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A C*-Algebraic Approach to Topological Phases for Insulators

Tesi di Laurea Magistrale in
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Abstract

Topological insulators are materials with very interesting properties from a physical point of view: they are electrical insulators in the bulk, while on the surface they can be characterised by the presence of robust currents. These properties are characterised by the "topological phase" of the material, i.e. their equivalence class with respect to continuous deformations in a given topology. This means that small external perturbations or microscopic irregularities of the material, which we can consider as "continuous" deformations of the insulator, will not affect the intrinsic physical properties of the phase.

Particular physical symmetries can be considered. Thanks to mathematical tools from operator algebra, it is possible to give a mathematical "structure" to the set of homotopy classes. In this paper I describe and comment with examples a possible classification. This classification is based on a particular approach to K-theory for C^*-algebras: the great advantage, which makes the novelty of the classification, is the ability to give a compact description for all types of symmetry.

Keywords: topological phases, operator algebra, C^*-algebras, K-theory

Abstract in lingua italiana

Gli isolanti topologici sono materiali che presentano proprietà molto interessanti dal punto di vista fisico: sono isolanti elettrici al loro interno, mentre in superficie possono essere caratterizzati dalla presenza di correnti robuste. Queste proprietà sono caratterizzate dalla "fase topologica" del materiale, cioè dalla loro classe di equivalenza rispetto alle deformazioni continue in una data topologia. Questo significa che piccole perturbazioni esterne o irregolarità microscopiche del materiale, che possiamo considerare come deformazioni "continue" dell'isolante, non avranno conseguenze sulle proprietà fisiche intrinseche della fase.

Particolari simmetrie fisiche possono essere considerate. Grazie a strumenti matematici provenienti dall'algebra degli operatori, è possibile dare una "struttura" matematica all'insieme delle classi di omotopia. In questo lavoro descrivo e commento con esempi una possibile classificazione. La classificazione è basata su un particolare approccio alla K-teoria per le C^*-algebre: il grande vantaggio, che rende la classificazione descritta innovativa, è la capacità di dare una descrizione compatta per tutti i tipi di simmetria.

Parole chiave: fasi topologiche, algebra degli operatori, C^*-algebre, K-teoria

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Introduction

This work is the result of a research internship carried out in collaboration with the University of Lyon (France). For me it was the first time I heard about topological insulators and before I had just a vague idea of what "operator algebra" means and what we can do with it. As a consequence, the great majority of the internship was dedicated to learn and familiarise with subjects at the same time from quantum physics and mathematics (in particular from solid physics, abstract algebra and operator theory). For this reason, the first two chapters of this work present a brief review of what I read about, as an introduction to the core of the subject. In the first chapter, I deal with the physics part. We will see the modelling of a simple example of a solid, namely a regular crystal. From quantum physics, we know that a physical system is described by the hamiltonian of the system (that is, by its energy). Even if the physical situation is quite simple, due to the huge number of atoms, several approximations are necessary: I will introduced the "tight binding approximation", which is a kind of spatial discretisation of the system. Then, we will be able to talk about the "band theory", which can help us to understand the difference of behaviour between a conductor and an insulator. Finally, we can introduce "topological insulators", their fundamental properties and what it means to classify them.

In quantum physics, the hamiltonian of a system is usually considered as a linear operator (for us, also bounded) on an Hilbert space. Therefore, an insulator is identified with its hamiltoninan. For some reasons I will explain, we can see hamiltonians in a particular subspace of the bounded linear operators: this subspace is a C^*-algebra. In the second chapter, we will see the definition of C^*-algebra and some of the properties that make it a key object of "operator algebra". The structure of a C^*-algebra can be investigated further thanks to K-theory: after giving a brief review of it, we will also see a particular approach to it (the Van Daele's K-theory), which is the central idea for the approach for the classification of topological insulators presented in the following chapter. Finally, in chapter 3 we enter in the core of the work. Here I present the approach proposed in the paper [5]: the goal of the paper is to classify topological insulators satisfying particular symmetry conditions. Modulo some technicalities (involving among others

Clifford algebras), the approach of Van Daele to K-theory applies *almost* straightforward to topological insulators and the author presents a compact classification.

In chapter 4, I present my part of "research work". I present some examples and exercises which helped me to give a less abstract understanding of the physical and mathematical objects I was dealing with. In particular I present the Haldande model, an example of topological insulator, and I show that it is a non-trivial insulator (we will discuss the concept of triviality). I also prove some results on the gradings and real structures on fundamental C^*-algebras, the key ingredients to talk about symmetries in C^*-algebras: I show which are the possible gradings and real structures and I explain the relation between these examples and the applications.

1 | Physical framework

From our point of view, an insulator is defined abstractly: it is a self-adjoint invertible element of a C^*-algebra. Why does this definition make sense? In quantum mechanics, the behaviour of a material is characterised by its hamiltonian. Moreover, hamiltonians are self-adjoint elements of $\mathcal{L}(H)$, the linear operators on a (separable) Hilbert space H: we identify the concrete material with an operator. For some deep reasons, which we will discuss in the next chapter, we can think the hamiltonian in a smaller subset of $\mathcal{L}(H)$: this choice leads us to see it in a C^*-algebra. We will see that also the property of being an inversible operator has a reasonable physical interpretation.

In this chapter we well review briefly some topics of solid-state physics in order to give a motivation, or at least an intuition, for the previous abstract definition. I will rely on the first three chapters of [2] to recall basic results and concepts (as, for example, the *tight binding approximation*, the Fermi energy or the Bloch theory) coming from physics of electrons in a solid, which are necessary to give a justification for the definition.

At the end of the section, we will discuss what are "topological phases" for insulators. We will see which are the properties of topological insulators and why they are particularly important for us.

1.1. General hamiltonian for a solid

We can simplify a solid as a collection of N_n atomic nuclei (for simplicity all identical) with mass M and electrical charge Ze and N_e electrons with mass m_0. We can then write the hamiltonian for this solid

$$
\begin{aligned}
H = & \frac{1}{2M}\sum_{i=1}^{N_n}\mathbf{P}_i^2 + \frac{1}{2m_0}\sum_{j=1}^{N_e}\mathbf{p}_j^2 \\
& + \frac{Z^2}{2}\sum_{i,j=1,i\neq j}^{N_n} V_c\left(\mathbf{R}_i - \mathbf{R}_j\right) - Z\sum_{i=1}^{N_n}\sum_{j=1}^{N_e} V_c\left(\mathbf{r}_j - \mathbf{R}_i\right) \\
& + \frac{1}{2}\sum_{i,j=1,i\neq j}^{N_e} V_c\left(\mathbf{r}_i - \mathbf{r}_j\right)
\end{aligned}
$$

Where R_i are the positions of the nuclei, r_j the positions of electrons, P_i and p_j are the momentum operators for the nuclei and electrons and the Coulomb potential is given by

$$V_c(\mathbf{r}) = \frac{e^2}{4\pi\epsilon_0|\mathbf{r}|}.$$

As the order of magnitude of atoms in a solid is of 10^{23}, it is impossible to compute a solution for the Schrödinger equation with the previous hamiltonian. An approximation becomes necessary. Then, we consider the following assumptions.

- We can neglect the kinetic energy of nuclei and suppose they are localised at fixed points R_i.
- We consider an average electron-electron interaction (this assumption is justified if the electrons are not too close). Then, we can introduce an "effective potential" V_{at} which sums up the interaction of the electron with one nucleus and all the other electrons.

We get the following approximated hamiltonian

$$
\begin{aligned}
H_e &= \frac{1}{2m_0}\sum_{j=1}^{N_e}\mathbf{p}_j^2 + \sum_{i=1}^{N_n}\sum_{j=1}^{N_e} V_{at}\left(\mathbf{r}_j - \mathbf{R}_i\right) \\
&= \sum_{j=1}^{N_e}\left[\frac{\mathbf{p}_j^2}{2m_0} + \sum_{i=1}^{N_n} V_{at}\left(\mathbf{r}_j - \mathbf{R}_i\right)\right] = \sum_{j=1}^{N_e} H_j
\end{aligned}
$$

This hamiltonian is separable. It is enough to study the hamiltoninan for one electron

$$H_1 = \frac{\mathbf{p}^2}{2m_0} + \sum_{l=1}^{N_n} V_{at}\left(\mathbf{r} - \mathbf{R}_l\right).$$

If $\psi_k(\mathrm{r})$ is a eigenvector of H_1 for the energy E_k, we can easily find an eigenvector Ψ for

H_e with respect to the energy E

$$\Psi\left(\mathrm{r}_1, \mathrm{r}_2, \ldots, \mathrm{r}_{N_e}\right) = \psi_{k_1}\left(\mathrm{r}_1\right)\psi_{k_2}\left(\mathrm{r}_2\right)\ldots\psi_{k_{N_e}}\left(\mathrm{r}_{N_e}\right),$$

$$E = \sum_{i=1}^{N_e} E_{k_i}.$$

However, we must satisfy the anti-symmetric condition for fermions given by the Pauli principle: as a consequence, we look for a linear combination of vector of the previous form which satisfies this constraint. Therefore, we get the following eigenvector (written using the so-called Slater determinant)

$$\Psi\left(\mathrm{r}_1, \mathrm{r}_2, \ldots, \mathrm{r}_{N_e}\right) = \frac{1}{\sqrt{N_e!}}\begin{vmatrix} \psi_{k_1}\left(\mathrm{r}_1\right) & \psi_{k_1}\left(\mathrm{r}_2\right) & \cdot & \cdot \\ \psi_{k_2}\left(\mathrm{r}_1\right) & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \psi_{k_{N_e-1}}\left(\mathrm{r}_{N_e}\right) \\ \psi_{k_{N_e}}\left(\mathrm{r}_1\right) & \cdot & \psi_{k_{N_e}}\left(\mathrm{r}_{N_e-1}\right) & \psi_{k_{N_e}}\left(\mathrm{r}_{N_e}\right) \end{vmatrix}$$

1.2. Tight binding approximation

In the "tight binding" approximation we consider a further assumption: the electrons are strongly bounded to the nuclei. We first consider the Schrödinger equation for an atom

$$\left[\frac{\mathrm{p}^2}{2m_0} + V_{at}(\mathrm{r})\right]\chi_n(\mathrm{r}) = E_n\chi_n(\mathrm{r})$$

where V_{at} is the potential of a neutral atom where the eigenstate of lowest energy $E_1, E_2 ...$ $E_n ... E_v$ are occupied by Z electrons. We want to study the last energy state χ_v of the solid with energy E_v.
$\{\chi_v\left(\mathrm{r} - \mathrm{R}_n\right)\}_n$ are the eigenfunctions corresponding to the potential centred in each site R_n. In the "tight binding" approximation, we do the hypothesis that we can write $\psi_k\left(\mathrm{r}\right)$ as a linear combination of the orbitals $\chi_v\left(\mathrm{r} - \mathrm{R}_n\right)$. If we note $|\mathbf{R}_l\rangle$ the state associated to the orbital $\chi_v\left(\mathrm{r} - \mathrm{R}_l\right)$, we get

$$|\psi_k\rangle = \frac{1}{\sqrt{N_n}}\sum_{l=1}^{N_n} a_{k,l}\,|\mathbf{R}_l\rangle$$

We also assume that $|\mathbf{R}_l\rangle$ form an orthonormal set. We define

$$V_l(\mathbf{r}) = \sum_{m=1, m\neq l}^{N_n} V_{at}\left(\mathbf{r} - \mathbf{R}_m\right)$$

and the **transfer integrals**

$$-t_{n,l} = \langle \mathbf{R}_n \left| V_l(\mathrm{r}) \right| \mathbf{R}_l \rangle$$

We get the equation

$$-\sum_{l=1}^{N_n} t_{n,l} a_{k,l} = (E_k - E_v)\, a_{k,n}$$

There is a non zero solution if $E_k - E_v$ is an eigenvalue of the matrix with elements $-t_{n,l}$: the problem is reduced to the computation of the solution of a linear system.

1.3. 1D chain of atoms

We can apply the previous approximation to a simple, but instructive, example. We consider a 1D chain of N_n atoms where a is the distance between them (see figure 1.1).

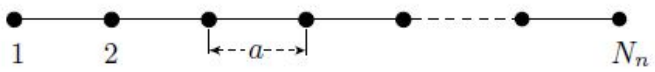


Figure 1.1: 1D chain of atoms.

We consider periodic conditions on the (finite) linear chain, i.e. we impose the condition

$$a_{k,n+N_n} = a_{k,n}$$

Thanks to the periodicity of V_{at} and the properties of χ_v, $t_{n,l}$ depends only on the difference $|n-l|$

$$t_{n,l} = t_{|n-l|}.$$

Moreover, as the translation operator commutes with the hamiltonian (the potential is translation invariant), we can apply Bloch's theorem. ψ_k has the form

$$\psi_k(x) = \mathrm{e}^{\mathrm{i}kx} u_k(x) \quad \text{where} \quad u_k(x+a) = u_k(x)$$

All previous considerations lead to a condition on k and we have

$$k = \frac{2\pi m}{N_n a}, \quad m \text{ integer}$$

Furthermore, thanks to the exponential decay with the distance of χ_v, we can assume

that $t_n = 0$ if $|n| > 1$ and we get a formula for the eigenvalues E_k

$$E_k = E_v - t_0 - 2t_1 \cos ka$$

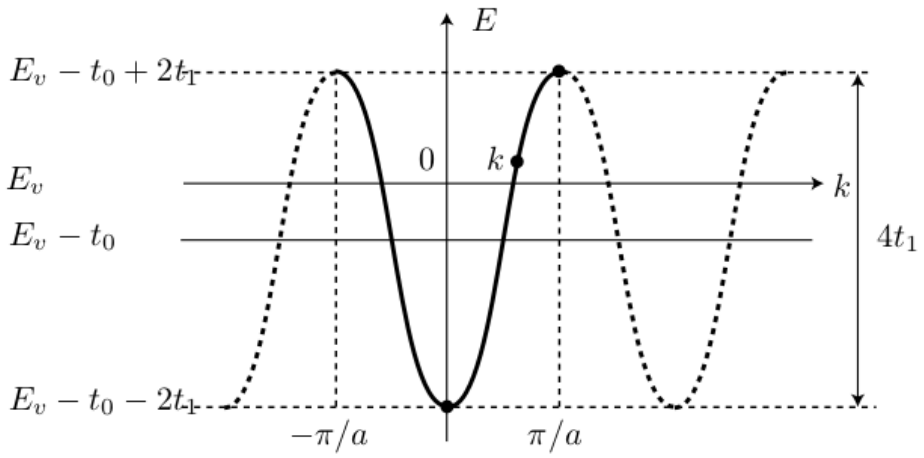


Figure 1.2: Tight binding approximation: energy band of the valence level for the 1D atom chain.

The interval $-\frac{\pi}{a} < k \leq \frac{\pi}{a}$ is called **first Brillouin zone**. In 1.2 we observe the existence of a band of permitted energies. We could also consider deeper energy levels, but in this case the electrons are more strongly bounded to the nucleus and the energy bands are much narrower than in the previous case: therefore, we can "forget" about them.

In the previous situation we observed just one band of energy, but it is not always the case. For example, we can consider the case in which the electrons are almost unbounded and the tight binding approximation does not hold. Now, we observe that the crystalline potential can be viewed as a perturbation. With the help of the perturbation theory (see [3] chapter 9) we get the energy bands represented in figure 1.3. We observe several bands of energy and, between them, some "gaps" in the spectrum: there are bands of forbidden energy.

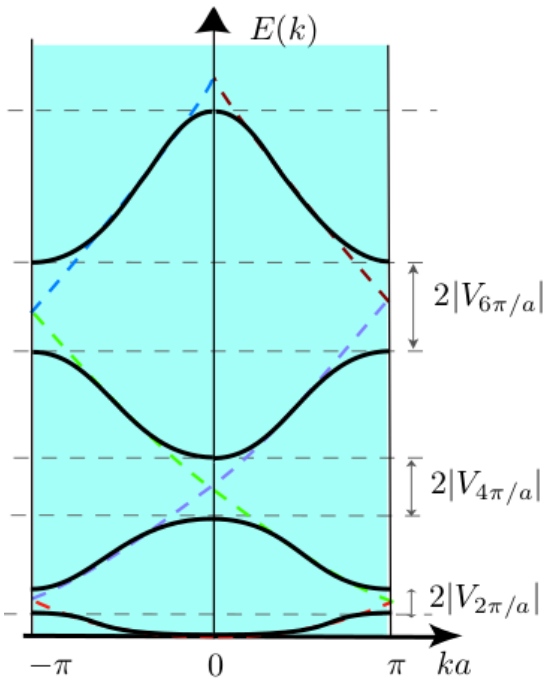


Figure 1.3: Almost free electrons.

1.4. Conductors and insulators

We can now give an explanation for a different behaviour of conductors and insulators.

If we consider the energy bands in the spectrum of a solid, we can imagine to fill a band with electrons coming from the most external atomic orbital of each atom: thanks to the Pauli principle, the electrons (which are fermions) cannot be in the same state and they will dispose themselves in states corresponding to increasing energy. We call **Fermi energy** the energy of the last electron added at $0K$ temperature. Two situations can occur. The last band of the solid containing electrons could be not completely full (see 1.4), i.e. the Fermi energy belongs to the spectrum. In this case, with an arbitrarily small amount of energy an electron can be excited in the band: the material is a conductor!

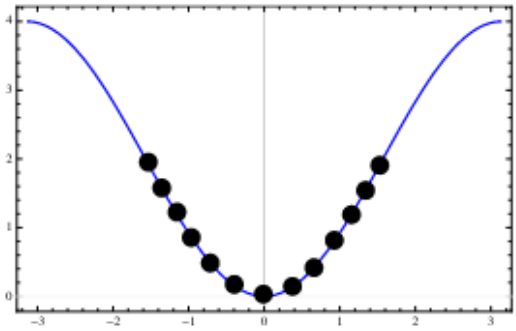


Figure 1.4: Energy band partially filled.

On the other hand, if the last band is full (see 1.5), a new electron must absorb enough energy to achieve the following empty band. The Fermi energy does not belong to the spectrum and the material is an insulator. At the beginning, we said that an insulator is an invertible element: indeed, by means of a translation of a real quantity of the spectrum of the insulator's hamiltonian, we can consider the Fermi energy at 0 and therefore, it is invertible.

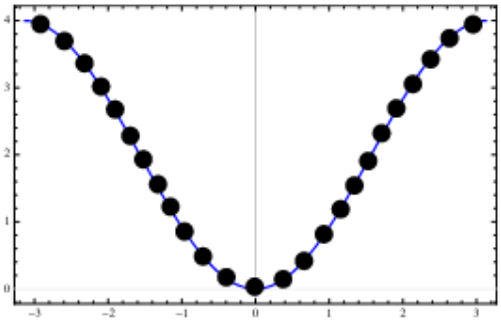


Figure 1.5: Full energy band.

1.5. Topological insulators

Given a physical situation, our goal is to classify the insulators, i.e. we want to put in the same class hamiltonians which preserve some fundamental characteristics of the solid, as for example symmetry conditions, locality of the operator or the spatial structure. We say that two insulators belong to the same class (the same topological phase) if we can find an homotopy (a continuous path with respect to a chosen topology) between them which does not close the gap; moreover, if we impose one or more symmetry conditions, the continuous path must respect the symmetry too. The very delicate aspect is to choose in which topological space hamiltonians live. This definition is reasonable because we can

look at the homotopy as a sequence of small perturbations (inevitable in the real world) of the hamiltonian and we are interested in physical phenomena which are stable to the perturbation and which we can see as an intrinsic feature of the topological phase. For these phenomena, we will be able to measure with great precision the quantities associated to them: this fact could have important application in technology (see [7], [12]).

One of the first examples of topological insulator was found experimentally in 1980, when the *quantum Hall* (QH) effect was discovered. The QH state provided the first example of a quantum state which is topologically distinct from all states of matter known before. We describe briefly the QH effect. We consider a two-dimensional electron gas at a very low temperature ($T < 4K$) subject to a strong perpendicular magnetic field ($B \sim \mathcal{O}(T)$). By applying a constant electric field $\mathbf{E}$, a constant current density $\mathbf{J}$ emerges. $\mathbf{E}$ and $\mathbf{J}$ are related by the conductivity σ.

$$\mathbf{J} = \sigma \mathbf{E}$$

where

$$\sigma = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ -\sigma_{xy} & -\sigma_{yy} \end{pmatrix}$$

The resistivity matrix ρ is simply the inverse of σ. Experimentally, we observe that the bulk of the sample is insulating and the electric current is carried only along the edge of the sample. Moreover, we observe a peculiar behaviour of the quantity ρ_{xy}: it is quantised (see figure 1.6) and given by

$$\rho_{xy} = \frac{2\pi\hbar}{e^2}\frac{1}{\nu}, \quad \nu \in \mathbb{Z}$$

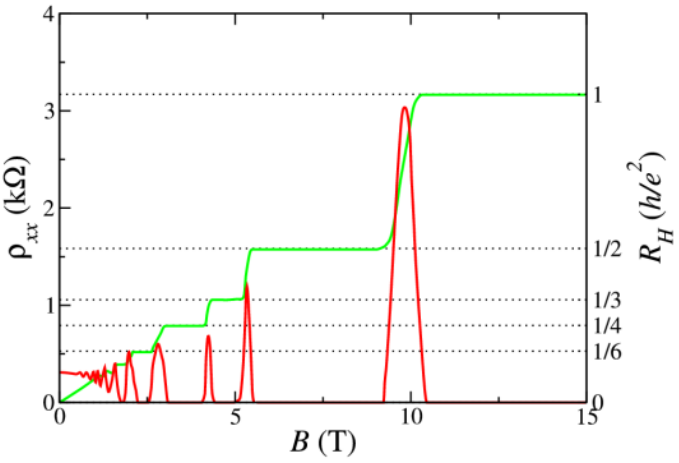


Figure 1.6: Resistivities as functions of the magnetic field, ρ_{xx} in red and ρ_{xy} in green.

The plateau values are independent of the sample details and the precise value of the

magnetic field: they are a topological property!

1.6. C^*-algebra for a crystal

We consider a crystal lattice in $\mathbb{Z}^d$ invariant with respect to the directions $a_1, a_2 ... a_d \in \mathbb{Z}^d$ and a periodic potential with the same periodicity of the lattice. For simplicity, let us consider just the case $d = 1$ with $a_1 = 1$. We consider also that electrons have N internal degrees of freedom, which can correspond, for example, to the their spin or to the presence of more types of atoms in the unit cell of the crystal (see example 4.1). Thanks to the tight binding approximation, we can assume that the spatial part of state function for each electron is characterised by the probability of being associated to one single nucleus of the lattice: for this reason we can take as underlying Hilbert space $\ell^2(\mathbb{Z}) \otimes \mathbb{C}^N$, where $\mathbb{C}^N$ stands for the internal degrees of freedom and it is called the *fiber*. Therefore, we can consider a sub-C^*-algebra $\mathcal{A}$ of periodic (i.e. commuting with the translation operator) operators of $\mathcal{B}(\ell^2(\mathbb{Z}) \otimes \mathbb{C}^N)$.
In order to have a better insight on this C^*-algebra, we introduce the Bloch-Floquet transform $\mathcal{F} : \ell^2(\mathbb{Z}) \to L^2(\mathbb{S}^1)$ (see [8], first chapter)

$$(\mathcal{F}\phi)(k) = (2\pi)^{-\frac{1}{2}} \sum_{x \in \mathbb{Z}} \phi(x) e^{-\mathrm{i}xk}$$

$\mathbb{S}^1$ is the Brillouin zone in the one dimensional case and in our case it is just the interval $(-\pi, \pi]$. We can see at the Bloch-Floquet transform as a discrete version of the Fourier transform. We can verify that $\mathcal{F}$ is unitary (it preserves scalar products) and it has inverse $\mathcal{F}^*$ given by

$$(\mathcal{F}^*\psi)(n) = (2\pi)^{-\frac{1}{2}} \int_{\mathbb{S}^1} \psi(k) e^{\mathrm{i}nk} \mathrm{d}k$$

The Bloch-Floquet transform is useful to partially diagonalise periodic operators (and for $N = 1$, i.e. no internal degree, it fully diagonalises them). Indeed, proposition 2.18 in [11] shows that for a periodic hamiltonian H, we can write

$$\mathcal{F}H\mathcal{F}^* = \int_{\mathbb{S}^1}^{\oplus} \mathrm{d}k H(k)$$

where in general $H(k) \in \mathcal{L}(L^2(\mathbb{S}^1))$ (linear operators over $L^2(\mathbb{S}^1)$) and, in particular in our case, $K(k)$ is a matrix of size N continuous in k. The meaning of the direct integral is

$$(\mathcal{F}H\mathcal{F}^*)(\psi)(k) = (H(k)(\psi))(k)$$

(see [9] for a rigorous introduction to the direct integral). The spectrum of $\mathcal{F}H\mathcal{F}^*$ is given by

$$\sigma(\mathcal{F}H\mathcal{F}^*) = \bigcup_{k\in\mathbb{S}^1} \sigma(H(k))$$

There is a compact formula to apply $\mathrm{Ad}_{\mathcal{F}}(\cdot) = \mathcal{F}(\cdot)\mathcal{F}^*$ to an hamiltonian, namely Peierls's substitution. Fix I a finite subset of $\mathbb{Z}$ and be $a_n \in M_n(\mathbb{C})$ for $n \in I$ given; define T the translation operator over $\ell^2(\mathbb{Z})$. Then, Peierls's substitution is given by

$$H = \sum_{n\in I} a_n T^i \mapsto \sum_{n\in I} a_n \mathrm{e}^{\mathrm{i}kn}$$

In section 4.1, I will present an easy example/exercise where we can see how the Bloch-Floquet transform helps us to compute the energy band of an hamiltonian.
Finally, we can show that $\mathrm{Ad}_{\mathcal{F}}(\cdot)$ is a isomorphism between $\mathcal{A}$ (the C^*-algebra in the "position" domain with N degrees of freedom) and $\mathcal{C}((\mathbb{S}^1)^d) \otimes M_N(\mathbb{C})$ (the tensor product between the continuous functions over the torus of dimension d and the operators over $\mathbb{C}^N$). The C^*-algebra which is usually considered is indeed

$$A = \mathcal{C}((\mathbb{S}^1)^d) \otimes M_N(\mathbb{C}).$$

2 | Mathematical framework

2.1. C^*-algebras: basic results

We briefly recall the definition and the fundamental results and theorems for a C^*-algebra. For this section, I mostly rely on [6].

Definition 1. A ($\mathbb{C}$-)C^*-*algebra* A is a $\mathbb{C}$-algebra with a norm and an *involution* $a \mapsto a^*$, $a \in A$, such that A is complete w.r.t. the norm, and such that $\|ab\| \leq \|a\|\|b\|$ and $\|a^*a\| = \|a\|^2$ for every a, b in A.

A C^*-algebra A is called *unital* if it has a multiplicative identity 1. We observe that a C^*-algebra is a particular type of Banach algebra. Some fundamental examples of C^*-algebras are:

- The scalar field $\mathbb{C}$ is a unital C^*-algebra with involution given by complex conjugation $\lambda \mapsto \bar{\lambda}$.
- If Ω is a locally compact Hausdorff space, then $\mathcal{C}_0(\Omega)$ is a C^*-algebra with involution $f \mapsto \bar{f}$.
- If H is a Hilbert space, then $\mathcal{B}(H)$ with the operator norm is a C^*-algebra.

As in the context of Banach algebras, an element $a \in A$ is *invertible* if there is an element $b \in A$ such that $ab = ba = 1$. We define the *spectrum* of an element to be:

$$\sigma(a) = \{\lambda \in \mathbb{C} \mid \lambda 1 - a \text{ is not invertible}\}$$

If A is not unital, there is a standard way to extend it to a unital C^*-algebra $\tilde{A}$. Therefore, we can extend the definition of spectrum of an element also in the case of non unital algebras as $\sigma_A(a) = \sigma_{\tilde{A}}(a)$. We can also define the *multiplier algebra* of A, $M(A)$, as the unital C*-algebra that is the largest unital C^*-algebra that contains A as proper ideal. In general $\tilde{A} \subseteq M(A)$.

Much of the reason for the interest in C^*-algebras comes from the following theorems. The first one is a characterisation of commutative C^*-algebras.

Theorem 2.1 (Gelfand). *Every* ***abelian*** *C^*-algebra is isometrically $*$-isomorphic to the C^*-algebra $\mathcal{C}_0(\Omega)$ for some locally compact Hausdorff space Ω.*

The second one allows us to see C^*-algebras as an "abstraction" of physical operators over an Hilbert space.

Theorem 2.2 (Gelfand-Naimark). *Every C^*-algebra is isomorphic to a sub-C^*-algebra of $\mathcal{B}(H)$ for some Hilbert space H.*

It is useful to give some definitions. An element $a \in A$ is called:

- *self-adjoint* if $a = a^*$;
- *normal* if $aa^* = a^*a$;
- *positive* if it is self-adjoint and $\sigma(a) \subseteq \mathbb{R}_+$;
- a *projection* if it is self-adjoint and $a^2 = a$;
- *unitary* if $aa^* = 1$ and $a^*a = 1$.

2.2. Why a C^*-algebra?

As we have already said several times, an hamiltonian h is a self-adjoint operator on an Hilbert space H. In our case, we assume furthermore that $h \in \mathcal{B}(H)$, the bounded linear operators on H. We identify each concrete material with its hamiltonian and a Fermi energy level, as they characterise completely its behaviour. An insulator is an hamiltonian h such that its Fermi level belongs to a "gap" in the spectrum of h. As we want to study the topological properties of the set of the insulators, we must choose a good topology for $\mathcal{B}(H)$. We could try with the **strong topology**. We say that $T_i \to T$ in the strong operator topology if and only if $\|T_i x - Tx\| \to 0$ for each x in H. For this, we have to keep in mind that in the literature about topological insulators, the "index theory" approach revealed very useful and we do not want to dispense with it. With the strong topology, the "index theory" of the algebra becomes trivial and therefore, it is not satisfying. We try with the **weak topology**, i.e. the weakest topology on the set of bounded operators on a Hilbert space H, such that the functional sending an operator T to the complex number $\langle Tx, y\rangle$ is continuous for any vectors x and y in H. However, in this way, we would have too many continuous paths! Therefore, we would have no topological information. Another "natural" candidate for the topology is the one given by the **operator norm**. Nevertheless, equipped with this norm, $\mathcal{B}(H)$ has a trivial K-theory (because it is not separable). In this optic, we would like to "restrict" $\mathcal{B}(H)$ in

order to use the operator norm. Moreover, for physical reasons, we are interested in local operators. Therefore, we consider the set of local operators and we take the closure with respect to the operator norm topology: we get a C^*-algebra!

If we are interested in the case of crystal structures, we would like to consider periodic hamiltonians: we restrict furthermore the C^*-algebra. In general, if no symmetry condition is imposed, there is no obstruction to do a translation of the spectrum of h, a self-adjoint element in the C^*-algebra, in order to consider the Fermi energy at 0: therefore, 0 does not belong to the spectrum of h and so this latter is an invertible element of the algebra. We define an *abstract insulator* as an invertible self-adjoint element of a C^*-algebra.

2.3. Symmetries

In the following, we will consider hamiltonians which could possibly satisfy one or more symmetry conditions. We assume that the symmetries act only on the fiber of the C^*-algebra, not on the "spatial" part of it. The "physical" symmetries are translated in algebraic conditions with the help of order two linear or anti-linear $*$-automorphism. We give the following definitions:

Definition 2. A **grading** on a (complex or real) C^*-algebra A is a $*$-automorphism γ of order two ($\gamma^2 = \mathrm{id}$).

Definition 3. A **real structure** on a complex graded C^*-algebra (A, γ) is an anti-linear $*$-automorphism $\mathfrak{r}$ of order two which commutes with the grading γ and preserves the norm.

Definition 4. A complex C^*-algebra with a real structure $(A, \mathfrak{r})$ is called a **Real C^*-algebra** or a $C^{*,r}$-algebra. The $\mathfrak{r}$-invariant elements furnish a real C^*-algebra which we call the real subalgebra of the $C^{*,r}$-algebra.

A graded C^*-algebra (A, γ) is a C^*-algebra A equipped with a grading γ. γ-invariant elements are called *even*, and elements with $\gamma(a) = -a$ are called *odd*.

In the following we will often consider special gradings, *inner* gradings and *balanced* gradings.

Definition 5. A grading γ is called **inner** if $\gamma = \mathrm{Ad}_\Gamma$ for some self-adjoint unitary Γ in A. The self-adjoint unitary Γ is called the generator of γ or the grading operator.

Definition 6. A grading on a C^*-algebra is called **balanced** if C^*-algebra contains an odd self-adjoint unitary e.

In our physical setting, the hypothesis of having a balanced grading is equivalent to say that it exists at least one insulator.

We have three relevant symmetries.

Definition 7. Let A be a C^*-algebra and $h \in A$ an abstract hamiltonian.

- h has **chiral** symmetry if there is a grading γ on A such that $\gamma(h) = -h$;
- h has **time reversal symmetry (TRS)** if there is a real structure $\mathfrak{t}$ on A such that $\mathfrak{t}(h) = h$;
- h has **particle hole symmetry (PHS)** if there is a real structure $\mathfrak{p}$ on A such that $\mathfrak{p}(h) = -h$.

We have that the product of a time reversal symmetry together with a particle hole symmetry yields a chiral symmetry. We thus have the following combinations:

- no symmetry
- chiral symmetry
- time reversal symmetry
- particle hole symmetry
- chiral symmetry and time reversal symmetry (and therefore, also particle hole symmetry).

These five cases will be refined (we will define an odd/even TRS and PHS) and we will obtain two complex cases and eight real cases.

2.4. Clifford algebras

Clifford algebras are a technical tool which will allow us to give us a unified framework to treat all cases of symmetries (the five cases of symmetries presented at the end of section 2.3).

We give a definition of Clifford algebra suited for our case.

Definition 8. The Clifford algebra $Cl_{r,s}$ is the graded real C^*-algebra generated by r self-adjoint generators $e_1, \ldots, e_r$ which square to 1 and s anti-self-adjoint generators $f_1, \ldots, f_s$ which square to -1 and all generators anti- commute pairwise. The grading is defined by declaring the generators to be odd.

Definition 9. The complex Clifford algebra $\mathbb{C}l_{r+s}$ is the complexification of $Cl_{r,s}$, $\mathbb{C}l_{r+s} = \mathbb{C} \otimes Cl_{r,s}$.

The generators define completely the grading, which is noted st. We remind the expression of the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Recall that the quaternions $\mathbb{H}$ form a real C^*-algebra which is spanned as a real vector space by $\{1, \mathrm{i}\sigma_x, \mathrm{i}\sigma_y, \mathrm{i}\sigma_z\}$. We consider $\mathbb{H}$ always as trivially graded. We give a list of useful properties for some examples of Clifford algebras.

- $(\mathbb{C}l_1, \mathrm{st}) \cong (\mathbb{C} \oplus \mathbb{C}, \phi)$ with grading $\phi(a, b) = (b, a)$ and generator $(1, -1)$. Indeed, ϕ is the only possible non-trivial grading on $\mathbb{C} \oplus \mathbb{C}$ (see 4.3.2).
- $(\mathbb{C}l_2, \mathrm{st}) \cong (M_2(\mathbb{C}), \mathrm{Ad}_{\sigma_z})$.
- $(Cl_{1,0}, \mathrm{st}) \cong (\mathbb{R} \oplus \mathbb{R}, \phi)$ with $\phi(a, b) = (b, a)$ and generator $(1, -1)$.
- $(Cl_{0,1}, \mathrm{st}) \cong (\{(a, \bar{a}) \in \mathbb{C} \oplus \mathbb{C}\}, \phi)$ with $\phi(a, b) = (b, a)$ and generator $(\mathrm{i}, -\mathrm{i})$.
- $(Cl_{1,1}, \mathrm{st}) \cong (M_2(\mathbb{R}), \mathrm{Ad}_{\sigma_z})$.
- $Cl_{2,0}$ is generated by σ_x and σ_y.
- $Cl_{0,2}$ is generated by $\mathrm{i}\sigma_x$ and $\mathrm{i}\sigma_y$.
- $(Cl_{0,3}, \mathrm{st}) \cong (\mathbb{H} \otimes Cl_{1,0}, \mathrm{id} \otimes \mathrm{st})$
- $(Cl_{3,0}, \mathrm{st}) \cong (\mathbb{H} \otimes Cl_{0,1}, \mathrm{id} \otimes \mathrm{st})$
- $(Cl_{0,4}, \mathrm{st}) \cong (\mathbb{H} \otimes Cl_{1,1}, \mathrm{id} \otimes \mathrm{st})$

The eight real Clifford algebras appearing in the previous list will be useful when considering the eight real cases related to TRS and PHS.

2.5. What we need from K-theory

In [10] we can find a friendly approach to K-theory for C^*-algebras. I will rely on this text to introduce this subject. Here we consider for simplicity the case of K-theory over a $\mathbb{C}$-C^*-algebra, the real case being more technical. In our context, the goal of K-theory is to associate to homotopy classes of particular elements in the C^*-algebra A (either projections or unitaries) an abelian group: it will be called $K_0(A)$ in the case of projections and $K_1(A)$ in the case of unitaries. This is a very nice feature because we

can give a structure to homotopy classes. This fact allows us to use tools from algebraic topology.

First of all, we have to introduce the *matrix algebra* for a C^*-algebra A: it is the algebra $M_n(A)$ equipped with the element-by-element involution defined by the involution on A and the (unique) norm that makes it a C^*-algebra. This algebra is necessary to talk about the *stabilisation* of A. The stabilisation of A is just the fact of replacing A with the set

$$\bigsqcup_{n\in\mathbb{N}} M_n(A)$$

2.5.1. $K_0(A)$

In this case, we focus on the projections of A. We denote with $\mathcal{P}(A)$ the set of projections of A. Then, we define

$$\mathcal{P}_n(A) = \mathcal{P}(M_n(A)) \quad \text{and} \quad \mathcal{P}_\infty(A) = \bigsqcup_{n\in\mathbb{N}} \mathcal{P}_n(A)$$

Define the equivalence relation $\sim_0$ on $\mathcal{P}_\infty(A)$ as follows. If $p \in \mathcal{P}_n(A)$ and $q \in \mathcal{P}_m(A)$, $p \sim_0 q$ if there is an element $v \in M_{m,n}(A)$ such that $p = v^*v$ and $q = vv^*$ (in the case $n = m$, this is also called the Murray-von Neumann equivalence). We also define the binary operation $\oplus$ on $\mathcal{P}_\infty(A)$ by

$$p \oplus q = \begin{pmatrix} p & 0 \\ 0 & q \end{pmatrix} \in \mathcal{P}_{n+m}(A), \quad p \in \mathcal{P}_n(A),\, q \in \mathcal{P}_m(A)$$

We introduced these new concepts, namely the stabilisation of A and the $\sim_0$ relation, because we can prove that, "up to stabilisation", the homotopy equivalence and $\sim_0$ are equivalent. Therefore, we can just focus on $\sim_0$ equivalence, as it is easier to handle.

Starting from the previous object, now we can define the semigroup $\mathcal{D}(A)$.

Definition 10. With $(\mathcal{P}_\infty(A), \sim_0, \oplus)$, set

$$\mathcal{D}(A) = \mathcal{P}_\infty(A)/\sim_0$$

For each $p \in \mathcal{P}_\infty(A)$ let $[p]_\mathcal{D}$ denote the equivalence class containing p. Define addition on $\mathcal{D}(A)$ by

$$[p]_\mathcal{D} + [q]_\mathcal{D} = [p \oplus q]_\mathcal{D}, \quad p, q \in \mathcal{P}_\infty(A)$$

It is easy to see that $(\mathcal{D}(A), +)$ is an abelian semigroup. Now, the construction of $K_0(A)$ is very simple (to fix ideas we just consider the case of an unital C^*-algebra, the non unital case being more technical). First, we define the *Grothendieck construction* which gives us an abelian group starting from an abelian semigroup: $K_0(A)$ is just the application of the Grothendieck construction to $(\mathcal{D}(A), +)$! The Grothendieck construction is nothing more than the generalisation of the construction of the set $\mathbb{Z}$ starting from $\mathbb{N}$.

Let $(S, +)$ be an abelian semigroup with the equivalence relation $\sim$ on $S \times S$

$$(x_1, y_1) \sim (x_2, y_2) \iff \exists z \in S \text{ s.t. } x_1 + y_2 + z = x_2 + y_1 + z$$

We define the group $G(S) = S \times S/\sim$, note with $\langle x, y\rangle$ the equivalence class of $(x, y) \in S \times S$ and define the addition:

$$\langle x_1, y_1\rangle + \langle x_2, y_2\rangle = \langle x_1 + x_2, y_1 + y_2\rangle$$

Take $y \in S$. The map

$$\gamma_S : S \to G(S), \quad x \mapsto \langle x + y, y\rangle$$

is independant of the choice of y and is called the *Grothendieck map*.

Definition 11. For an unital C^*-algebra A define

$$K_0(A) = G(\mathcal{D}(A))$$

Define $[\cdot]_0 : \mathcal{P}_\infty(A) \to K_0(A)$ by

$$[p]_0 = \gamma([p]_{\mathcal{D}}) \in K_0(A), \quad p \in \mathcal{P}_\infty(A)$$

where $\gamma = \gamma_{\mathcal{D}(A)}$ is the Grothendieck map of $\mathcal{D}(A)$.

A very important property of $K_0(A)$ is its uniqueness in an "universal" way. Moreover, we can show that $K_0(A)$ is a *functor* from the category of unital C^*-algebras to the category of abelian groups.

2.5.2. $K_1(A)$

Now we focus on the set of unitary elements of A, $\mathcal{U}(M_n(A))$. We define

$$\mathcal{U}_n(A) = \mathcal{U}(M_n(A)) \quad \text{and} \quad \mathcal{U}_\infty(A) = \bigsqcup_{n\in\mathbb{N}} \mathcal{U}_n(A)$$

Again, we define the binary operation $\oplus$ on $\mathcal{U}_\infty(A)$ by

$$u \oplus v = \begin{pmatrix} u & 0 \\ 0 & v \end{pmatrix} \in \mathcal{U}_{n+m}(A), \quad u \in \mathcal{U}_n(A),\, v \in \mathcal{U}_m(A)$$

Define the equivalence relation $\sim_1$ on $\mathcal{U}_\infty(A)$ as follows. If $u \in \mathcal{U}_n(A)$ and $v \in \mathcal{U}_m(A)$, $u \sim_1 v$ if there exists a natural number $k \geq \max\{m, n\}$ such that $u \oplus 1_{k-n} \sim_h v \oplus 1_{k-m}$ in $\mathcal{U}_k(A)$, where 1_r is the unity of $M_r(A)$ and $\sim_h$ is the homotopy equivalence in $M_r(A)$. The following definition of $K_1(A)$ is valid without further precaution also when A is a non-unital C^*-algebra.

Definition 12. For each C^*-algebra A define

$$K_1(A) = \mathcal{U}_\infty(\tilde{A})/\sim_1$$

Let $[u]_1 \in K_1(A)$ denote the equivalence class containing $u \in \mathcal{U}_\infty(\tilde{A})$. Define addition on $\mathcal{K}_\infty(A)$ by

$$[u]_1 + [v]_1 = [u \oplus v]_1, \quad u, v \in \mathcal{U}_\infty(\tilde{A})$$

The properties for $K_1(A)$ are analogous to those of $K_0(A)$. In particular, $K_1(A)$ is a *functor* from the category of C^*-algebras to the category of abelian groups.

2.5.3. Higher order $K_n(A)$ groups

A very important result about K-theory for complex C^*-algebras is

$$K_n(A) \cong K_{n-2}(A), \quad n \geq 2$$

This is the so-called Bott periodicity. For this reason, we just have to construct $K_0(A)$ and $K_1(A)$. In the case of real C^*-algebras, we have a richer landscape:

$$K_n(A) \cong K_{n-8}(A), \quad n \geq 8$$

2.6. Van Daele's approach to K-theory

In [13], A. Van Daele proposes a new approach to K-theory for Banach algebras (not just for C^*-algebras, but we will apply this theory just to the C^*-algebra case) in a particular situation: here, we want to associate an abelian group to the homotopy classes of a subset of the elements of the Banach algebra which satisfy a symmetry condition. This is exactly

what we want to obtain physically and Van Daele's approach applies directly to our case. Finally, in some cases, Van Daele manages to link (i.e. find an isomorphism between) his K-groups and the standard K-groups (those presented in 2.5).

Let A be a real or complex C^*-algebra with a grading α. Also in this case, we just consider the case of an unital C^*-algebra (in Van Daele's paper also the non-unital case is treated). We define

$$\mathscr{F}(A,\alpha) = \{a \in A \mid a \text{ self-adjoint and unitary, } \alpha(a) = -a\}$$

We first assume that $\mathscr{F}(A,\alpha)$ is not empty, i.e. the grading is balanced (physically it means that we have at least an insulator). We denote by $F(A,\alpha)$ the set of homotopy equivalence classes of $\mathscr{F}(A,\alpha)$.
We let

$$\mathscr{F}_n(A,\alpha) = \mathscr{F}\left(M_n(A),\alpha_n\right) \quad \text{and} \quad F_n(A) = F\left(M_n(A),\alpha_n\right)$$

where α_n is application of α element-by-element on $M_n(A)$. Analogously to the construction of $K_0(A)$ and $K_1(A)$, we define the direct sum as a map from $\mathscr{F}_n(A) \times \mathscr{F}_m(A)$ to $\mathscr{F}_{m+n}(A)$.

Definition 13. Choose an element $e \in \mathscr{F}(A,\alpha)$ and define $DK_e(A) = \varinjlim F_n(A,\alpha)$ where the inductive limit is taken with respect to the maps $x \to x \oplus e$ from $\mathscr{F}_n(A,\alpha)$ to $\mathscr{F}_{n+1}(A,\alpha)$. We will denote by $[x]$ the image of x in the inductive limit.

It is interesting that we have to choose a reference element e: physically, it means that we must choose a reference insulator. We have the following propositions.

Proposition 2.1. *The direct sum induces an abelian semi-group structure on $DK_e(A)$. The neutral element is $[e]$.*

Proposition 2.2. *If e and $-e$ are homotopic in $\mathscr{F}(A,\alpha)$ then $DK_e(A)$ is a group.*

Now we can define the Van Daele K-group $DK(A)$. The definition is quite technical, as it must deal with several special cases (for example, when $\mathscr{F}(A)$ is empty); we refer to Van Daele's paper for the notation.

Definition 14. Let $DK(A)$ be the group $DK_e(M_4(A))$ where on $M_4(A)$ the automorphism γ (depending on α) and the explicit element $e \in M_4(A)$ are given in [13] paragraph 3.

We have the following proposition.

Proposition 2.3. *If A has an element $e_0 \in \mathscr{F}(A)$ then $DK(A)$ is the Grothendieck group*

of the semi-group $DK_{e_0}(A)$.

Remark. We can also consider a symmetry with respect to a real structure $\mathfrak{r}$. If $(A, \gamma, \mathfrak{r})$ is a graded unital $C^{*,r}$-algebra, we define

$$\mathscr{F}(A, \gamma, \mathfrak{r}) := \left\{x \in A : x^* = x^{-1}, \gamma(x) = -x, \mathfrak{r}(x) = x\right\}$$

Definition 15. Let $(A, \gamma, \mathfrak{r})$ be a graded unital $C^{*,r}$-algebra. Suppose that $\mathscr{F}(A, \gamma, \mathfrak{r})$ contains an element e which is homotopic to $-e$ in $\mathscr{F}(A, \gamma, \mathfrak{r})$. The K-group of Van Daele is

$$DK_e(A, \gamma, \mathfrak{r}) := DK_e(A^{\mathfrak{r}}, \gamma).$$

We can define for an algebra (A, γ) with a choice of an odd self-adjoint unitary $e \in A$ as $GV_e(A, \gamma)$, the Grothendieck construction applied to the semigroup

$$V_e(A, \gamma) := \bigsqcup_{n \in \mathbb{N}} \mathscr{F}\left(M_n(A), \gamma_n\right) / \sim_h^e$$

We could show that $GV_e(A, \gamma)$ and $DK(A)$. This remark allows us to give the following important result.

Corollary 2.2.1. *Consider two odd self-adjoint unitaries $x \in M_n(A)$, $y \in M_m(A)$. x and y define the same class in $DK(A)$ if and only if there exist k such that $x \oplus e_k \oplus -e_{n+k}$ is homotopic to $y \oplus e_{n+k-m} \oplus -e_{n+k}$ in $\mathscr{F}(M_{2(n+k)}(A), \gamma)$.*

Before introducing Van Daele's higher K-groups, we give a useful result. We have

$$DK_e\left(A \hat{\otimes} Cl_{r,s}, \gamma \otimes \mathrm{st}\right) \cong DK_e\left(A \hat{\otimes} Cl_{r+1,s+1}, \gamma \otimes \mathrm{st}\right)$$

In particular, it implies that $DK_e\left(A \hat{\otimes} Cl_{r,s}, \gamma \otimes \mathrm{st}\right)$ depends only on the difference $s - r$. The key result to obtain the previous isomorphism is

$$(A \otimes \mathbb{C}l_2, \gamma \otimes \mathrm{st}) \cong (M_2(A), \gamma_2)$$

where the isomorphism depends on the choice of the reference element e.

We show here Van Daele's higher K-groups.

Definition 16. Let (A, γ) be a unital graded complex or real C^*-algebra containing an odd self-adjoint unitary e. The K_n-group of (A, γ) in Van Daele's formulation is

$$K_n(A,\gamma) := DK_e\left(A\hat{\otimes}Cl_{1,n}, \gamma\otimes \mathrm{st}\right).$$

For $C^{*,r}$-algebras, it is defined as $K_n(A,\gamma,\mathfrak{r}) = K_n(A^{\mathfrak{r}},\gamma)$

We remark that the definition of K_n depends on the choice of a base point. A fundamental property of the K-groups $K_n(A,\gamma)$ is their periodicity. We have $K_n = K_{n-8}$ and if we are in the complex case we also have $K_n = K_{n-2}$.

We conclude this section with a list of useful results in some particular cases. We will use this results in chapter 3.

- If the algebra is trivially graded:

  1. case of a complex C^*-algebra (A,id)
     Van Daele shows that

     $$K_n(A,\mathrm{id}) = DK\left(A\otimes \mathbb{C}l_{n+1}, \mathrm{id}\otimes \mathrm{st}\right) \cong KU_n(A)$$

     where $KU_n(A)$ is the standard K_n-group (n taken modulo 2) of A seen as ungraded complex C^*-algebra. In particular, in the case $n=0$, the isomorphism is given by $\mathrm{sgn}(h) \mapsto p_F(h)$, where $\mathrm{sgn}(h)$ is the spectral flattening of h and $p_F(h)$ is the Fermi projector (we will define them in chapter 4).

  2. case of a $C^{*,r}$-algebra $(A,\mathrm{id},\mathfrak{r})$
     We have

     $$DK\left(A\otimes \mathbb{C}l_{r+s}, \mathrm{id}\otimes \mathrm{st}, \mathfrak{r}\otimes \mathfrak{l}_{r,s}\right) \cong K_{s-r+1}\left(A^{\mathfrak{r}},\mathrm{id}\right) \cong KO_{s-r+1}\left(A^{\mathfrak{r}}\right)$$

     where $\mathfrak{l}_{r,s}$ are real structures on $\mathbb{C}l_{r+s}$ such that $\mathbb{C}l_{r+s}^{\mathfrak{l}_{r,s}} = Cl_{r,s}$ and $KO_n(A)$ is the K_n-group of A seen as real ungraded C^*-algebra.

- If the grading of the algebra is inner:

  1. case of a complex C^*-algebra (A,γ)
     We have

     $$DK(A,\gamma) \cong K_1(A,\mathrm{id}) \cong KU_1(A)$$

  2. case of a $C^{*,r}$-algebra $(A,\gamma,\mathfrak{r})$, where $\gamma = \mathrm{Ad}_\Gamma$
     If $\mathfrak{r}(\Gamma) = \Gamma$, then

     $$DK(A,\gamma,\mathfrak{r}) \cong K_1\left(A^{\mathfrak{r}},\mathrm{id}\right) \cong KO_1\left(A^{\mathfrak{r}}\right)$$

If $\mathfrak{r}(\Gamma) = -\Gamma$, then

$$DK(A, \gamma, \mathfrak{r}) \cong K_{-1}\left(A^{\mathfrak{r}}, \mathrm{id}\right) \cong KO_{-1}\left(A^{\mathfrak{r}}\right)$$

3 | Description of the approach

In this chapter, we outline the goals and the main steps presented in the paper [5].

3.1. Goals

Paper [5] has two main goals. The first one is to give a classification of the possible "physical frameworks". Indeed, in section 2.3 we saw that there are five possible cases of symmetries: each case corresponds to a specific physical situation and they are potentially infinitely many. Considering further assumptions to simplify the mathematical problem, the author presents a compact classification of possible symmetries. The key idea is to consider a reference real structure: in this way, it is possible to define a relation between all the other real structures and classify them.

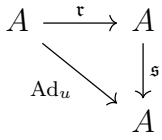
The second goal is the original one: given one of the previous cases of symmetry, we want to give a description of the algebraic structure of the topological phases. Also in this case, the idea is to choose a reference element (a "trivial" insulator) and to define an equivalence relation. Then, it is possible to apply Van Daele's construction to obtain an abelian group.

3.2. Classification of real structures

We cannot study all possible real structures, they are too many. Therefore, we decide to fix a reference real structure and we define two notions of equivalence between the real structures: we define the concept of *inner related* (weaker equivalence relation) and *inner conjugated* (stronger equivalence relation).

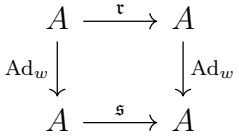
Definition 17. Let A be a graded complex C^*-algebra with two real structures $\mathfrak{r}$, $\mathfrak{s}$. We call them **inner related** if there exists a unitary u (the generator of $\mathfrak{s}\circ\mathfrak{r}$) in the multiplier algebra of A such that $\mathfrak{s}\circ\mathfrak{r} = \mathrm{Ad}_u$.

If $\mathfrak{r}$ and $\mathfrak{s}$ are inner related with generator u, then the following diagram commutes.



Definition 18. Let A be a graded complex C^*-algebra with two real structures $\mathfrak{r}$, $\mathfrak{s}$. We call them **inner conjugate** if there exists a unitary w in the multiplier algebra of A such that $\mathfrak{s} \circ \mathrm{Ad}_w = \mathrm{Ad}_w \circ \mathfrak{r}$ and Ad_w preserves the grading.

If $\mathfrak{r}$ and $\mathfrak{s}$ are inner conjugate, then the following diagram (using w of the definition) commutes.



Inner conjugation is a stronger equivalence relation than inner relation. Indeed, we can show that (lemma 4.11 in [5]), if $\mathfrak{r}$ and $\mathfrak{s}$ are inner conjugate then it exists a unitary $w \in A$ such that they are also inner related with generator given by $w\mathfrak{r}(w^*)$.

Definition 19. Let (A, γ) be a graded C^*-algebra with two inner related real structures $\mathfrak{r}$, $\mathfrak{s}$. The relative signs between $\mathfrak{r}$ and $\mathfrak{s}$ are

$$\eta_{\mathfrak{r},\mathfrak{s}} = \left(\eta^1_{\mathfrak{r},\mathfrak{s}}, \eta^2_{\mathfrak{r},\mathfrak{s}}\right) := (u\mathfrak{r}(u), u\gamma(u)^*)$$

where u is any generator for $\mathfrak{s} \circ \mathfrak{r}$.

An important result obtained in the paper is Corollary 4.14: it states that, under further technical hypothesis, given a reference real structure, up to stabilisation and inner conjugation, there is a **finite number of real structures** inner related to the first one. Below we determine these real structures for a class of algebras which is usually considered in condensed matter (see chapter 4 for some examples and a further discussion of Corollary 4.14). We will achieve a compact description of K-groups for all real structures inner related to a reference real structure.

3.3. How to use Van Daele's construction

The goal is to classify hamiltonians (i.e. self-adjoint invertible elements of a C^*-algebra) which satisfy one of the symmetry conditions presented at the end of paragraph 2.3. Van Daele's construction (presented in 2.6) allows us to obtain a K-group corresponding to

the homotopy classes in the set of **unitary** self-adjoint elements which satisfy a chiral symmetry. We will see how to adapt each case in order to apply Van Daele's construction. In some cases, it could seem an artificial and too complicated procedure: for example, in the case of "no symmetry" we introduce an artificial chiral-symmetry to apply the construction. However, we can argue that Van Daele gives us a common framework to treat in a compact way different situations. Moreover, this approach can handle at the same time the commutative case and the non-commutative one. An explanation is needed. In chapter 1, we have considered the case of a crystal with a periodic potential: to describe this physical situation, we can choose a commutative C^*-algebra, namely the algebra of continuous functions over the Brioullin zone. The approximation to a periodic crystal is typical in physics and often effective, but we can easily realise that in "real life" crystals are not perfect and that a perturbation of the periodicity is inevitable. We get that disorder destroys commutativity. For this reason, we would like to consider both cases.

In the paper, the author associates to each symmetry case a K-group (a Van Daele K-group or a standard one). Two classifications are presented. The first one is a "rough" classification, under minimal assumptions. The second is finer and it is a classification with respect to a reference real structure. The classifications can be improved if we assume the grading to be inner.

Before entering in the description of the classification, we give a general result which is fundamental to apply Van Daele's construction to all cases of symmetry. In a C^*-algebra A, any invertible self-adjoint element h is homotopic to a self-adjoint unitary, namely its sign $\mathrm{sgn}(h)$; this is referred to as *spectral flattening*. To define $\mathrm{sgn}(h)$, we introduce the *Fermi projector* of h, $p_F(h)$. If we think A represented on a Hilbert space using theorem 2.2, $p_F(h)$ is the projector on the eigenspaces corresponding to the eigenvalues below the Fermi energy (in our case, the negative eigenvalues). If $p_F^{\perp}(h)$ is the projection on the orthogonal of the previous subspace, then $\mathrm{sgn}(h)$ can be defined as

$$\mathrm{sgn}(h) = p_F(h) - p_F^{\perp}(h)$$

$\mathrm{sgn}(h)$ is clearly self-adjoint and unitary. It is easy to see that $\mathrm{sgn}(h)$ "flatten" the negative part of spectrum of h to -1 and the positive part to $+1$. It can be shown that there is a continuous path between $\mathrm{sgn}(h)$ and h which preserves the symmetry condition (if any). In this way, we are allowed to consider just unitary self-adjoint elements, as all generic self-adjoint elements are in the same homotopy class of one of them.

3.3.1. Rough classification

We consider the graded (A, γ), with, for simplicity, A unital. Most of the following results are still valid in the non-unital case.

No symmetry

No symmetry is equivalent to a trivial grading, $\gamma = \mathrm{id}$. Therefore, there is no odd element. The trick to recover an odd element is to extend the algebra A to $A \otimes \mathbb{C}l_1$. Indeed, the map $(x, -x) \mapsto x$ from the self-adjoint odd unitaries of $(A \otimes \mathbb{C}l_1, \mathrm{id} \otimes \mathrm{st})$ to the self-adjoint unitaries of (A, id) is a bijection (we consider the isomorphism between $\mathbb{C}l_1$ and $\mathbb{C} \otimes \mathbb{C}$, as reminded in 2.4). The advantage is that now each insulator is associated to an odd element of a C^*-algebra and we can apply straightforwardly Van Daele's construction. Thanks to the results showed in 2.6, we get the K-group

$$DK\left(A \otimes \mathbb{C}l_1, \mathrm{id} \otimes \phi\right) = K_0(A, \mathrm{id}) \cong KU_0(A)$$

The isomorphism is given by $\mathrm{sgn}(h) \mapsto p_F(h)$.

Chiral symmetry

Now the grading γ is non trivial and we assume that the grading is balanced, i.e. it exists at least a self-adjoint odd element (otherwise, the grading is not physically very interesting). We can use without further precaution Van Daele's construction, which gives the K-group

$$DK(A, \gamma) = K_1(A, \gamma)$$

In this case, we need A to be unital. Moreover, as there is no element a self-adjoint with stricly positive spectrum and chiral symmetry (if $\lambda > 0 \in \mathrm{sp}(a)$, then $-\lambda \in \mathrm{sp}(a)$), there is no trivial reference insulator and we must choose a non-trivial reference.

Time reversal symmetry

We consider the trivially graded $C^{*,r}$-algebra $(A, \mathfrak{t})$. Analogously to the case without symmetry, we consider $(A \otimes \mathbb{C}l_1, \mathrm{id} \otimes \phi, \mathfrak{t} \otimes \mathfrak{c})$ ($\mathfrak{c}$ is the complex conjugation) and we identify an odd self-adjoint unitary h with the element $h \otimes (1, -1)$ in $A \otimes \mathbb{C}l_1$ which is odd and $\mathfrak{t} \otimes \mathfrak{c}$-invariant. Therefore, we get the K-group

$$DK\left(A \otimes \mathbb{C}l_1, \mathrm{id} \otimes \phi, \mathfrak{t} \otimes \mathfrak{l}_{1,1}\right) = K_0\left(A^{\mathfrak{t}}, \mathrm{id}\right) \cong KO_0\left(A^{\mathfrak{t}}\right)$$

Particle hole symmetry

We consider the trivially graded $C^{*,r}$-algebra $(A, \mathfrak{p})$. Now we consider the algebra

$$(A \otimes \mathbb{C}l_1, \mathrm{id} \otimes \phi, \mathfrak{p} \otimes \phi \circ \mathfrak{c})$$

We see that the element $h \otimes (1, -1)$ is invariant with respect to the new real structure. We get the K-group

$$\begin{aligned} DK\left(A \otimes \mathbb{C}l_1, \mathrm{id} \otimes \phi, \mathfrak{p} \otimes \phi \circ \mathfrak{c}\right) = DK\left(A^{\mathfrak{p}} \otimes Cl_{0,1}, \mathrm{id} \otimes \phi\right) = K_2\left(A^{\mathfrak{p}}, \mathrm{id}\right) \\ \cong KO_2\left(A^{\mathfrak{p}}\right). \end{aligned}$$

Chiral symmetry and time reversal symmetry

We have a real structure $\mathfrak{t}$ and the grading γ is balanced. We get immediately the K-group

$$DK(A, \gamma, \mathfrak{t}) = K_1(A^{\mathfrak{t}}, \gamma)$$

If the grading is inner, we get a finer classification. We say that a grading $\gamma = \mathrm{Ad}_\Gamma$ is **real** with respect to the real structure $\mathfrak{t}$ if $\mathfrak{t}(\Gamma) = \Gamma$, **imaginary** if $\mathfrak{t}(\Gamma) = -\Gamma$. We have

Symmetries	K-group
Only inner chiral	$KU_1(A)$
Real inner chiral	$KO_1\left(A^{\mathfrak{t}}\right)$
Imag. inner chiral	$KO_{-1}\left(A^{\mathfrak{t}}\right)$

3.3.2. Classification w.r.t. a reference real structure

We assume that there is a "more natural" real structure $\mathfrak{f}$ over the C^*-algebra: it will serve as a reference real structure. We choose to classify only the real structures which are inner related to $\mathfrak{f}$. From 3.2 we know that up to stabilisation and inner conjugation, there is a finite number of real structures inner related to $\mathfrak{f}$. The great advantage is that now we just have to consider a finite number of cases. Indeed, if γ is a grading and $\mathfrak{r}$ and $\mathfrak{s}$ are two inner conjugate real structures, we have that $(A, \gamma, \mathfrak{r})$ and $(A, \gamma, \mathfrak{s})$ are isomorphic as graded C^*-algebras equipped with a real structure: therefore, the DK-groups are isomorphic and we just have to focus on one real structure for each inner conjugation "equivalence class". We give the following definition.

Definition 20. A real symmetry $\mathfrak{r}$ is called even (odd) if the relative sign $\eta^1_{\mathfrak{r},\mathfrak{f}}$ to the

reference structure $\mathfrak{f}$ is $+1$ (-1).

In the case of chiral symmetry and time reversal symmetry $\mathfrak{t}$, in the "rough" case we found that the K-group was $K_1(A^{\mathfrak{t}}, \gamma)$. Now we can describe better this latter. Indeed, we find that it is isomorphic to the K-groups of the table

$\eta_{\mathfrak{t},\mathfrak{f}}$	K-group	K-group (inner case)
$(+1,+1)$	$K_1\left(A^{\mathfrak{f}}, \gamma\right)$	$KO_1(A^{\mathfrak{f}})$
$(+1,-1)$	$K_{-1}\left(A^{\mathfrak{f}\circ\gamma}, \gamma\right)$	$KO_{-1}(A^{\mathfrak{f}})$
$(-1,+1)$	$K_5\left(A^{\mathfrak{f}}, \gamma\right)$	$KO_3(A^{\mathfrak{f}})$
$(-1,-1)$	$K_3\left(A^{\mathfrak{f}\circ\gamma}, \gamma\right)$	$KO_5(A^{\mathfrak{f}})$

Again, if we assume the grading to be inner, we can get a finer classification.

If the grading is trivial, again we tensor with $\mathbb{C}l_1$ to restore odd elements. We get

Symmetry	$\eta^{(1)}_{\mathfrak{r},\mathfrak{f}}$	$\mathfrak{s}$	K-group
TRS even	$+1$	$+1$	$KO_0\left(A^{\mathfrak{f}}\right)$
TRS odd	-1	$+1$	$KO_4\left(A^{\mathfrak{f}}\right)$
PHS even	$+1$	-1	$KO_2\left(A^{\mathfrak{f}}\right)$
PHS odd	-1	-1	$KO_6\left(A^{\mathfrak{f}}\right)$

Where we noted with $\mathfrak{s} = +1$ or -1 the real structure over $\mathbb{C}l_1$ which gives $Cl_{1,0}$ or $Cl_{0,1}$. The K-group in the table is $KO_0\left(A^{\mathfrak{t}}\right)$ or $KO_2\left(A^{\mathfrak{p}}\right)$, for TRS or PHS, respectively (we obtained these groups in the "rough" classification).

4 | Comments and examples

Here we see some "practical" examples of what we have discussed in the previous chapters. I will discuss some examples and show some explicit computations: they were for me very useful exercises which helped me to understand better the kind of objects I was dealing with. At the same time, these examples are fundamental and a reference for further development.

In the first two sections, we will consider two explicit hamiltonians and we discuss their properties as insulators. In the second case, we can show the non-triviality of the insulator; this proof gives us the opportunity to introduce the important notion of *Chern number*. In the third part we will discuss and do explicit calculation to find gradings and real structures in some easy (but fundamental) cases.

4.1. Energy band of a simple periodic hamiltonian

As in 1.6, we consider the Hilbert space $\ell^2(\mathbb{Z})$ (we neglect the internal degrees of freedom). We define T as the right-shift operator in $\mathcal{B}(\ell^2(\mathbb{Z}))$

$$(T\psi)(n) = \psi(n-1)$$

and the periodic operator V

$$(V\psi)(n) = \psi(n)V(n) \quad V(n) = (-1)^n a,\ a \in \mathbb{R}_+$$

We propose the following hamiltonian:

$$H = T + T^* + V$$

The term $T + T^*$ is a kind of discretisation of the laplacian operator over $L^2(\mathbb{R})$. We want to compute the energy bands for this hamiltonian. We would like to use Bloch's theory to partially diagonalise H. However, to do this, we need that H commutes with the translation operator, which it is not the case. Nevertheless, we observe that H commutes

with T^2: to recover the commutativity with the "simple" translation, it is enough to consider the fundamental cell of the crystal as made of two points (figure 4.1).

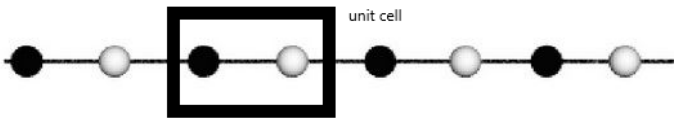


Figure 4.1: Unit cell of a 1D chain of atoms.

To see it, we observe

$$\ell^2(\mathbb{Z}) = \ell^2(\mathbb{Z}_{\text{even}}) \oplus \ell^2(\mathbb{Z}_{\text{odd}}) \simeq \ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$$

We see each couple of points as a single point with two internal degrees of freedom. We note with $\delta_n \otimes (1,0)$ and $\delta_n \otimes (0,1)$ the vectors of the basis for the nth-cell. Using this basis, we can rewrite the operator T

$$T(\delta_n \otimes (1,0)) = \delta_n \otimes (0,1) \quad \text{and} \quad T(\delta_n \otimes (0,1)) = \delta_{n+1} \otimes (1,0)$$

We can introduce the translation operator with respect to the newly introduced unit cell

$$S(\delta_n \otimes v) = \delta_{n+1} \otimes v$$

We can write the representation of T in the new basis

$$T = \begin{pmatrix} 0 & S \\ 1 & 0 \end{pmatrix}$$

Therefore,

$$H = \begin{pmatrix} a & 1+S \\ 1+S^* & -a \end{pmatrix}$$

Using Peiels's substitution (see 1.6) to partially diagonalise H, we get

$$H \mapsto \hat{H} = \begin{pmatrix} a & 1+\mathrm{e}^{\mathrm{i}k} \\ 1+\mathrm{e}^{-\mathrm{i}k} & -a \end{pmatrix}$$

We compute the characteristic polynomial of $\hat{H}$

$$P(\lambda) = (\lambda+a)(\lambda-a) - (1+\mathrm{e}^{\mathrm{i}k})(1+\mathrm{e}^{-\mathrm{i}k}) = \lambda^2 - a^2 - 2 - 2\cos k$$

The eigenvalues $E(k)$ of $\hat{H}$ are (figure 4.2)

$$E(k) = \pm\sqrt{2\cos k + 2 + a^2}$$

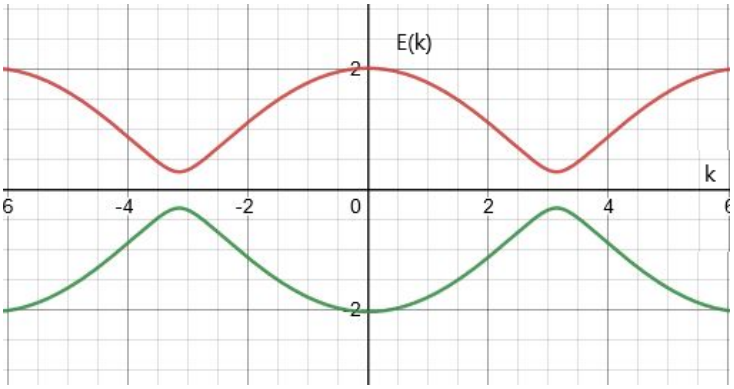


Figure 4.2: Bands in the spectrum of H ($a = 0.25$).

If we set the Fermi energy at 0, we see that the material is an insulator.

4.2. A non-trivial insulator: Haldane's model

An insulator with strictly positive spectrum corresponds to the physical situation where the Fermi level is under the first value of energy which is possible for an electron: it is an empty insulator! If the spectrum is strictly negative, we have an insulator which is completely filled up. We define these two types of insulators as *trivial*. If we consider the topological classes of equivalence, we say in general that an insulator is trivial if it is in the same homotopy class as the empty or full insulator. We could find an explicit continuous path between them, but in general it may be an hard task. Another way is to compute the *Chern number* of the insulator: it is an integer which is an invariant for the homotopy class and it is zero if and only if the insulator is trivial. We will see here a famous example of a non-trivial insulator, and, to show its non-triviality, we will compute the Chern number. We refer to [4] for the details of the description of the physical framework. We consider a two band model displaying a topological insulating phase, namely the model proposed by Haldane. We consider a tight-binding model of spinless electrons on a two-dimensional hexagonal (honeycomb) lattice. The unit cell contains two types of atoms A and B (see figure 4.3)

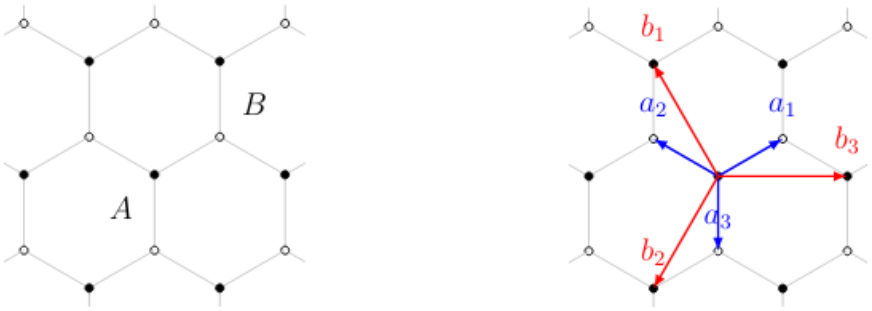


Figure 4.3: Honeycomb lattice used in Haldane's model.

The lattice parameter a, defined as the shortest distance between nearest neighbours, sets the unit of length: $a = 1$. We define the vectors

$$b_1 = \begin{pmatrix} -\sqrt{3}/2 \\ 3/2 \end{pmatrix} \quad b_2 = \begin{pmatrix} -\sqrt{3}/2 \\ -3/2 \end{pmatrix} \quad b_3 = -b_1 - b_2 = \begin{pmatrix} \sqrt{3} \\ 0 \end{pmatrix}$$

b_1 and b_2 are a basis for the Bravais lattice and we get a basis for the reciprocal lattice $\{b_1^*, b_2^*\}$ (to have an introduction to the notions of Bravais and reciprocal lattice, see [2]) imposing

$$b_i b_j^\star = 2\pi\delta_{ij}, \quad i \in \{1, 2\}$$

We get the basis

$$b_1^\star = 2\pi \begin{pmatrix} -1/\sqrt{3} \\ 1/3 \end{pmatrix} \quad b_2^\star = 2\pi \begin{pmatrix} -1/\sqrt{3} \\ -1/3 \end{pmatrix}$$

We consider as Hilbert space $\mathcal{H}$ of square integrable functions over the sites of type A and B. The form of the hamiltonian for Haldane's model is:

$$\hat{H} = t \sum_{\langle i,j \rangle} |i\rangle\langle j| + t_2 \sum_{\langle\langle i,j \rangle\rangle} |i\rangle\langle j| + M \left[\sum_{i \in A} |i\rangle\langle i| - \sum_{j \in B} |j\rangle\langle j| \right]$$

where $|i\rangle$ represents an electronic state localised at site i , $\langle i, j\rangle$ represents nearest neighbours lattice sites i and j, $\langle\langle i, j\rangle\rangle$ represents second nearest neighbours sites i, j, $i \in A$ represents sites in the sublattice A (resp. $i \in B$ in the sublattice B) and t and t_2 are hopping parameters. The first term represents the transition of the electron from one site to the nearest neighbour sites (the nearest neighbour hopping term), while the second term stands for the transition to the second neighbour sites. The third term contains a projection on the sites of type A and a projection on sites of type B. Using the Bloch-Floquet

transform, we obtain the following hamiltonian:

$$H(k) = \sum_{j\in\{0,x,y,z\}} h^j(k)\sigma_j$$

where σ_j are the Pauli matrices ($\sigma_0 = I_2$) and h_j are real functions given by

$$h_0 = 2t_2 \cos\phi \sum_{i=1}^{3} \cos(k\cdot b_i) \qquad h_z = M - 2t_2 \sin\phi \sum_{i=1}^{3} \sin(k\cdot b_i)$$
$$h_x = t\left[1 + \cos(k\cdot b_1) + \cos(k\cdot b_2)\right] \quad h_y = t\left[\sin(k\cdot b_1) - \sin(k\cdot b_2)\right]$$

The parameter ϕ is the Aharonov-Bohm phase due to the local magnetic flux.

We notice, as it should be, that for n, $m \in \mathbb{Z}$

$$\vec{h}(k + nb_1^* + mb_2^*) = \vec{h}(k).$$

The periodicity of $\vec{h}(k)$ with respect to the translations by b_1^* and b_2^* allows us to identify the opposite sides in the parallelogram corresponding to b_1^* and b_2^*: we get the torus S (see figure 4.4). This torus is the *Brioullin zone* of the crystal.

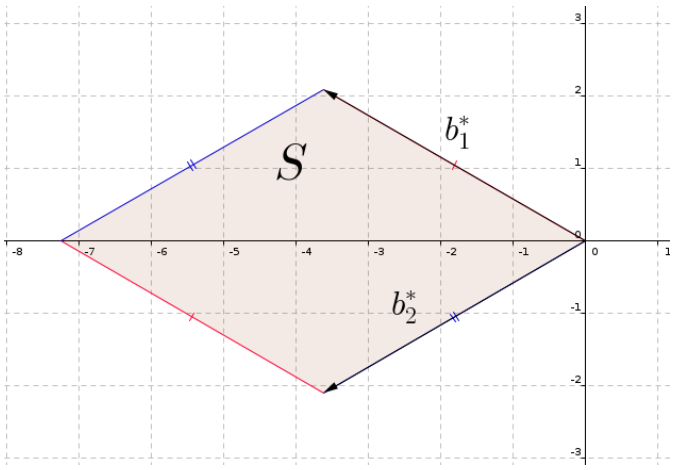


Figure 4.4: Brioullin zone (quasimomentum space).

We can easily compute the eigenvalues $\epsilon_\pm$ of $H(k)$

$$\epsilon_\pm(k) = h_0(k) \pm h(k)$$

where $h(k) = \sqrt{h_x^2 + h_y^2 + h_z^2}$. Therefore, the insulator has two bands. We see that, when $h(k) > 0\ \forall k$ (which corresponds, as we will see later, to the condition $\frac{M}{t_2} \neq \pm 3\sqrt{3}\sin(\phi)$),

the energy bands are separated. The material is an insulator whenever the lower band is completely filled up and the upper one is empty. We are interested in the topology of the filled band. Therefore, we look for the eigenvector $u(k)$ of $H(k)$ corresponding to $\epsilon_-(k)$ (i.e. such that $H(k)u(k) = \epsilon_-(k)u(k)$). We find

$$u(k) = \begin{pmatrix} h_z(k) - h(k) \\ h_x(k) + \mathrm{i}h_y(k) \end{pmatrix}$$

We must be careful: this vector is an eigenvector only for the values of k where $u \neq \vec{0}$. We define $\hat{u}$ the normalisation of u and consider the projection operator $P(k) = |\hat{u}(k)\rangle\langle\hat{u}(k)|$, the projection along the $\hat{u}(k)$. The first *Chern number* is defined as (see [8] for an introduction with more details)

$$c_1 = \frac{1}{2\pi\mathrm{i}} \int_S \mathrm{Tr}(P)\mathrm{d}P\mathrm{d}P$$

While we might not be able to extend $\hat{u}$ to a continuous non-zero eigenvector over all of S, this can be done for P. Therefore, the previous integral is well defined. However, to compute c_1 practically, we can consider a surface $S_\varepsilon \subset S$, where we exclude from S a "small" surface of measure of order ε containing the singularities of $\hat{u}$, and C_ε its boundary: we can show the following formula

$$\int_{S_\varepsilon} \mathrm{Tr}(P)\mathrm{d}P\mathrm{d}P = \int_{C_\varepsilon} \langle\hat{u}|\mathrm{d}\hat{u}\rangle = \int_0^1 \langle\hat{u}(m(t))|\mathrm{d}\hat{u}(m(t))\rangle \mathrm{d}t \tag{4.1}$$

where $\mathrm{d}\hat{u}(m(t)) = \mathrm{d}_t\hat{u}(m(t))$, with $m(t)$ a parametrisation of C_ε. With this formula, we get

$$c_1 = \lim_{\varepsilon\to 0} \frac{1}{2\pi\mathrm{i}} \int_{C_\varepsilon} \langle\hat{u}|\mathrm{d}\hat{u}\rangle$$

We give a proof of 4.1. Using the properties of the exterior derivative d, we get

$$\mathrm{d}P\mathrm{d}P = |\mathrm{d}\hat{u}\rangle\langle\hat{u}|\mathrm{d}\hat{u}\rangle\langle\hat{u}| + |\hat{u}\rangle\langle\mathrm{d}\hat{u}|\mathrm{d}\hat{u}\rangle\langle\hat{u}| + |\mathrm{d}\hat{u}\rangle\langle\hat{u}|\hat{u}\rangle\langle\mathrm{d}\hat{u}| + |\hat{u}\rangle\langle\mathrm{d}\hat{u}|\hat{u}\rangle\langle\mathrm{d}\hat{u}|$$

Last identity holds for points, at which $\hat{u}$ is well defined and C^1. Then

$$\mathrm{Tr}(P\mathrm{d}P\mathrm{d}P) = \langle\hat{u}|\mathrm{d}\hat{u}\rangle\langle\hat{u}|\mathrm{d}\hat{u}\rangle + \langle\mathrm{d}\hat{u}|\mathrm{d}\hat{u}\rangle + \langle\hat{u}|\mathrm{d}\hat{u}\rangle\langle\mathrm{d}\hat{u}|\hat{u}\rangle + \langle\mathrm{d}\hat{u}|\hat{u}\rangle\langle\mathrm{d}\hat{u}|\hat{u}\rangle$$

The last two terms give $\langle\hat{u}|\mathrm{d}\hat{u}\rangle\langle\mathrm{d}\hat{u}|\hat{u}\rangle + \langle\mathrm{d}\hat{u}|\hat{u}\rangle\langle\mathrm{d}\hat{u}|\hat{u}\rangle = (\mathrm{d}\langle\hat{u}|\hat{u}\rangle)\langle\mathrm{d}\hat{u}|\hat{u}\rangle = 0$ as $\langle\hat{u}|\hat{u}\rangle = 1$. Furthermore $\langle\hat{u}|\mathrm{d}\hat{u}\rangle\langle\hat{u}|\mathrm{d}\hat{u}\rangle$ is the square of a scalar valued 1-form, hence also 0 (a property

of the exterior derivative). Hence

$$\mathrm{Tr}(P\mathrm{d}P\mathrm{d}P) = \langle \mathrm{d}\hat{u}|\mathrm{d}\hat{u}\rangle$$

Finally, using the Stokes theorem, we get

$$\int_{S_\varepsilon} \mathrm{Tr}(P)\mathrm{d}P\mathrm{d}P = \int_{S_\varepsilon} \langle \mathrm{d}\hat{u}|\mathrm{d}\hat{u}\rangle = \int_{C_\varepsilon} \langle \hat{u}|\mathrm{d}\hat{u}\rangle$$

The singularities of $u(k)$ correspond to the values of k for which $u(k) = \vec{0}$ (namely where $u(k)$ is not an eigenvector for $H(k)$). The second component of $u(k)$ is zero if and only if $h_x(k) = h_y(k) = 0$ (remember that $h_x(k)$, $h_y(k)$ are real functions):

$$h_x(k) = h_y(k) = 0 \iff \sin k \cdot b_2 = \sin k \cdot b_1 \wedge 1 + \cos k \cdot b_1 + \cos k \cdot b_2 = 0$$

We define the auxiliary scalar values $\tilde{k}_1 = k \cdot b_1$ and $\tilde{k}_2 = k \cdot b_2$ and $\tilde{k}$ as the corresponding value of k. If $\sin \tilde{k}_1 = \sin \tilde{k}_2$, then either $\tilde{k}_1 = \tilde{k}_2$, either $\tilde{k}_1 + \tilde{k}_2 = \pi$. In the first case we get

$$1 + 2\cos \tilde{k}_1 = 0 \Rightarrow \tilde{k}_1 = \pm\frac{2\pi}{3}$$

In the second case, we get the contradiction

$$1 = -\cos \tilde{k}_1 - \cos \tilde{k}_2 = -\cos \tilde{k}_1 + \cos \tilde{k}_1 = 0$$

Therefore, $\tilde{k}_1 = \tilde{k}_2 = \pm\frac{2\pi}{3}$. When $\tilde{k}_1 = \tilde{k}_2 = \frac{2\pi}{3}$, we have in the standard basis of $\mathbb{R}^2$

$$\tilde{k} = \begin{pmatrix} -4\pi\frac{\sqrt{3}}{9} \\ 0 \end{pmatrix} = K_1^*$$

and

$$h_z(K_1^*) = M - 2t_2 \sin\phi(2\sin \tilde{k}_1 + \sin(-\tilde{k}_1 - \tilde{k}_2))) = M - 3\sqrt{3}t_2 \sin\phi,$$

while if $\tilde{k}_1 = \tilde{k}_2 = -\frac{2\pi}{3}$

$$\tilde{k} = \begin{pmatrix} 4\pi\frac{\sqrt{3}}{9} \\ 0 \end{pmatrix}$$

which is the same point on the torus as

$$\tilde{k} + b_1^* + b_2^* = \begin{pmatrix} -2\pi\frac{4\sqrt{3}}{9} \\ 0 \end{pmatrix} = K_2^*$$

and

$$h_z(K_2^*) = M + 3\sqrt{3}t_2 \sin\phi$$

By the way, we observe that $h(k) \neq 0\ \forall k$ if and only if $h_z(K_1^*)$, $h_z(K_1^*) \neq 0$, i.e. $\frac{M}{t_2} \neq \pm 3\sqrt{3}t_2 \sin\phi$

When the second component of $u(k)$ is zero, we have that the first one becomes

$$h_z(k) - h(k) = h_z(k) - |h_z(k)|$$

Therefore, $u(k)$ vanishes for $k = K_1^*$ (respectively K_2^*) if $h_z(K_1^*) \geq 0$ (respectively $h_z(K_2^*) \geq 0$). To fix ideas, we assume that $t_2 > 0$ and $\sin(\phi) > 0$. We get the following table

$\frac{M}{t_2}$	$-3\sqrt{3}\sin(\phi)$		$3\sqrt{3}\sin(\phi)$
$u(K_1^*)$	$\neq \vec{0}$	$\neq \vec{0}$	$= \vec{0}$
$u(K_2^*)$	$\neq \vec{0}$	$= \vec{0}$	$= \vec{0}$

We choose $K^* \in \{K_1^*, K_2^*\}$ such that $h_x(K^*) = 0$, we set $\varepsilon > 0$ and we define a curve C_ε with the map

$$m(t) = K^* + \varepsilon(\cos(2\pi t)b_1^* + \sin(2\pi t)b_2^*), \quad t \in [0, 1)$$

Developing h_x and h_y around the point K^*, on C_ε we can write

$$(h_x + \mathrm{i}h_y)(k) = c(k)\varepsilon\xi(k) + o(\varepsilon)$$

where $c \in \mathcal{O}(1)$, $c(k) > 0$ and $\xi(k) \in \mathbb{S}^1 \subset \mathbb{C}$. We saw previously that if $h_z(K^*) < 0$, then $\hat{u}(K^*)$ is properly defined. Therefore, we focus just on the case $h_z(K^*) > 0$.

Using a Taylor expansion, we remark that

$$h_z - h = h_z\left(1 - \sqrt{1 + \frac{h_x^2 + h_y^2}{h_z^2}}\right) = h_z\left(1 - 1 - \frac{(c\varepsilon)^2}{2h_z^2}\right) + o(\varepsilon^2) = \mathcal{O}(\varepsilon^2).$$

We can write

$$u = \begin{pmatrix} 0 \\ c\varepsilon\xi \end{pmatrix} + \mathcal{O}(\varepsilon^2)$$

and we have $|u| \simeq c\varepsilon$. Then

$$\hat{u} = \begin{pmatrix} 0 \\ \xi \end{pmatrix} + \mathcal{O}(\varepsilon) \simeq \begin{pmatrix} 0 \\ \xi \end{pmatrix}$$

Finally, $\langle \hat{u} | \mathrm{d}\hat{u} \rangle = \bar{\xi}\mathrm{d}\xi + \mathcal{O}(\varepsilon)$ We define the map

$$\begin{aligned} \gamma : [0,1] &\to \mathbb{C} \\ t &\mapsto \xi(m(t)) \end{aligned}$$

We can link the formula for $\langle \hat{u} | \mathrm{d}\hat{u} \rangle$ and the index for the curve γ. Indeed

$$\begin{aligned} 2\pi\mathrm{i} \cdot \mathrm{ind}_\gamma(0) &= \int_0^1 \frac{\gamma'(t)}{\gamma(t)}\mathrm{d}t = \int_0^1 \frac{\bar{\gamma}(t)\gamma'(t)}{|\gamma(t)|^2}\mathrm{d}t = \int_{C_\varepsilon} \bar{\xi}\mathrm{d}\xi \\ &= \int_{C_\varepsilon} \langle \hat{u} | \mathrm{d}\hat{u} \rangle + \mathcal{O}(\varepsilon) \\ &= 2\pi\mathrm{i} \cdot c_1 + \mathcal{O}(\varepsilon) \end{aligned}$$

Here the $\mathcal{O}(\varepsilon)$ must be 0, as we know that $\mathrm{ind}_\gamma(0)$ and c_1 must be integer. Moreover, if we define

$$\begin{aligned} \phi : [0,1] &\to \mathbb{C} \\ t &\mapsto (h_x + \mathrm{i}h_y)(m(t)) \end{aligned}$$

we see that, by definition of ξ, $\mathrm{ind}_\gamma(0) = \mathrm{ind}_\phi(0)$. One way to compute $\mathrm{ind}_\phi(0)$ is using the formula:

$$\begin{aligned} \mathrm{ind}_\phi(0) = &\,\mathrm{card}\left(\{s \in [0,1) \text{ s.t. } h_x(m(s)) = 0, h_y(m(s)) > 0, h_x'(m(s)) < 0\}\right) \\ &- \mathrm{card}\left(\{s \in [0,1) \text{ s.t. } h_x(m(s)) = 0, h_y(m(s)) > 0, h_x'(m(s)) > 0\}\right) \end{aligned}$$

Using the previous formula, we are just counting how many times we are crossing the positive side of the imaginary axis; the sign of the derivative defines if the curve is crossing it clock or anti-clockwise. For $i \in \{1,2\}$ we define the maps

$$\rho_i(t) = K_i^* + \varepsilon(\cos(2\pi t)b_1^* + \sin(2\pi t)b_2^*), \quad t \in [0,1)$$

and the curve in $\mathbb{C}$

$$\begin{aligned} \phi_i : [0,1] &\to \mathbb{C} \\ t &\mapsto (h_x + \mathrm{i}h_y)(\rho_i(t)) \end{aligned}$$

First we consider $i = 1$. We look for $\bar{s}$ s.t. $h_x(\rho_1(\bar{s})) = 0$.

$$h_x(\rho_1(s)) = t\left(1 + \cos\left(\frac{2}{3}\pi + 2\pi\varepsilon\cos(2\pi s)\right) + \cos\left(\frac{2}{3}\pi + 2\pi\varepsilon\sin(2\pi s)\right)\right)$$

We define

$$f_1(s) = \cos\left(\frac{2}{3}\pi + 2\pi\varepsilon\cos(2\pi s)\right)$$
$$f_2(s) = \cos\left(\frac{2}{3}\pi + 2\pi\varepsilon\sin(2\pi s)\right)$$

We sum up in the following table the qualitative behaviour of $h_x(\rho_1(s))$ (up and down-going arrows mean that the functions are strictly increasing and decreasing on the interval).

s	0	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{3}{4}$	1
f_1	$< -\frac{1}{2}$ ↗	$-\frac{1}{2}$ ↗	$> -\frac{1}{2}$ ↘	$-\frac{1}{2}$ ↘	$< -\frac{1}{2}$
f_2	$-\frac{1}{2}$ ↘	$< -\frac{1}{2}$ ↗	$-\frac{1}{2}$ ↗	$> -\frac{1}{2}$ ↘	$< -\frac{1}{2}$
$h_x(\rho_1(s)) = t(f_1 + f_2)$	< -1 →	< -1 ↗	> -1 →	> -1 ↘	< -1

From the previous table we see that it exists $\bar{s}_1 \in (\frac{1}{4}, \frac{1}{2})$ and $\bar{s}_2 \in (\frac{3}{4}, 1)$ such that $\bar{s}_1$ and $\bar{s}_2$ are the only solutions of $h_x(\rho_1(s)) = 0$. We must check the sign of $h_y(\rho_1(\bar{s}_i))$.

$$h_y(\rho_1(s)) = t\left(\sin\left(\frac{2}{3}\pi + 2\pi\varepsilon\cos(2\pi s)\right) - \sin\left(\frac{2}{3}\pi + 2\pi\varepsilon\sin(2\pi s)\right)\right)$$

We easily see that just $\bar{s}_1$ satisfies $h_y(\rho_1(\bar{s}_1)) > 0$.

We note with ∂_1 and ∂_2 the derivatives in the directions b_1^* and b_2^*. To simplify the computation of $\partial_s h_x(\rho_1(s))$, we will use the following relations (coming from the conditions $b_i b_j^\star = 2\pi\delta_{ij}$ when $i \in \{1, 2\}$)

$$\partial_1(k \cdot b_1) = 2\pi \qquad \partial_1(k \cdot b_2) = 0 \qquad \partial_1(k \cdot b_3) = -2\pi$$
$$\partial_2(k \cdot b_1) = 0 \qquad \partial_2(k \cdot b_2) = 2\pi \qquad \partial_2(k \cdot b_3) = -2\pi$$

We compute $\partial_s h_x(\rho_1(s))$

$$\begin{aligned}\partial_s h_x(\rho_1(s)) &= (\partial_1 h_x, \partial_2 h_x)(\rho_1(s)) \cdot \mathrm{d}_s\rho_1(s)\\ &= (-2\pi t\sin(\rho_1(s)\cdot b_1), -2\pi t\sin(\rho_1(s)\cdot b_2)) \cdot (-2\pi\varepsilon\sin(2\pi s), 2\pi\varepsilon\cos(2\pi s))\\ &= \alpha\left(\sin\left(\frac{2}{3}\pi + 2\pi\varepsilon\cos(2\pi s)\right)\sin(2\pi s) - \sin\left(\frac{2}{3}\pi + 2\pi\varepsilon\sin(2\pi s)\right)\cos(2\pi s)\right)\\ &\quad (\alpha > 0)\end{aligned}$$

We verify that $\partial_s h_x(\rho_1(\bar{s}_1)) > 0$ and therefore

$$\mathrm{ind}_{\phi_1}(0) = -1$$

Now we consider $i = 2$.

$$h_x(\rho_2(s)) = t\left(1 + \cos\left(\frac{2}{3}\pi - 2\pi\varepsilon\cos(2\pi s)\right) + \cos\left(\frac{2}{3}\pi - 2\pi\varepsilon\sin(2\pi s)\right)\right)$$

We define

$$g_1(s) = \cos\left(\frac{2}{3}\pi - 2\pi\varepsilon\cos(2\pi s)\right)$$
$$g_2(s) = \cos\left(\frac{2}{3}\pi - 2\pi\varepsilon\sin(2\pi s)\right)$$

s	0	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{3}{4}$	1
g_1	$> -\frac{1}{2}$ ↘	$-\frac{1}{2}$ ↘	$< -\frac{1}{2}$ ↗	$-\frac{1}{2}$ ↗	$> -\frac{1}{2}$
g_2	$-\frac{1}{2}$ ↗	$> -\frac{1}{2}$ ↘	$-\frac{1}{2}$ ↘	$< -\frac{1}{2}$ ↗	$-\frac{1}{2}$
$h_x(\rho_2(s)) = t(g_1 + g_2)$	> -1 →	> -1 ↘	< -1 →	< -1 ↗	> -1

Again, from the previous table we see that it exists $\bar{q}_1 \in (\frac{1}{4}, \frac{1}{2})$ and $\bar{q}_2 \in (\frac{3}{4}, 1)$ such that

$\bar{q}_1$ and $\bar{q}_2$ are the only solutions of $h_x(\rho_2(s)) = 0$.

$$\begin{aligned} h_y(\rho_2(s)) &= t\left(\sin\left(-\frac{2}{3}\pi + 2\pi\varepsilon\cos(2\pi s)\right) - \sin\left(-\frac{2}{3}\pi + 2\pi\varepsilon\sin(2\pi s)\right)\right) \\ &= t\left(\sin\left(\frac{2}{3}\pi - 2\pi\varepsilon\sin(2\pi s)\right) - \sin\left(\frac{2}{3}\pi - 2\pi\varepsilon\cos(2\pi s)\right)\right) \end{aligned}$$

Just $\bar{q}_1$ satisfies $h_y(\rho_2(\bar{q}_1)) > 0$.

We compute $\partial_s h_x(\rho_2(s))$

$$\begin{aligned} \partial_s h_x(\rho_2(s)) &= (-2\pi t\sin(\rho_2(s)\cdot b_1), -2\pi t\sin(\rho_2(s)\cdot b_2))\cdot(-2\pi\varepsilon\sin(2\pi s), 2\pi\varepsilon\cos(2\pi s)) \\ &= \alpha\left(\sin\left(\frac{2}{3}\pi - 2\pi\varepsilon\sin(2\pi s)\right)\cos(2\pi s) - \sin\left(\frac{2}{3}\pi - 2\pi\varepsilon\cos(2\pi s)\right)\sin(2\pi s)\right) \\ &(\alpha > 0) \end{aligned}$$

We verify that $\partial_s h_x(\rho_2(\bar{q}_1)) < 0$ and therefore

$$\mathrm{ind}_{\phi_2}(0) = 1.$$

The Chern number c_1 is given by

$$c_1 = \mathrm{ind}_{\phi_1}(0) + \mathrm{ind}_{\phi_2}(0)$$

(in the previous formula we set $\mathrm{ind}_{\phi_i}(0)$ to 0 when $u(K_i^*) \neq \vec{0}$). Finally, we obtain the following table summing up the results.

$\frac{M}{t_2}$	$-3\sqrt{3}\sin(\phi)$		$3\sqrt{3}\sin(\phi)$
$\mathrm{ind}_{\phi_1}(0)$	0	0	-1
$\mathrm{ind}_{\phi_2}(0)$	0	1	1
c_1	0	1	0

When $-3\sqrt{3}\sin(\phi) < \frac{M}{t_2} < 3\sqrt{3}\sin(\phi)$ the Haldane insulator is not trivial!

4.3. Gradings and real structures on examples

In order to understand better the nature of gradings and real structures, it was very useful for me to practise on some examples. Moreover, even if we will focus on the easiest cases, the following examples are fundamental as they recur often when dealing with topological

insulators. In this section I will show how to find the possible gradings and real structures in the case of the C^*-algebras $\mathbb{C}$, $\mathbb{C}\oplus\mathbb{C}$, $M_2(\mathbb{C})$ and $M_n(\mathbb{C})$.

In the following, we will often use the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

These matrices anti-commute pairwise, are self-adjoint and they square to the identity (therefore, they are unitary).

4.3.1. $\mathbb{C}$

This case is extremely simple. The only possible grading is the identity. Indeed, if γ is a grading, then we have $\gamma(1) = 1$ and therefore, by $\mathbb{C}$-linearity, $\forall a \in \mathbb{C}$, $\gamma(a) = a$. If $\mathfrak{r}$ is a real structure, by anti-linearity, $\mathfrak{r}(a) = \bar{a} \cdot \mathfrak{r}(1) = \bar{a}$ and therefore, the only possible real structure is the complex conjugation (which of course commutes with the identity).

4.3.2. $\mathbb{C}\oplus\mathbb{C}$

Let γ be a grading over $\mathbb{C}\oplus\mathbb{C}$. If we choose a basis for the finite dimensional vector space $\mathbb{C}\oplus\mathbb{C}$ (for example $\{(1,0),(0,1)\}$), by $\mathbb{C}$-linearity we can represent γ via a matrix M,

$$M = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

γ preserves the unity $(1,1)$: we get the condition $a+b=c+d=1$. The condition $\gamma^2 = \mathrm{id}$ implies $M^2 = I_2$ which gives

$$\begin{pmatrix} a^2+(1-a)(1-d) & (a+d)(1-a) \\ (a+d)(1-d) & d^2+(1-a)(1-d) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

If $a+d=0$, we just obtain $\gamma = \mathrm{id}$. If $a+d \neq 0$, the condition for γ of preserving the multiplication implies

$$M = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

and therefore, $\gamma(s,t) = (t,s)$ (the "flip" automorphism). In this case there are just two possible gradings. The trivial grading is of course not balanced (there is no odd element), while the second one is balanced ($(1,-1)$ is an odd element squaring to the identity). We consider the flip automorphism as the standard grading for $\mathbb{C}\oplus\mathbb{C}$.

We look for the real structures (which, by definition, commute with the grading). First of all, we remark that $\mathfrak{r}$ is anti-linear if and only if $\bar{\mathfrak{r}}$ is $\mathbb{C}$-linear. As before, we can say that $\bar{\mathfrak{r}}$ is represented by the matrix N. The commuting condition between $\bar{N}$ and M forces N to be under the form

$$N = \begin{pmatrix} a & b \\ b & a \end{pmatrix}$$

The condition $\mathfrak{r}^2 = \mathrm{id}$ gives $\bar{N}N = I_2$. Therefore

$$\begin{pmatrix} |a|^2 + |d|^2 & \bar{a}b + \bar{b}a \\ \bar{a}b + \bar{b}a & |a|^2 + |d|^2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$\mathfrak{r}$ preserves the multiplication. We get that

- either $a = 1$ and $b = 0$: the corresponding real structure is

$$\mathfrak{r}(s, t) = (\bar{s}, \bar{t})$$

- either $a = 0$ and $b = 1$: the corresponding real structure is

$$\mathfrak{r}(s, t) = (\bar{t}, \bar{s})$$

4.3.3. $M_2(\mathbb{C})$

Thanks to Skolem-Noether theorem, we know that for every $\mathbb{C}$-linear automorphism γ on $M_2(\mathbb{C})$ it exists $\sigma \in M_2(\mathbb{C})$ such that $\gamma = \mathrm{Ad}_\sigma$. $\gamma^2 = \mathrm{id}$, therefore, $\forall M \in M_2(\mathbb{C})$

$$\sigma^2 M (\sigma^{-1})^2 = M \Rightarrow \sigma^2 M = M\sigma^2$$

i.e. σ^2 commutes with all matrices of $M_2(\mathbb{C})$. As a consequence, we have $\sigma^2 = \lambda I$. As we can multiply σ by a scalar without modifying the grading γ, we can choose $\lambda = 1$ and then the eigenvalues of σ are contained in $\{1, -1\}$. There are two possibilities:

- either $\sigma = I$: γ is the trivial grading;
- either σ is similar to σ_z. Up to a changing of the basis, the only non-trivial grading is $\gamma = \mathrm{Ad}_{\sigma_z}$

Once more, the trivial grading is not balanced. On the other hand, σ_x is odd and squares to I: Ad_{σ_z} is balanced.

If $\mathfrak{r}$ is a real structure over $M_2(\mathbb{C})$, then $\bar{\mathfrak{r}}$ is a $\mathbb{C}$-linear automorphism: therefore it exists

$\sigma \in M_2(\mathbb{C})$ such that $\mathfrak{r} = \overline{\mathrm{Ad}_\sigma}$. We note with $\mathfrak{c}$ the complex conjugation. $\mathfrak{r}$ commutes with the grading γ, so

$$\mathrm{Ad}_{\sigma_z} \circ \mathfrak{c} \circ \mathrm{Ad}_\sigma = \mathfrak{c} \circ \mathrm{Ad}_\sigma \circ \mathrm{Ad}_{\sigma_z} \iff \mathrm{Ad}_{\sigma_z\sigma} = \mathrm{Ad}_{\sigma\sigma_z}$$

$$\iff (\sigma\sigma_z)^{-1}(\sigma_z\sigma)M = M(\sigma\sigma_z)^{-1}(\sigma_z\sigma) \quad \forall M \in M_2(\mathbb{C})$$

$$\iff (\sigma\sigma_z)^{-1}(\sigma_z\sigma) = \mu I \quad \mu \in \mathbb{C}$$

and therefore

$$\sigma_z\sigma = \mu\sigma\sigma_z$$

There is a unique decomposition of σ in an even term and a odd one, namely $\sigma = \sigma_{ev} + \sigma_{odd}$ with

$$\sigma_{ev} = \frac{1}{2}(\sigma + \gamma(\sigma)) \quad \sigma_{odd} = \frac{1}{2}(\sigma - \gamma(\sigma))$$

On one side we have

$$\mathrm{Ad}_{\sigma_z}(\sigma) = \sigma_z\sigma\sigma_z = \mu\sigma = \mu\sigma_{ev} + \mu\sigma_{odd}$$

and on the other

$$\mathrm{Ad}_{\sigma_z}(\sigma) = \gamma(\sigma_{ev}) + \gamma(\sigma_{odd}) = \sigma_{ev} - \sigma_{odd}$$

Therefore, we have

$$(1-\mu)\sigma_{ev} = 0 \quad \text{and} \quad (1+\mu)\sigma_{odd} = 0$$

So

$$\sigma_z\sigma = \pm\sigma\sigma_z \tag{4.2}$$

The condition $\mathfrak{r}^2 = \mathrm{id}$ gives $\bar{\sigma}\sigma M = M\bar{\sigma}\sigma$, $\forall M \in M_2(\mathbb{C})$ and therefore

$$\bar{\sigma}\sigma = \lambda I \quad \lambda \in \mathbb{C} \tag{4.3}$$

Finally, the condition $\mathfrak{r}(M^*) = (\mathfrak{r}(M))^*$ gives $\sigma^*\sigma M = M\sigma^*\sigma$, $\forall M \in M_2(\mathbb{C})$ and therefore

$$\sigma^*\sigma = \eta I \quad \eta \in \mathbb{C} \tag{4.4}$$

Now, we can put 4.2, 4.3 and 4.4 together.

- **Case 1**, $\sigma_z\sigma = \sigma\sigma_z$. In this case σ is a diagonal matrix. Equation 4.3 gives (remember that we can multiply σ by a scalar)

$$\sigma = \sigma_\theta = \begin{pmatrix} 1 & 0 \\ 0 & \mathrm{e}^{\mathrm{i}\theta} \end{pmatrix} \quad \theta \in (0, 2\pi]$$

- **Case 2**, $\sigma_z\sigma = -\sigma\sigma_z$. σ is a off-diagonal matrix.

$$\sigma = \begin{pmatrix} 0 & b \\ c & 0 \end{pmatrix}$$

Equation 4.3 implies that $\bar{b}c$ is real and equation 4.4 that $|b| = |c|$. These two condition imply $b = \pm c$. Therefore, $\sigma = \sigma_x$ or $\sigma = \mathrm{i}\sigma_y$

We define the real structures $r_\theta = c \circ \mathrm{Ad}_{\sigma_\theta}$, $r_x = c \circ \mathrm{Ad}_{\sigma_x}$ and $r_y = c \circ \mathrm{Ad}_{\mathrm{i}\sigma_y}$. We see that there are infinitely many real structures. However, we see that the real structures r_θ are quite "similar": we would like to say that they are equivalent. Indeed, we can prove that they are inner conjugate (definition 18): we fix $\theta \in (0, 2\pi]$ and we show that $r_0 = c \circ \mathrm{Ad}_{\sigma_0}$ and r_θ are inner conjugate. We define

$$w_\theta = \begin{pmatrix} 1 & 0 \\ 0 & \mathrm{e}^{\frac{\mathrm{i}\theta}{2}} \end{pmatrix}$$

and we verify that w_θ satisfies:

- $w_\theta^* w_\theta = I$ (w_θ is a unitary)
- $r_0(w_\theta M w_\theta^*) = w_\theta r_\theta(M) w_\theta^*$, $\forall M \in M_2(\mathbb{C})$
- $\mathrm{Ad}_{\sigma_z} \circ \mathrm{Ad}_{w_\theta} = \mathrm{Ad}_{w_\theta} \circ \mathrm{Ad}_{\sigma_z}$

Now, we would like to prove that between r_0, r_x and r_y there are no inner conjugate couple. We just show the case r_0 and r_x are not inner conjugate, the other cases being analogous. If r_0 and r_x are inner conjugate via the unitary w, from $r_0(wMw^*) = wr_x(M)w^*$, $\forall M \in M_2(\mathbb{C})$ we get

$$w\sigma_x = \lambda\bar{w}$$

From $\mathrm{Ad}_{\sigma_z} \circ \mathrm{Ad}_w = \mathrm{Ad}_w \circ \mathrm{Ad}_{\sigma_z}$ we get

$$\sigma_z w = \mu w \sigma_z$$

As before (decomposition of w in even and odd elements), we find $\mu = \pm 1$. In both cases, we find a contradiction with the previous equation.

Remark. We have just found that in the case $M_2(\mathbb{C})$, up to inner conjugation, we have three possible real structures. It is interesting to compare this result to the Corollary 4.15 of [5].

Corollary 4.0.1. *Up to stabilization and inner conjugation, there are four different bal-*

anced graded real structures on $M_n(\mathbb{C})$ [...].

It means that three out of four real structures of $M_n(\mathbb{C})$ appear in the $n = 2$ case. To find the fourth real structure, we must consider the stabilisation of $M_2(\mathbb{C})$.

4.3.4. $M_n(\mathbb{C})$

If γ is a grading, then there exists $\Gamma \in M_n(\mathbb{C})$ such that $\gamma = \mathrm{Ad}_\Gamma$. With the same computations as in the case of the gradings over $M_2(\mathbb{C})$, we can show that, up to changing of the basis, Γ can be one of the $\Gamma_k \in M_n(\mathbb{C})$

$$\Gamma_k = \begin{pmatrix} I_k & 0_{k,n-k} \\ 0_{n-k,k} & -I_{n-k} \end{pmatrix}, \quad k \in \{0, 1 \dots n\}$$

We are interested in *balanced* gradings, namely a grading for which it exists $M \in M_n(\mathbb{C})$ such that (1) $\gamma(M) = -M$ and (2) $M^* = M = M^{-1}$. From (1)

$$-M = -\begin{pmatrix} M_1 & M_2 \\ M_3 & M_4 \end{pmatrix} = \Gamma M \Gamma = \begin{pmatrix} M_1 & -M_2 \\ -M_3 & M_4 \end{pmatrix}$$

we have that M has the shape

$$M = \begin{pmatrix} 0 & M_2 \\ M_3 & 0 \end{pmatrix}$$

with $M_2 \in M_{k,n-k}(\mathbb{C})$ and $M_3 \in M_{n-k,k}(\mathbb{C})$. This shape implies

$$M \begin{pmatrix} \mathbb{C}^k \\ 0_{n-k} \end{pmatrix} = \begin{pmatrix} 0_k \\ \mathbb{C}_{n-k} \end{pmatrix} \quad \text{and} \quad M \begin{pmatrix} 0_k \\ \mathbb{C}_{n-k} \end{pmatrix} = \begin{pmatrix} \mathbb{C}_k \\ 0_{n-k} \end{pmatrix}$$

From (2) we have that M is invertible, therefore, from previous condition, $k = n - k$ and so $n = 2k$. To sum up,

- if n is **even**, there is **one and only one** balanced grading $\gamma = \mathrm{Ad}_{\Gamma_{n/2}}$;
- if n is **odd**, there is **no** balanced grading.

Now we look for real structures. From corollary 4.0.1, we know that we there are just four real structures. We obtain three of them just extending the ones we found in the case $n = 2$. Indeed, we can see $M_n(\mathbb{C})$ as $M_k(M_2(\mathbb{C})) \simeq M_k(\mathbb{C}) \otimes M_2(\mathbb{C})$: we extend $\mathfrak{r}$ real structure over $M_2(\mathbb{C})$ with $\mathfrak{c} \otimes \mathfrak{r}$ ($\mathfrak{c}$ is the entry-wise complex conjugation) over $M_k(\mathbb{C}) \otimes M_2(\mathbb{C})$ (we apply $\mathfrak{r}$ to each 2×2 bloc of the matrix). To find the last real structure, as described in the proof of 4.0.1, we must realise the last possibility for the

sign (see definition 19). The last real structure appears over $M_2(\mathbb{C}) \otimes M_2(\mathbb{C})$. It is defined as

$$r_4 = \mathrm{Ad}_{\sigma_y} \circ \mathfrak{c} \otimes \mathfrak{c}$$

We can "extend" this last real structure to $M_k(M_4(\mathbb{C})) \simeq M_k(\mathbb{C}) \otimes M_4(\mathbb{C})$ with $\mathfrak{c} \otimes r_4$. To sum up, the four real structures up to stabilisation and inner conjugation on $M_n(\mathbb{C})$ are

Real structures on $M_n(\mathbb{C})$

	n	**real structure**
r_1	2	$\mathfrak{c}$
r_2	2	$\mathrm{Ad}_{\sigma_x} \circ \mathfrak{c}$
r_3	2	$\mathrm{Ad}_{\sigma_y} \circ \mathfrak{c}$
r_4	4	$\mathrm{Ad}_{\sigma_y} \circ \mathfrak{c} \otimes \mathfrak{c}$

4.3.5. Link with the classification of topological phases

As we saw at the end of 1.6, the typical C^*-algebra which is considered in the applications is

$$A = \mathcal{C}((\mathbb{S}^1)^d) \otimes M_N(\mathbb{C})$$

where $\mathcal{C}((\mathbb{S}^1)^d)$ stands for the spatial part and $M_N(\mathbb{C})$ acts on the internal degrees of freedom. Following the approach described in chapter 3, when there is no chiral symmetry we must tensor the C^*-algebra with $\mathbb{C}l_1$ to recover the existence of an odd element and to use Van Daele's theory

$$\mathcal{C}((\mathbb{S}^1)^d) \otimes M_N(\mathbb{C}) \otimes \mathbb{C}l_1.$$

It is easy to see that

$$M_N(\mathbb{C}) \otimes \mathbb{C}l_1 \cong M_N(\mathbb{C}) \oplus M_N(\mathbb{C}).$$

We can see how the study of the real structures over C^*-algebras of the type $M_N(\mathbb{C})$ is important, as they appear recurrently.

5 | Conclusions and future developments

Let us conclude this work with an overview of possible applications in technology of topological insulators. We have seen that the key property of topological phases is the stability to exterior perturbations in the sense that we can find physical properties which are highly robust to noise. For example we mentioned the Chern number and the Hall transversal resistivity. Another example could be edge currents: we can easily imagine to use these materials to encode information with a low risk of error. This is why topological insulators are extremely interesting for the development of quantum computers, in particular for the topological quantum computers (see [7]). Aside from quantum computers, other promising applications are in the field of photodetectors, magnetic devices, field-effect transistors and lasers: a review can be found in [12].

I hope that with this work I could give a glimpse of why mathematics has a fundamental role to study these materials. Using C^*-algebras and K-theory we can obtain a fine description of the possible physical frameworks and of the structure of the set of topological phases. It is charming the idea that through mathematics we can predict the existence of a material which still does not exist! Then, it will be the task of the chemist/engineer to "build" in practice the hamiltonian which was postulated by the mathematician.

Concerning the continuation of this project, the idea is to compare the mathematical approach to classify topological phases of [5] to another one, namely the one presented in [1]. Also in the second approach Van Daele's picture is used to classify topological phases but taking a different starting point: it would be interesting to find the link between the results of the two approaches and determine if they are equivalent.

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