that it requires including extra symmetries (the Poincaré group), though there are a few exceptions[14]. Furthermore this topological construction has not been derived from an analytical point of view as in [16], [17], [33] and the present work. Non the less in the physics literature there are some examples of systems considered to be Bosonic SPT phases which have been shown to have non-trivial quantum computational power [89]. Due to the relation between quantum computation and contextuality, this would suggest that a form of contextuality is hidden in Bosonic SPT phases since it is believed to be the necessary ingredient for non-trivial quantum computation. If such computational power extends to Fermionic SPT phases there should be a connection between quantum contextuality and topological phases or quantum contextuality and topological Fermi surfaces corresponding to Fermionic SPT phases with boundary.

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