Quasicrystals, C*-algebras and K-theory

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Abstract

Quasicrystals are a phase between crystals and amorphous materials, exhibiting long-range order without periodicity. We review attempts to provide a theory of electronic transport in quasicrystals that may generalize Bloch theory. To this end, we introduce groupoid C*-algebras, and use these to develop Noncommutative Topology. This can be used to obtain a noncommutative C*-algebra of observables in the aperiodic case that is a generalization of its periodic counterpart. The K-theory of this C*-algebra is used to obtain a labelling of the gaps in the spectrum of one-electron Hamiltonians, and this labelling can be linked to the value of the integrated density of states on the gaps. Finally, we study a well-known one-dimensional quasiperiodic example.

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Chapter 1

Introduction

Intuitively, a crystal is thought of as a solid, in which the atoms are configured in an "ordered" way. This order is reflected by the discreteness of the diffraction spectrum of a crystal, showing sharp spots (Bragg peaks), which is in contrast to the continuous -"blurred"- diffraction spectrum of unordered materials such as glass. For a long time, it was thought that the only way to get long range order was by periodicity. Specifically, it was thought that periodicity was essential to get a discrete diffraction spectrum. Since only 2-, 3-, 4- or 6-fold symmetry are compatible with periodicity (the "crystallographic restriction"), the only symmetries that could occur in diffraction spectra were of this kind.

Therefore, it came as a surprise to the world of crystallographers when Schechtman *et al* reported in 1984 that they had made alloys of Al with 10-14 at.% Mn, Fe or Cr showing a discrete diffraction spectrum with a forbidden five-fold symmetry. Their article *Metallic Phase with Long-Range Orientational Order and No Translational Symmetry* meant a revolution in crystallography. Soon afterwards, many others constructed alloys with forbidden symmetries, using various techniques. Until now, five-fold, eight-fold, ten-fold and twelve-fold symmetries have been observed. During the eighties and nineties, the quality of the samples continued to increase, and the level of impurities has now reached the same level as in classical crystalline samples.

The new discovered phase between crystal and amorphous metal was called **quasicrystal**, and it is characterized by the fact that its diffraction spectrum is on the one hand discrete, i.e., it consists δ -functions (the Bragg peaks), and on the other hand shows a symmetry forbidden by the crystallographic restriction. The structure of d-dimensional quasicrystals (e.g. d = 3) can be modeled by projecting an n dimensional periodic lattice (with n > d) onto a d-dimensional subspace. This "projection method" can be used to obtain quasiperiodic point sets, as we will show in Chapter 2. In this chapter, it is also shown that d-dimensional tilings are an effective tool to describe quasicrystals. A different

method to obtain quasiperiodic sets, the so-called substitution method, is also explained. A one-dimensional quasiperiodic tiling called the "Fibonacci chain" will serve as a basic example of these constructions.

When the level of impurities in the quasiperiodic alloys gradually decreased, it became possible to measure the physical properties of quasicrystals in a reproducible way. Among the physical properties that are of interest are of course the electronic transport properties. It appeared that quasicrystals generically have the following electronic behaviour:

- 1. They have a very high resistivity, up to 10^3 times as large as the resistivity of periodic alloys made of the same components.
- 2. The resistivity increases with improved sample quality, which indicates that the conducting of electrons is mainly caused by impurities. Note that in ordinary metals, the situation is the other way round.
- 3. The lower the temperature, the higher the resistivity. This is typical semiconductor behaviour; for metals, the situation is the opposite.

During the last decades, people have searched for explanations of this anomalous behaviour. To set up a theory that describes electronic motion in quasicrystals, one should try to generalize the methods that have already been developed for crystals. Now the main tool to describe electronic motion in crystals is Bloch theory, developed in the late twenties. It allows to compute the spectrum of Hamiltonians describing the motion of an electron in a crystal, where the interactions with other electrons and with phonons (lattice vibrations) are neglected. Bloch theory can be used to show that in crystals, electronic wave functions are extended, and that the spectrum of the one-electron Hamiltonian is absolutely continuous, exhibiting a typical band structure. This band structure can be used to obtain conductivity properties of the crystal.

However, Bloch theory cannot be applied to quasicrystals, because it crucially depends on the periodicity of the medium. Therefore, to describe electronic motion in quasicrystals, one has to find different methods.

In the late eighties, J. Bellissard proposed to use the mathematical framework of Noncommutative Geometry, mainly developed by A. Connes, to describe electronic transport in aperiodic media. In 1994, his approach lead to a successful explanation of the well-known plateaus in the plot of conductivity versus magnetic field of the Integer Quantum Hall Effect, explaining why these plateaus are so robust under perturbations. For quasicrystals, his approach leads to the labelling of the gaps in the spectrum of the one-electron Hamiltonian by the value of the integrated density of states on these gaps. This is the main subject of this thesis.

For this gap labelling, we only use Noncommutative Topology, which is simpler than noncommutative geometry. The idea is to begin with a topological space X that is (locally) compact and Hausdorff. The topology is described by the open subsets of X, and it can be shown that all topological data are carried by the continuous, complex-valued functions on X. These functions form a commutative algebra C(X) under pointwise multiplication, and one can give this algebra the structure of a C*-algebra by defining involution * and norm $\|\cdot\|$ in an obvious way. Now an important theorem by Gelfand and Naimark states that every commutative C*-algebra can be seen as the C*-algebra of continuous functions on a (locally) compact Hausdorff space, called the structure space. This theorem can be used to form a dictionary between the topological and the C*-algebraic side.

The philosophy of noncommutative topology is now to view the C*-algebra as the main data, instead of the underlying space, and to generalize this to arbitrary (not necessarily commutative) C*-algebras. An important theorem of Gelfand and Naimark characterizes noncommutative C*-algebras by stating that every C*-algebra is isomorphic to a C*-subalgebra of $\mathcal{B}(\mathcal{H})$, the C*-algebra of bounded operators on some Hilbert space \mathcal{H} . People have tried to find noncommutative analogues of the structure space, and especially the pure state space and the space of unitary equivalence classes of irreducible representations were considered to be good candidates. These matters were developed mainly before the eighties. We will review this in Chapter 3.

Then, during the eighties, A. Connes found a way to use noncommutative C^{*}algebras to describe the topology of non-Hausdorff spaces. For non-Hausdorff spaces, the C^{*}-algebra of continuous functions is too small to carry all the relevant topological information. However, it turned out that non-Hausdorff spaces that are quotients by a certain equivalence relation can be described by the groupoid C^{*}-algebra of the equivalence relation. This noncommutative C^{*}algebra contains all the relevant topological data. The above will be the subject of Chapter 4.

To analyze topological properties, people often use certain topological invariants. The noncommutative analogues of the structure space might serve as such invariants. However, it turned out that there is a better topological invariant at hand, namely K-theory. C*-algebraic K-theory consists of two functors, K_0 and K_1 , that assign abelian groups $K_0(A)$ and $K_1(A)$ to an arbitrary C*-algebra A. We will mainly use the K_0 -group, whose elements are obtained from the projections in a so-called stabilized version of the C*-algebra. This will be the subject of Chapter 5.

An important example of a non-Hausdorff quotient space that can effectively be described by noncommutative topology is the space of Penrose tilings. This example, designed by A. Connes, will be the subject of Chapter 6. Penrose constructed such a tiling of the plane in 1974. It was the first example of a tiling by two different tiles that covers the plane in a way such that on the one hand, the tiling is not periodic, but on the other hand, every finite patch in the tiling repeats itself infinitely often. This tiling is an important example of a quasiperiodic tiling constructed by the substitution method, and it has been used a lot to model two-dimensional quasicrystals. It turns out that the K-theory of the noncommutative C*-algebra associated to the space of Penrose tilings can be used to measure the density of the two different tiles in a Penrose tiling.

The construction of the noncommutative space of Penrose tilings has been generalized to arbitrary tilings by J. Kellendonk. This space, which basically consists of all translates of a fixed *d*-dimensional tiling, is called the "hull". We define this hull in Chapter 8, and form its noncommutative C^* -algebra in the same way as in Chapter 6. We will also compare the differences and similarities between the hull and the space of Penrose tilings.

The physical motivation for the construction of the hull is the following: the motion of an electron in a (quasi-)crystal can be modeled by the motion of the electron on the tiling that is associated to the (quasi-)crystal. However, keeping the electron in the origin and moving the tiling around will lead to an equivalent description. Therefore, the set of all translates of the tiling can be used to describe the motion of an electron in the tiling. We also define a discrete version of the hull, to describe the discrete model of an electron hopping from tile to tile. The discrete model is simpler to compute, and it turns out that it contains the same data as the continuous model, which is reflected by the fact that C*-algebra of the discrete hull is stably equivalent to the C*-algebra of the continuous hull.

The abstract noncommutative C*-algebra of the hull turns out to be the C*algebra of observables. To show this, we first review Bloch theory in Chapter 7. Then we use the translates of the resolvent of the periodic Hamiltonian to build the C*-algebra of observables, which turns out to be isomorphic to $C(\mathcal{B}) \otimes \mathcal{K}$, the stabilized version of the commutative C*-algebra of continuous functions on the Brillouin zone \mathcal{B} . In Chapter 8, it is then shown that for a periodic tiling by unit tiles, the C*-algebra of the hull reduces to the periodic C*-algebra of observables. This justifies the fact that the C*-algebra of the hull can be seen as the noncommutative generalization of the C*-algebra of observables to the general, not necessarily periodic case. In other words, we have

 $\begin{array}{rcl} \text{commutative topology} & \longleftrightarrow & \text{noncommutative topology} \\ & & & & & & & \\ \text{periodic media} & & & & & & \\ \end{array}$

where the right hand side is a generalization of the left hand side.

The question arises what we can do with this C*-algebra of observables. Of course, we can try to classify different tilings using topological invariants such as K-theory, but this will not help us in the description of electronic motion in quasicrystals. However, it turns out that if an operator, such as a quasiperiodic Hamiltonian, is "affiliated" to a certain C*-algebra, its spectral projections on gaps in the spectrum belong to this C*-algebra. Because the K_0 -group is constructed from equivalence classes of projections in the stabilized version of the

C*-algebra, it can be used to label these gaps. Moreover, it turns out that via an equation designed by Shubin in 1979, called "Shubin's formula", a trace on the K_0 -group links the gap labels with the value of the integrated density of states on it. Now the density of states is an important quantity in solid state physics, which is in fact accessible by experiments. Complete knowledge of the integrated density of states gives complete knowledge of the spectrum, which can in turn be used to derive conductivity properties of the medium. The above is the subject of Chapter 9.

So it turns out that using an abstract topological invariant of a fairly abstract C^* -algebra can be used to describe electronic motion in quasicrystals, as a generalization of Bloch theory. However, there are some problems that prevent us from obtaining quantitative results. For example, the gap labelling is not one-to-one, which means that we only have a set of *possible* gap labels. We don't know which elements of this set actually occur as gap labels, because some gaps may be closed. This problem, among others, is discussed in the last section for the "Almost Mathieu operator", which describes a one-dimensional quasiperiodic model. In conclusion, noncommutative topology and K-theory prove to be useful tools in the description of electronic motion in quasicrystals, but the theory is yet far from complete.

Chapter 2

Crystals and Tilings

In this chapter, we will show how crystals can be modeled by a point lattice, and generalize this to aperiodic solids using Delone sets. We explain how diffraction spectra can be used to determine the structure of solids. By proving the crystal-lographic restriction, we see that the five-fold symmetry found by Schechtman *et. al.* in 1984 [48] in diffraction spectra of certain alloys is in conflict with periodicity. This shows that there exist aperiodic solids using tiling theory, and we'll review two methods to obtain quasiperiodicity, namely the projection method and the substitution method. Finally, we review some electronic transport properties of quasicrystals.

2.1 Mathematical Crystallography

Definition 2.1.1 A point set $\Lambda \subset \mathbb{R}^d$ is said to be **discrete** if for every $x, y \in \Lambda$, there exists a positive real number r, such that $|x - y| \geq 2r$. If an r can be found such that $|x - y| \geq 2r \ \forall x, y \in \Lambda$, then Λ is **uniformly discrete**. A point set Λ is called **relatively dense** in \mathbb{R}^d if there is a positive real number R such that every sphere of radius greater than R contains at least one point of Λ in its interior. If Λ is both uniformly discrete and relatively dense, it is called a **Delone set** or (R, r)-set.

Delone sets will be used to describe the positions of atoms in a solid.

Definition 2.1.2 A subset $\Gamma \subset \mathbb{R}^d$ is called a **(Bravais) lattice** if it is a free \mathbb{Z} -module generated by d linearly independent vectors, that is,

$$\Gamma = \mathbb{Z}v_1 \oplus \mathbb{Z}v_2 \oplus \dots \oplus \mathbb{Z}v_d.$$

Note that Γ can be seen as a discrete subgroup of \mathbb{R}^d , isomorphic to \mathbb{Z}^d . Therefore, the factor group \mathbb{R}^d/Γ is compact. Orbits under the group action of Γ on \mathbb{R}^d are uniformly discrete subsets of \mathbb{R}^d . Since the vectors v_i span \mathbb{R}^d , each orbit lies relatively dense in \mathbb{R}^d . Therefore, the orbits of a lattice are Delone sets. In some cases, it will be useful to identify the orbit with the lattice itself, although strictly speaking [49], we should reserve the name "lattice" for the \mathbb{Z} -module, calling the (discrete) orbit of a lattice a **point lattice**.

Definition 2.1.3 A set $S \subseteq \mathbb{R}^d$ is called **periodic** if there is a nonzero vector $t \in \mathbb{R}^d$, called a **period** of S, such that S + t = S, where S + t is defined as

$$S + t := \{s + t \mid s \in S\}$$

S is called crystallographic if its periods form a lattice.

From the above definitions, it is clear that a point lattice is a crystallographic set S. The symmetry group of S consists of translations (by periodicity), and certain orthogonal transformations, i.e. combinations of reflections, inversions and rotations. We will call the general group of isometric transformations that leave the crystallographic set invariant the **space group**, and its subgroup of translations the **translation group**.

Remark 2.1.4 Note that a lattice Γ can be identified with the translation group of the point lattice.

Taking the quotient of the space group by the translation group, we get the group of orthogonal symmetries, a subgroup of O(d), that is called the **point group** of the set (these transformations always leave one point invariant). The point group symmetries of a crystallographic set are restricted by the **crystal-lographic restriction**:

Proposition 2.1.5 Let S be a crystallographic point set in \mathbb{R}^d , and let R be an orthogonal transformation that maps S into itself.

- 1. The order of R is finite, i.e. $R^k = Id$ for some $k \in \mathbb{N}$.
- 2. k is restricted to $\{1, 2, 3, 4, 6\}$ in the case that n = 2 or n = 3.

In other words, only reflections and 2-,3-,4- and 6-fold rotations are possible.

Proof: The proof is taken from [49]. The first statement is clear, since the periods of S form a \mathbb{Z} -module of finite dimension d. For the second statement, observe by a suitable choice of a basis in \mathbb{R}^d , any orthogonal transformation R

can be written as

$$R = \begin{pmatrix} A_1 & 0 & \dots & \dots \\ 0 & A_2 & 0 & \\ \vdots & 0 & \ddots & \\ \vdots & & & A_k \end{pmatrix}$$

where each A_i can be either 1, -1 or a 2 × 2-matrix of the form

$$\left(\begin{array}{cc}\cos\theta & -\sin\theta\\\sin\theta & \cos\theta\end{array}\right)$$

and all other entries are zero. Since an orthogonal transformation of an *n*-dimensional crystallographic set can also be written as an element of $GL(n,\mathbb{Z})$, we see that R is conjugate (by a change of basis) to an element in $GL(n,\mathbb{Z})$. The latter has integer valued trace, and since traces are invariant under a change of basis, the trace of R is integer valued too. Thus, in dimension n = 2 or n = 3, we get

$$2\cos\theta \in \mathbb{Z}$$

Using that $|\cos \theta| \le 1 \ \forall \theta$, it follows that $\cos \theta \in \{0, \pm \frac{1}{2}, \pm 1\}$, and we see that $\theta \in \{0, \pi, \pi/2, 2\pi/3, 2\pi/6\}$. \Box

Remark 2.1.6 If one regards a crystal as a crystallographic set with an atom placed at each point, Proposition 2.1.5 states that a crystal with 5-fold or k-fold symmetry, where k > 6, is impossible. However, we will see that nonetheless there are solids with some sort of long range order (though not periodicity), that exhibit these symmetries. These solids will be called quasicrystals; a precise definition is given in the following section.

Definition 2.1.7 For a lattice
$$\Gamma \in \mathbb{R}^d$$
, the **dual lattice** Γ^* is defined as
 $\Gamma^* := \{ y \in \mathbb{R}^d \mid x \cdot y \in \mathbb{Z} \text{ for all } x \in \Gamma \}.$ (2.1)

It follows immediately from the definition that the dual of a dual lattice is equal to the original lattice, i.e.

$$(\Gamma^*)^* = \Gamma.$$

Remark 2.1.8 In crystallography, the dual lattice is often called the **reciprocal lattice**. Just as the lattice can be seen as a group of translations acting on the "real" space \mathbb{R}^d , the reciprocal lattice can be seen as a group of translations acting on momentum space or k-space. In describing the reciprocal lattice, a frequently used convention is to define Γ^* as the space of vectors $k \in \mathbb{R}^d$ for which, for all $x \in \Gamma$,

$$e^{ik \cdot x} = 1. \tag{2.2}$$

This definition of Γ^* differs from the original one by a factor of 2π . It has the advantage that in this way it is clearer that the dual lattice Γ^* is essentially just the Fourier transform of the "real" lattice Γ .

2.2 Diffraction

The symmetry properties of crystals have been extensively studied by looking at their diffraction spectra. The following is a short introduction; for more information, see e.g. [2, 3, 26, 49].

Figure 2.1: Discrete diffraction spectrum of a crystal, showing sharp spots (the Bragg peaks), with 4- and 6-fold symmetry, respectively

Visible light or x-rays diffract when they meet an obstacle, and interference of such waves leads to a diffraction pattern. In a similar way, the scattering of electrons or neutrons is used to obtain a diffraction pattern, from which properties of the structure of the object can be deduced. If the obstacle is a crystal, the periodicity of the positions of the atoms leads to a discrete spectrum with sharp peaks of high intensity, the so called **Bragg peaks**. This is due to the famous **Bragg condition**, stating that only for rays with incident angle θ , satisfying

$$n\lambda = 2d\sin\theta,\tag{2.3}$$

a peak is formed in the spectrum. Here, n is an integer, λ is the wavelength of the ray, d is the spacing between the atoms (the period of the point lattice), and θ is the angle between the incident beam and the plane of reflection. Note that in this formulation the crystal is regarded as a collection of parallel planes consisting of atoms spaced a distance d apart. Furthermore, it is assumed that the angle of reflection always equals the angle of incidence (**specular** reflection), as is the case with ordinary reflection of light in a mirror. Of course, the planes of reflection also differ by a spacing d, and it is clear that the reflected rays of two different planes interfere constructively if and only if the path difference is an integer multiple of the wavelength of the beam. Now, the path difference between two consecutive planes is precisely $2d\sin\theta$, and the Bragg condition follows. The only problem is that there are in general many ways to regard a crystal as a collection of parallel planes.

A condition equivalent to the Bragg condition is the **Laue condition**. The von Laue approach has the advantage that we don't have to divide the crystal in parallel planes. One regards a crystal as a collection of microscopic objects (atoms, ions or small sets of those), each placed at a point in a crystallographic set. An incoming beam is scattered by these objects in all possible directions, so no assumption of specular reflection is made. The only assumption is that the wavelength of the scattered beam is the same as the wavelength of the incoming beam, which was also implicitly assumed in the Bragg picture. This is the same as assuming that the scattering is elastic, i.e. there is no energy of the incoming beam transferred to the crystal. Now, if **d** is a displacement vector between two scatterers, and $\hat{\mathbf{n}}$ is the direction of an incident ray, with wavelength λ and wave vector $\mathbf{k} = 2\pi \hat{\mathbf{n}}/\lambda$, a scattered ray will be observed in the direction $\hat{\mathbf{n}}$ if and only if the path difference between the rays scattered by the two scatterers

is an integral multiple of the wavelength, or

$$\mathbf{d} \cdot (\mathbf{\hat{n}} - \mathbf{\hat{n}}') = m\lambda.$$

Multiplying both sides by $2\pi/\lambda$ gives

$$\mathbf{d} \cdot (\mathbf{k} - \mathbf{k}') = 2\pi m,$$

where m is an integer. It easy to see that the generalization to a crystallographic set of scatterers with lattice Γ yields

$$\mathbf{R} \cdot (\mathbf{k} - \mathbf{k}') = 2\pi m$$
, for all $\mathbf{R} \in \Gamma$,

where m is an integer, or equivalently

$$e^{i(k-k')\cdot R} = 1$$
, for all $\mathbf{R} \in \Gamma$. (2.4)

Thus, constructive interference will take place if and only if the change in wave vector, $\mathbf{k} - \mathbf{k}'$, is an element of the reciprocal lattice (cf. (2.2)). This is the Laue condition. It is not difficult to show that the Laue condition and the Bragg condition are equivalent, see [2].

The von Laue formulation has the advantage that one does not have to consider planes in the crystal, and in this way it is more natural than Bragg's formulation. Now, consider an incident beam with wave vector \mathbf{k} , and suppose the wave vector \mathbf{k}' satisfies the Laue condition. Thus, in the diffraction spectrum, we see a peak of intensity $J(\mathbf{k}')$ at \mathbf{k}' . This intensity is the square of the amplitude, i.e.

$$J(\mathbf{k}') = |A(\mathbf{k}')|^2.$$

Now the amplitude $A(\mathbf{k}')$ is the Fourier transform of the atomic distribution $\rho(\mathbf{x})$. Using the fact that

$$\mathcal{F}(f \ast g) = \mathcal{F}(f)\mathcal{F}(g),$$

where \mathcal{F} denotes the Fourier transform and * denotes the convolution product, we get the following commuting diagram:

$$\rho(\mathbf{x}) \xrightarrow{convolution} \rho(\mathbf{x}) * \overline{\rho(-\mathbf{x})}$$

$$\uparrow^{\mathcal{F}} \qquad \uparrow^{\mathcal{F}} \qquad \uparrow^{\mathcal{F}} \qquad (2.5)$$

$$A(\mathbf{k}) \xrightarrow{squaring} J(\mathbf{k})$$

We call this diagram a **Wiener diagram**, following [49]. Now the main problem in using diffraction spectra to obtain the real structure of a crystal is the fact that we only know the lower right corner of the diagram, and we want to know the upper left corner. What we miss is a phase factor. There are ways to get the unknown information by a "direct method", which means going via $A(\mathbf{k})$, Figure 2.2: Diffraction spectra with eight-fold and ten-fold symmetry, respectively

or by "deconvolution" of $\rho(\mathbf{x}) * \rho(-\mathbf{x})$, which is known as Patterson analysis. We won't go into detail; the main thing is that once we have the diffraction spectrum, it is still difficult to determine the real crystal structure.

In Proposition 2.1.5, we have seen that for a crystallographic set, which is periodic, the only rotation symmetries allowed are 2-,3-,4- and 6-fold. So if one would find a crystal with a diffraction spectrum with, for instance, 5-fold rotational symmetry, this would not be a true crystal, since it could not be periodic by the crystallographic restriction. However, in 1984, Schechtman et al. [48] found out that rapidly cooled alloys of Al with 10 - 14 at.% Mn, Fe or Cr form a structure with icosahedral symmetry, which was apparent in fivefold symmetry axes in their electron diffraction spectra. This was, of course, a revolution in crystallography: until then, it was believed that only true (i.e., periodic) crystals could have a discrete diffraction spectrum. Later, various other alloys with symmetries forbidden by the crystallographic restriction were produced [26], see Figure 2.2 for examples of diffraction spectra with 8- and 10-fold symmetry. The long range order in these alloys is not due to translation invariance, like in crystals. Nevertheless, there is long range order, which can be described by quasiperiodicity. Therefore, this new phase between amorphous materials and crystallographic periodic order was called a quasicrystal.

Remark 2.2.1 It is important to realize that quasicrystals are truly different from crystals. In particular, they cannot be described as crystals with defects or impurities. There are various intermediate phases between ordered crystals and unordered amorphous materials. On the one hand, amorphous materials do not have a discrete diffraction spectrum, whereas, on the other hand, the diffraction spectrum of a crystal is discrete. Solids in between, are often called **aperiodic** [3]. As such, quasicrystals are aperiodic media, but they are the ones that are closest to crystals, having a discrete diffraction spectrum, in contrast to amorphous materials. In fact, the only property of crystals that quasicrystals don't have is periodicity.

2.3 Tilings

A useful concept of describing a crystal is by associating a tiling to it. A twodimensional **tiling** is essentially a covering of the plane by tiles, such that they do not overlap, and such that there are no gaps between them. Later, we will give a precise definition. The concept of a two-dimensional tiling can, of course, be extended to higher dimensions, and in general we will think of tiles as polyhedra. In crystallography, one can associate a tiling to a lattice by defining a **unit cell** as a subset of \mathbb{R}^d whose edges are parallel to the basis vectors of the lattice. These unit cells then form tiles, which form a periodic tiling of \mathbb{R}^d , since the lattice consists precisely of the periods of a crystallographic set. Note that there are many ways to define the unit cell, so that the tiling associated to a lattice is in no sense unique. Let us now give a precise definition of a tiling.

Definition 2.3.1 A tiling T is a countable set of closed subsets t_i of \mathbb{R}^d , $T = \{t_1, t_2, ...\}$, each of positive Lebesgue measure, such that $\bigcup_{i=1}^{\infty} t_i = \mathbb{R}^d$ and $(t_i \setminus \partial t_i) \cap (t_j \setminus \partial t_j) = \emptyset$ if $i \neq j$, i.e. the tiles do not overlap, but can have a boundary ∂t in common.

Two tiles t_1 and t_2 are **congruent** if there is a symmetry transformation R (i.e., R is a rotation and/or a translation), such that $t_1 = Rt_2$. If t_1 and t_2 are congruent, they are copies of the same tile t, called a **prototile**. Note that a prototile is nothing more than an equivalence class under congruence. All tilings we consider will have a finite set of different prototiles. Without this assumption, it would be possible to have any kind of long range order. Furthermore, we will assume that every tile is homeomorphic to the closed unit disk $\overline{B_1(0)}$. Practically, this means that tiles contain no "holes". Moreover, we assume that given a tile, its boundary can only be covered by other tiles in a finite number of ways (see [40]).

We have remarked already that one can associate a tiling to a lattice. An elegant choice is the **Voronoi construction**. We will apply this construction to a Delone set, of which a point lattice is a special example.

Definition 2.3.2 Let $\Lambda \subset \mathbb{R}^d$ be a Delone set. The Voronoi cell V(x) of a point $x \in \Lambda$ is defined as the subset of points in \mathbb{R}^d that lie at least as close to x as to any other point of Λ , i.e.

$$V(x) := \left\{ v \in \mathbb{R}^d \mid |x - v| \le |y - v| \text{ for all } y \in \Lambda \right\}.$$

$$(2.6)$$

It is clear that this construction precisely yields a tiling by convex polyhedra without overlaps or gaps (see Figure 2.3). In particular, in this way a crystal can be modeled [2]. In the case of a point lattice, the Voronoi cell is also called a **Wigner-Seitz cell**.

Figure 2.3: Construction of a Voronoi cell

Remark 2.3.3 If Γ is a lattice in \mathbb{R}^d , the quotient \mathbb{R}^d/Γ , which is a compact group, can be seen as a unit cell. We will identify \mathbb{R}^d/Γ with the Voronoi unit cell \mathcal{V} around the origin.

The Voronoi construction can also be applied in reciprocal space. The Voronoi cells of the dual lattice Γ^* are called **Brillouin zones**. The first Brillouin zone \mathcal{B} , which is the Voronoi cell of k = 0, will be identified with \mathbb{R}^d/Γ^* .

The Voronoi construction is a way to obtain tilings from Delone sets. On the other hand, starting with a tiling, one can associate a Delone set to it by puncturing each tile at a particular place (or at more places), and calling these punctures the points of the Delone set. For example, for a tiling by polyhedra, the vertices of the polyhedra form a point lattice. In this way, we obtain a correspondence between tilings and Delone sets, which is of course in no sense one-to-one. For example, starting with a periodic tiling of regular triangles in \mathbb{R}^2 , one can view the vertices of the triangles as a point lattice. The Voronoi tiling of this point lattice is a tiling by regular hexagons, which is of course different from the original tiling.

Of course, if one had taken the middle points of the triangles as point lattice and then carried out the Voronoi construction, one would have obtained the original tiling. However, in general the tiles are not regular polyhedra, and in that case the tiling is not a Voronoi tiling of some Delone set. We will frequently use the correspondence between Delone sets and tilings. In particular, many properties defined for tilings also hold for their associated Delone set, and vice versa.

Starting with a tiling T of \mathbb{R}^d , we can define for any $x \in \mathbb{R}^d T + x$ by

$$T + x := \{t + x \mid t \in T\}.$$

Evidently, T + x is again a tiling of \mathbb{R}^d .

Definition 2.3.4 A tiling T is periodic if there is an $x \in \mathbb{R}^d$ such that T+x = T. If $T + x \neq T$ for any $x \in \mathbb{R}^d$, T is called **aperiodic**.

Note that in this definition, a periodic tiling in d dimensions does not necessarily exhibit periodicity in d independent directions. Periodicity in one direction is enough. However, in most cases, we will see a periodic tiling T as a tiling corresponding to a point lattice Γ , such that the tiles of T are copies of the unit cell $\mathcal{V} = \mathbb{R}^d / \Gamma$.

2.4 Quasiperiodicity

Next, we will focus on tilings that serve as a model for quasicrystals, i.e. quasiperiodic tilings. Quasiperiodicity comes from the theory of almost periodic functions, developed in the 1930's by Harald Bohr, the younger brother of Niels Bohr (see [4] and the references therein). The basic example of an almost periodic function is

$$f(x) := \sin(x) + \sin(\tau x).$$
 (2.7)

If τ is rational, f(x) is clearly periodic. However, if τ is irrational, for example

$$\tau = \frac{1 + \sqrt{5}}{2},$$

the famous **golden ratio**, f(x) is not periodic anymore, lacking translation invariance over some period. Nevertheless, for every $\epsilon > 0$, one can find $t \in \mathbb{R}$ such that $|f(x) - f(x+t)| < \epsilon$, for all $x \in \mathbb{R}$. Moreover, such "almost-translations" lie relatively dense in \mathbb{R} , which is reflected in the following definition:

Definition 2.4.1 A continuous function $f : \mathbb{R} \to \mathbb{R}$ is almost periodic if for every $\epsilon > 0$, there is a $\delta > 0$, such that every interval $[x_0, x_0 + \delta]$ contains at least one t such that $|f(x) - f(x+t)| < \epsilon$, for all $x \in \mathbb{R}$.

Almost periodic functions can be approximated by trigonometric polynomials, generalizing the concept of Fourier series. In these generalized Fourier series, the base frequencies are pairwise incommensurate. If the number of base frequencies is finite, as in the example above, the function is called **quasiperiodic**. A quasiperiodic function can always be seen as a section of a periodic function in more variables. For example, the above function f(x) can be seen as

$$f(x) = \sin(x) + \sin(y) \upharpoonright_{y=\tau x} .$$

This concept can also be used to define obtain quasicrystallographic sets. Starting with a crystallographic set in \mathbb{R}^n , one can obtain a quasicrystallographic set in \mathbb{R}^d , with d < n, by taking a suitable section. This is called the **cut and project method**, or simply the **projection method**. The basic example is the so called Fibonacci chain, treated in [4, 49, 26] and by many other authors. We start with the lattice \mathbb{Z}^2 in the plane. We cut the plane by a line with irrational slope, called E_{\parallel} . Next, we define E_{\perp} to be the line perpendicular to E_{\parallel} through the origin, and restrict it to a "window" or "acceptance domain" M, for example with the width of the unit cell. In this way, we form a strip parallel to E_{\parallel} . We project all points inside the strip to E_{\parallel} , hereby obtaining a one dimensional sequence of intervals, and it is easy to see that this sequence is periodic if and only if the slope of the E_{\parallel} is rational. If the slope of E_{\parallel} is $1/\tau$, we obtain a **Fibonacci string** of long (L) and short (S) intervals, which differ by a factor τ (see Figure 2.4). This sequence is quasiperiodic. An example of a Fibonacci string is

Note that although the Fibonacci string is one-dimensional, it can be used in the analysis of three-dimensional quasicrystals that are periodic in two directions. These quasicrystals can be seen as Fibonacci chains of periodically arranged layers.

Figure 2.4: Fibonacci chain obtained via the projection method

The projection method can be generalized to other dimensions (see e.g. [11]). We define it in the following way:

Here, Γ is a point lattice in $\mathbb{R}^d \times \mathbb{R}^n$, and π_{\parallel} and π_{\perp} are the obvious projections. π_{\parallel} restricted to Γ is injective, and $\pi_{\perp}(\Gamma)$ is dense in \mathbb{R}^n . \mathbb{R}^d is called the "physical space", and \mathbb{R}^n is called the "internal space". For a subset M of the internal space \mathbb{R}^n (the "acceptance domain"), the point set $\Lambda(M) \subset \mathbb{R}^d$ is defined as

$$\Lambda(M) := \{ \pi_{\parallel}(a) \mid a \in \Gamma \text{ such that } \pi_{\perp}(a) \in M \}.$$

Note that for every $a \in \Gamma$, we have

$$\Lambda(M + \pi_{\perp}(a)) = \Lambda(M) + \pi_{\parallel}(a).$$

In this way, an irrational cut of an n + d-dimensional periodic point lattice Γ leads to a *d*-dimensional quasiperiodic point set $\Lambda(M)$. Of course, one can try to approximate a quasicrystal by looking at rational cuts. In the above example of the Fibonacci string, one can look at $\frac{1}{1}, \frac{2}{1}, \frac{3}{2}, \frac{5}{3}, \ldots$, using the fact that the golden ratio τ can be expressed as the following continued fraction:

$$\tau = 1 + \frac{1}{1 + \frac{1}{1 + \frac{1}{1 + \dots}}},$$

cf. below. It is clear that the closer the rational number gets to τ , the more the cuts coincide. However, the rational cut is periodic, so the closer the approximation is, the larger the period. In general, this means that we can approximate a quasicrystal by crystals with very large unit cells. In particular, we can compute properties (for example electronic properties, such as conductance) of the periodic approximants, and see if the properties of the quasicrystal can be seen as a limit case in some way [54].

Let's have another look at the Fibonacci string. Originally, the Fibonacci numbers ${\cal F}_n$ were defined by the sequence

$$1, 1, 2, 3, 5, 8, 13, 21, 34, \dots, (2.10)$$

or, recursively, by

$$F_{n+1} = F_n + F_{n-1}, (2.11)$$

with initial values $F_1 = 1$; $F_2 = 1$. Then τ is the limit

$$\tau = \lim_{n \to \infty} \frac{F_{n+1}}{F_n},$$

which is an alternative way to write the above continued fraction. The Fibonacci numbers can be considered to be counting the total number of intervals (L and S) under the growing condition

$$L \mapsto LS; \quad S \mapsto L.$$
 (2.12)

In this way, we can build a Fibonacci string by substituting every L and every S in each step according to the rules (2.12). We get:

$$S$$

$$L$$

$$LS$$

$$LSLLS$$

$$LSLLSLSLLSLLS$$

$$...$$

$$(2.13)$$

One can show that an infinite Fibonacci string generated by the above **substitution method** can always also be generated by the projection method [49]. Note that from the substitution scheme, it is immediate that every S is always followed by an L, i.e. SS never occurs.

The substitution method can be generalized to other substitutions, and to higher dimensions. An important 2-dimensional example of a substitution tiling is the Penrose tiling, which we will describe later in detail (cf. Chapter 6).

2.5 Properties of quasicrystals

We have described the structure of a quasicrystal as it arises from its diffraction spectrum. Let us summarize the properties that characterize a quasicrystal (see, for example, [54]):

- 1. The diffraction spectrum is discrete, i.e. it exists of δ -functions (the Bragg peaks).
- 2. The positions of the δ -functions can be specified with a set of n integers, where n is bigger than the spatial dimension d of the quasicrystal.
- 3. The diffraction pattern has a rotational symmetry forbidden by the crystallographic restriction.

The second point describes the fact that a quasicrystal can be obtained as a cut of a higher dimensional point lattice. For example, For a 3-dimensional quasicrystal, the diffraction spectrum can be generated by 6 basis vectors.

Remark 2.5.1 Note that it is in principle very difficult to predict how a quasicrystal "grows". This is clear in the one-dimensional case. If we consider a finite string of a periodic chain of L's and S's, for example

...LSLSLSLSLSLSL...,

we can predict that the next letter will be an S on both sides. However, if we consider a Fibonacci string, for example

it is impossible to say whether at the left side an L or an S has to be attached (on the right side, of course, we know that the next letter will be an L, because SSis forbidden in a Fibonacci chain). In general, we see that we cannot predict the growth of a quasicrystal by looking at a finite patch. Instead, we have to have knowledge of the whole quasicrystal to predict the growth. In particular, this would imply that the place of a new atom depends on its interaction with all the other atoms, instead of its interaction with only a finite (local) neighbourhood. This is of course physically not very probable. For more on this interesting problem, see [26].

Now, we would like to investigate other important properties of quasicrystals. In particular, we would want to formulate a theory of electronic transport in quasicrystals. Since quasicrystals are formed of metals, mostly with Al, their resistivity was expected to be of the order of the resistivity of the crystalline systems composed of the same metallic elements. However, in experiments, the following facts have been observed for quasicrystals [54]:

- 1. In general, they have a very high resistivity, i.e. their conductance is very low, compared to metals. Resistivity of quasicrystals at room temperature is typically of the order of $10^{-3}\Omega cm$ or higher, compared to $10^{-6}\Omega cm$ for metals.
- 2. The conductance lowers with improved sample quality, which indicates that the conducting of electrons is mainly caused by impurities. Note that in metals, the situation is the other way round, i.e. impurities lower the conductivity.
- 3. The resistivity increases if one lowers the temperature, i.e. $\frac{\partial \rho}{\partial T} < 0$. Once again, for metals, the situation is the other way round, i.e. the resistivity gets lower at lower temperatures.

To develop a theory that can explain these facts, one looks mainly at the spectrum of a one electron Hamiltonian, and its density of states. For crystals, the main tool in investigating electronic transport properties is Bloch theory, but this cannot be applied to quasicrystals, because it depends crucially on the periodicity of the crystal. In Chapter 7, we will define the spectrum and the density of states, and review Bloch theory. Then we will try to generalize it to aperiodic solids, using operator-algebraic techniques and noncommutative topology. Therefore, in the next chapters, we will introduce these techniques, and review the construction of the noncommutative space of Penrose tilings by Connes [15], which is in fact a starting point for the introduction of noncommutative topology in the world of tilings and quasicrystals.

Chapter 3

C*-algebras and noncommutative topology

C*-algebras have been extensively studied in the past decades, see e.g. [17, 18, 19, 38, 56]. Basically, a C*-algebra is a *-algebra that is also a Banach space (i.e., a complete normed space), satisfying some conditions that link the algebraic properties with the Banach space properties. The main examples of C*-algebras are the set C(X) of continuous functions on a compact Hausdorff space X, and the set $\mathcal{B}(\mathcal{H})$ of bounded operators on a Hilbert space \mathcal{H} . The former is commutative, whereas the latter is noncommutative.

One of the main advantages of C^{*}-algebras is that due to the involution *, there is a notion of self-adjointness in C^{*}-algebra. Since in quantum physics, observables are given by self-adjoint operators, the set of observables has a natural C^{*}-algebraic structure. In particular, one can define positivity in C^{*}-algebras. C^{*}-algebras have been used to construct a solid mathematical basis for Heisenberg's formulation of quantum mechanics in terms of "matrix mechanics". For more on C^{*}-algebras in physics, see e.g. [25, 33].

In mathematics, one of the most important subjects where C*-algebras are extensively used is noncommutative geometry, as developed by Connes [15]. We will only look at some part of it, namely noncommutative topology.

The first step in the philosophy of noncommutative topology is to describe the topological properties of a locally compact Hausdorff space X in terms of the algebraic properties of the commutative C*-algebra associated to X that consists of the continuous functions on X. In this way, we will get a "dictionary" between topology and algebra. Since every topological property of the space X can be described in terms of algebraic properties of the C*-algebra, we can hope to use the algebraic description as a definition for general, not necessarily commutative C*-algebras. From a noncommutative C*-algebra, we can then go "back" via

the dictionary, obtaining a so called "noncommutative" space, the structure space of the C*-algebra. In most cases, the last step is not needed anymore, and one just views the noncommutative C*-algebra itself as the noncommutative space (although it is not a topological space itself). In particular, topological invariants such as K-theory can be described in C*-algebraic terms, and may then be generalized to a general K-theory for arbitrary C*-algebras.

Noncommutative topology turns out to be especially useful in describing topological properties of non-Hausdorff spaces. Since in a non-Hausdorff space, basically there are not enough open sets to separate points, the commutative C*-algebra of continuous functions will not fully describe the topological properties in this case. However, for spaces X that can be seen as a quotient Y/R, where R is an equivalence relation, it turns out that there is a noncommutative groupoid C*-algebra $C^*(R)$ that contains all interesting information. We postpone the the construction of groupoid C*-algebras to Chapter 4, treating the non-Hausdorff case in Chapter 5.

Now, let us define what a C*-algebra is. We begin with the concept of a *-algebra.

Definition 3.0.2 A *-algebra A is an associative algebra (over \mathbb{C}) with an involution, *i.e.*, a map * : A \rightarrow A satisfying ($\forall a, b \in A, \forall \lambda \in \mathbb{C}$):

1. $(\lambda a)^* = \overline{\lambda} a^*;$ 2. $a^{**} = a;$ 3. $(ab)^* = b^* a^*;$

To make a C*-algebra of it, we have to define a norm such that certain conditions are satisfied:

Definition 3.0.3 A C*-algebra is a *-algebra A that is also a Banach space (i.e. a complete normed space), such that $\forall a, b \in A$, the "Banach algebra condition" and the "C*-condition" are satisfied:

$$\|ab\| \le \|a\| \|b\| \tag{3.1}$$

$$||aa^*|| = ||a||^2. \tag{3.2}$$

Next, we will review the basic examples of commutative C^* -algebras and noncommutative C^* -algebras. The basic theorems are Theorem 3.1.2 and Theorem 3.2.2. The first one states that indeed every commutative C^* -algebra can be seen as the C*-algebra of continuous functions on some locally compact Hausdorff space, and is a justification for the existence of a "dictionary" between topology and algebra. The second one states that every noncommutative C*-algebra is a *-subalgebra of the C*-algebra of bounded operators on some Hilbert space.

3.1 The commutative case

Before we can develop a dictionary between the topological and the algebraic points of view, we first need a bijective correspondence between the two sides. Let us start with a topological space X that is compact and Hausdorff. Associated to this space X there is a *-algebra, namely C(X), the space of continuous functions on X, equipped with pointwise multiplication and involution:

$$(fg)(x) := f(x)g(x).$$
$$f^*(x) := \overline{f(x)}.$$

We equip C(X) with the **sup-norm**, defined by

$$||f||_{\infty} := \sup_{x \in X} |f(x)|.$$

In this norm, C(X) is complete, and it satisfies the Banach algebra condition (3.1) and the C^{*}-condition (3.2):

$$\|fg\|_{\infty} = \sup_{x \in X} |f(x)g(x)| \le \sup_{x \in X} |f(x)||g(x)| \le \|f\|_{\infty} \|g\|_{\infty},$$
$$\|f^*f\|_{\infty} = \sup_{x \in X} |f^*(x)f(x)| = \sup_{x \in X} |\overline{f(x)}f(x)| = \sup_{x \in X} |f(x)|^2 = \|f\|_{\infty}^2$$

Thus, C(X) becomes a C*-algebra. Note that it is commutative, and that it has a unit, 1_X . So to each compact Hausdorff space X, a commutative, unital C*-algebra can be associated. As we will see, the converse is also true.

Definition 3.1.1 Let A be a commutative C*-algebra with unit. The structure space $\Delta(A)$ of A is defined as the space of characters of A, i.e., of nonzero linear maps $\omega : A \to \mathbb{C}$ for which, $\forall a, b \in A$,

$$\omega(ab) = \omega(a)\omega(b). \tag{3.3}$$

Since every $\omega \in \Delta(A)$ is nonzero, it immediately follows from (3.3) that $\omega(I) = 1$, where $I \in A$ is the unit of A. It can be shown [32] that $\Delta(A) \subseteq A^*$, where A^* is the dual of A. Now A^* can be equipped with a topology, the so called **weak*-topology**, where $\omega_n \to \omega$ iff $\omega_n(a) \to \omega(a)$ for all $a \in A$ (this topology is essentially the same as the weak operator topology of Definition 4.2.7). Therefore, $\Delta(A)$, equipped with the relative weak*-topology, is a topological space. It can be shown [32] that $\Delta(A)$ is compact and Hausdorff in this topology.

Next, we embed A in A^{**} by the map $a \mapsto \hat{a}$, where

$$\hat{a}(\omega) := \omega(a). \tag{3.4}$$

Restricting the domain of \hat{a} to $\Delta(A) \subseteq A^*$, this defines a function on $\Delta(A)$, which is easily seen to be continuous in the relative weak*-topology: let $a \in A$.

Then, if $\omega_n \to \omega$, by definition, $\omega_n(b) \to \omega(b) \forall b \in A$, in particular $\omega_n(a) \to \omega(a)$. But this means that $\hat{a}(\omega_n) \to \hat{a}(\omega)$, so \hat{a} is continuous. Moreover, $\hat{:} A \to C(\Delta(A))$, called the **Gelfand transform**, is a homomorphism of C*-algebras. This follows easily by combining equations (3.4) and (3.3). In fact, we have the following theorem of Gelfand and Naimark:

Theorem 3.1.2 Let A be a commutative C^* -algebra with unit and let $X = \Delta(A)$ be its structure space. Then the Gelfand transform is an isomorphism between A and C(X), the C*-algebra of continuous functions on X.

For the proof of this theorem, we refer to [32]. In categorical language, the theorem can be refined as follows: Define CH as the category of compact Hausdorff spaces and continuous mappings, and CCA as the category of commutative unital C*-algebras and unit-preserving homomorphisms. Next, extend C to a contravariant functor from CH to CCA, and Δ to a contravariant functor from CCA to CH. Then, the theorem states that $C \circ \Delta$ is similar to id_{CCA} (see Definition 4.1.10), restating that every commutative C*-algebra A is isomorphic to $C(\Delta(A))$.

The converse is also true: $\Delta \circ C$ is similar to id_{CH} , that is, every compact Hausdorff space X is homeomorphic to $\Delta(C(X))$. This can be seen by defining the **evaluation map** $\epsilon: X \to \Delta(C(X)); x \mapsto \epsilon_x$, with

$$\epsilon_x(f) := f(x). \tag{3.5}$$

Clearly, ϵ_x is a character for all $x \in X$, and ϵ can be shown to be the desired homeomorphism.

In particular, two commutative C*-algebras are isomorphic if and only if their structure spaces are homeomorphic, and, conversely, two topological spaces X and Y are homeomorphic if and only if their associated function algebras C(X) and C(Y) are isomorphic. Hence we now have the required bijective correspondence between the topological side and the algebraic side.

Remark 3.1.3 Theorem 3.1.2 can be extended to the case of non-unital commutative C*-algebras. It can be shown that the structure space of a non-unital C*-algebra A is locally compact and Hausdorff. In this case, the Gelfand transform is an isomorphism between a C*-algebra A and $C_0(\Delta(A))$, the C*-algebra of continuous functions with values tending to zero at infinity, in the sense that if $f \in C_0(\Delta(A)), \forall \epsilon > 0$, there is a compact $K \subset \Delta(A)$ such that $\sup_{x \in \Delta(A) \setminus K} |f(x)| < \epsilon$.

3.2 The noncommutative case

The basic example of a noncommutative C*-algebra is the algebra $\mathcal{B}(\mathcal{H})$ of bounded operators on a Hilbert space \mathcal{H} :

Proposition 3.2.1 Let \mathcal{H} be a Hilbert space. Then $\mathcal{B}(\mathcal{H})$ is a C^* -algebra with operator product and involution $*: \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$, defined by $\langle \psi, A^* \varphi \rangle_{\mathcal{H}} := \langle A\psi, \varphi \rangle_{\mathcal{H}}$, for $\psi, \varphi \in \mathcal{H}$, $A \in \mathcal{B}(\mathcal{H})$. The norm on $\mathcal{B}(\mathcal{H})$ is the operator norm

$$||A||_{op} := \sup \{ ||A\psi||_{\mathcal{H}} \mid \psi \in \mathcal{H}, ||\psi||_{\mathcal{H}} = 1 \}$$
(3.6)

Proof: With this norm, $\mathcal{B}(\mathcal{H})$ satisfies (3.1) and (3.2):

$$||AB||_{op} = \sup \{ ||AB\psi||_{\mathcal{H}} \mid \psi \in \mathcal{H}, ||\psi||_{\mathcal{H}} = 1 \}$$

$$\leq \sup \{ ||A||_{op} ||B\psi||_{\mathcal{H}} \mid \psi \in \mathcal{H}, ||\psi||_{\mathcal{H}} = 1 \} = ||A||_{op} ||B||_{op},$$

where the inequality comes from the fact that $A \in \mathcal{B}(\mathcal{H})$ is bounded. Moreover, this leads to

$$\|A^*A\psi\| = \langle A\psi, A\psi \rangle = \langle \psi, A^*A\psi \rangle \le \|\psi\| \|A^*A\psi\| \le \|A^*A\| \|\psi\|^2 \Rightarrow$$
$$\|A\|^2 \le \|A^*A\| \le \|A^*\| \|A\|.$$
(3.7)

Therefore, $||A|| \leq ||A^*||$. Interchanging A and A^* (which is allowed by the fact that $(A^*)^* = A$), we get

$$||A^*|| = ||A||. \tag{3.8}$$

Finally, combining (3.7) and (3.8), we get

$$||A^*A|| = ||A||^2$$

which is (4.5). Since the bounded operators on a Hilbert space form a Banach space, $\mathcal{B}(\mathcal{H})$ is complete. \Box

In fact, the next theorem by Gelfand and Naimark states that every C*-algebra can be seen as a *-subalgebra of the C*-algebra of bounded operators on some Hilbert space, which shows that $\mathcal{B}(\mathcal{H})$ is indeed the basic example of a noncommutative C*-algebra, just as C(X) is the basic example in the commutative case.

Theorem 3.2.2 Every C^{*}-algebra is isomorphic to a norm-closed *-subalgebra of $\mathcal{B}(\mathcal{H})$, for some Hilbert space \mathcal{H} .

The proof of this theorem uses the so called GNS-construction. We will postpone the (sketch of the) proof until we have given the required definitions.

What we need is a noncommutative analogue of the structure space, as defined in Definition 3.1.1 for the commutative case. This will be the noncommutative space associated to a noncommutative C*-algebra A. There are three candidates: first of all, the space Prim(A) consisting of all the primitive ideals of A. Secondly, one has the space \hat{A} of equivalence classes (under unitary transformations) of irreducible representations of the C*-algebra on a Hilbert space. Thirdly, one might consider the space P(A) of all pure states on A. We will define all these objects, and indicate why these spaces could serve as noncommutative structure space. We will see that there is a natural surjective map from \hat{A} to Prim(A) and a natural surjective map from P(A) to \hat{A} :

$$Prim(A) \longleftarrow \hat{A} \longleftarrow P(A) \tag{3.9}$$

In the commutative case, both maps become bijections, and all three candidates reduce to the space $\Delta(A)$ of characters on A. In the noncommutative case, it turns out that in general, Prim(A) is too small, whereas P(A) is too large, leaving \hat{A} as the best candidate. Therefore, we will mainly focus on the irreducible representations.

Unfortunately, it is difficult to formulate a noncommutative analogue for Theorem 3.1.2. One would expect that a noncommutative C*-algebra A is isomorphic to the C*-algebra $C(\hat{A}, \mathcal{B}(\mathcal{H}))$ of continuous functions on the noncommutative structure space \hat{A} , with values in the C*-algebra of operators $\mathcal{B}(\mathcal{H})$ of Theorem 3.2.2. However, it is difficult to define continuity in this case, since different classes of representations (which are the elements of \hat{A}) have different Hilbert spaces on which they act. Therefore, we need the concept of Hilbert bundles.

But let us begin with some basic definitions.

Definition 3.2.3 A representation of a C^* -algebra A on a Hilbert space \mathcal{H} is a *-homomorphism from A to $\mathcal{B}(\mathcal{H})$.

Note that the characters of Definition 3.1.1 can in fact be seen as representations on a one-dimensional Hilbert space $\mathcal{H}^{(1)}$: recall that all finite-dimensional Hilbert spaces of the same dimension n are isomorphic to \mathbb{C}^n , i.e., a finite dimensional Hilbert space is, up to isomorphism, completely characterized by its dimension. It follows that for an n-dimensional Hilbert space $\mathcal{H}^{(n)}$, $\mathcal{B}(\mathcal{H}^{(n)}) =$ $\mathcal{B}(\mathbb{C}^n) = M_n(\mathbb{C})$, the algebra of n-dimensional matrices over \mathbb{C} . In particular, $\mathcal{B}(\mathcal{H}^{(1)}) = \mathbb{C}$, and hence the characters that form the commutative structure space can be seen as representations on a one dimensional Hilbert space $\mathcal{H}^{(1)}$.

Definition 3.2.4 A representation π of a C*-algebra A on a Hilbert space \mathcal{H} is called **irreducible** if the only closed subspaces of \mathcal{H} that are stable under $\pi(A)$ are 0 and \mathcal{H} .

Thus, an irreducible representation π of A on \mathcal{H} cannot be "reduced" to a direct sum of two nonzero representations π_1 and π_2 on \mathcal{H}_1 and \mathcal{H}_2 respectively, such that $\pi_1(A)\mathcal{H}_1 \subseteq \mathcal{H}_1$ and $\pi_2(A)\mathcal{H}_2 \subseteq \mathcal{H}_2$. Note that there is a similar notion of irreducibility in group representation theory.

We have seen that the characters that form the structure space of a commutative algebra can be seen as one dimensional representations. The converse is true for irreducible representations [19]:

Proposition 3.2.5 Every irreducible representation of a commutative C^* -algebra is one-dimensional, i.e., a scalar multiple of the identity.

The proof is immediate from **Schur's lemma**, which, like its well known grouptheoretic equivalent, states that a representation π is irreducible if and only if the only operators in $\mathcal{B}(\mathcal{H})$ that commute with $\pi(a)$ for all $a \in A$ are multiples of the identity. A proof of Schur's lemma can, for example, be found in [33].

Definition 3.2.6 Two representations π_1, π_2 of a C*-algebra on Hilbert spaces $\mathcal{H}_1, \mathcal{H}_2$ respectively, are called **unitary equivalent**, denoted by $\pi_1 \sim_u \pi_2$, if there exists a unitary isomorphism $U : \mathcal{H}_1 \to \mathcal{H}_2$ such that $U\pi_1(a)U^* = \pi_2(a)$ for all $a \in A$.

Remark 3.2.7 Note that in the commutative case, by Proposition 3.2.5, two irreducible representations are unitarily equivalent if and only if they are equal. Therefore, in the case that A is commutative, the space \hat{A} of equivalence classes of irreducible representations of A coincides with the space $\Delta(A)$ of characters of A.

Of course, the next step is to define a topology on \hat{A} , such that it becomes a locally compact space. We use a topology inherited from Prim(A). Therefore, we first define what a primitive ideal is.

Definition 3.2.8 A left (right) ideal of a C*-algebra A is a norm-closed subset $J \subseteq A$, such that for every $j \in J$, $aj \in J$ ($ja \in J$), $\forall a \in A$. An ideal is both a right and left ideal.

It is easy to see that the kernel of a *-homomorphism $\psi : A \to B$ is an ideal in A. In particular, for a representation π of a C*-algebra A on a Hilbert space \mathcal{H} , $ker(\pi)$ is an ideal of A. This motivates the definition of a primitive ideal:

Definition 3.2.9 An ideal of a C^* -algebra is called **primitive** if it is the kernel of an irreducible representation. The set of all primitive ideals of a C^* -algebra A is denoted by Prim(A).

There is a natural surjection from \hat{A} onto Prim(A), given by $[\pi] \mapsto ker(\pi)$, where $[\pi]$ is the unitary equivalence class of an irreducible representation π of A. Since unitarily equivalent representations have the same kernel, this surjection is independent of the choice of representative in the equivalence class.

Next, we will topologize Prim(A). Following [19], given any subset W of Prim(A), define the **hull-kernel closure** \overline{W} of W to be

$$\overline{W} := \big\{ I \in Prim(A) \mid I \supset \bigcap_{J \in W} J \big\}.$$

It can be shown [19] that this closure operator satisfies the Kuratowski closure axioms, i.e.

- 1. $\overline{\emptyset} = \emptyset;$ 2. $\overline{W} \supset W;$ 3. $\overline{\overline{W}} = \overline{W};$
- 4. $\overline{V \cup W} = \overline{V} \cup \overline{W}$.

Then we define the **hull-kernel topology** \mathcal{T} on Prim(A) by

 $\mathcal{T} := \{ Prim(A) - W \mid W \in Prim(A); W = \overline{W} \}.$

Kuratowski has shown that this construction indeed gives a topology of open subsets, whose closure operation is precisely the closure operation we began with. The surjection $[\pi] \mapsto ker(\pi)$ of \hat{A} onto Prim(A) enables us to pull back the hull-kernel topology to a topology on \hat{A} . It can be shown that in this topology, \hat{A} is locally compact for every C*-algebra A[19]. However, in general, \hat{A} will not be Hausdorff.

We now turn to the third candidate for the structure space, the space of pure states P(A). To define states on a C*-algebra, we need the notion of positivity. But first, we need to define the spectrum of an element $a \in A$.

Definition 3.2.10 Let A be a unital C*-algebra. The resolvent $\rho(a)$ of an element $a \in A$ is the set of all $\lambda \in \mathbb{C}$ for which $a - \lambda I$ is invertible in A. The spectrum $\sigma(a)$ of $a \in A$ is the complement of $\rho(a)$ in \mathbb{C} , i.e.

 $\sigma(a) := \{ \lambda \in \mathbb{C} \mid a - \lambda I \text{ is not invertible in } A \}.$

It is easy to see that for a matrix $M \in M_n(\mathbb{C})$, the spectrum $\sigma(M)$ coincides with the set of eigenvalues of M. However, in the infinite-dimensional case, the situation is more complicated. We will see this in Chapter 7. In the case that A has no unit, A can be enlarged to a C*-algebra with unit,

$$\hat{A} := \{ a + \mu I \mid a \in A, \ \mu \in \mathbb{C} \}.$$

Then the spectrum of $a \in A$ is defined as the spectrum of a as an element of \tilde{A} (more generally, one can show that if $A \subseteq B$, then $\sigma_A(a) = \sigma_B(a)$ for all $a \in A$).

Definition 3.2.11 An element $a \in A$ is positive if $a = b^*b$ for some $b \in A$. Equivalently, $a \in A$ is positive if $a = a^*$ and $\sigma(A) \subset \mathbb{R}^+$.

Note that this definition coincides with the usual one in the case that A = C(X): a function $f \in C(X)$ is positive if $f(x) \ge 0 \ \forall x \in X$. Then f can be written as $f = |\sqrt{f}|^2$, with $\sqrt{f}(x) := \sqrt{f(x)}$. Defining $g := \sqrt{f}$, we get for all $x \in X$:

$$f(x) = |g(x)|^2 = \overline{g(x)}g(x) = g^*(x)g(x) \Rightarrow f = g^*g.$$

Definition 3.2.12 A state on a C*-algebra A is a linear functional $\omega : A \to \mathbb{C}$, that is positive and normalized, i.e., $\forall a \in A$:

$$\omega(a^*a) \ge 0,\tag{3.10}$$

$$\|\omega\| = 1. \tag{3.11}$$

Here, the norm of ω is defined by $\|\omega\| := \sup\{|\omega(a)| \mid \|a\| = 1\}$. The state space S(A) of A is the space of all states on A.

Observe that the boundedness of ω is a consequence of its positivity [32], so that the supremum in the definition of the norm exists. In the case that A has a unit I, the supremum is reached for a = I, so in the unital case, we have

$$\|\omega\| = \omega(I) = 1. \tag{3.12}$$

Recall that a subset C of a vector space V is **convex** if $\forall v, w \in C, \forall \lambda \in [0, 1]$, the convex sum $\lambda v + (1 - \lambda)w$ belongs to C.

Proposition 3.2.13 Let A be a unital C^* -algebra. Then S(A) is a compact convex set.

Proof: The proof of compactness is more or less the same as the proof of compactness of $\Delta(A)$, the structure space in the commutative case. We refer again to [32]. Convexity follows immediately from (3.12). In the case that A has no unit, we use the fact that the convexity part of the proposition holds for the unitization \tilde{A} . Restricting every state on \tilde{A} to a state on A, the convexity part of the proposition holds for arbitrary C*-algebras.

Definition 3.2.14 The **boundary** of a convex set K is the set of points that cannot be written non-trivially as a convex sum of two other points. Elements of the boundary of S(A), denoted by P(A), are called **pure states**, a state that is not pure is called a **mixed state**.

Remark 3.2.15 The notion of a state is well known from quantum mechanics. Here, a state is a vector ψ in a Hilbert space \mathcal{H} with norm $\|\psi\|_{\mathcal{H}} = 1$. The quantum mechanical observables can be seen as selfadjoint operators on the space of vector states. Note that each vector state ψ defines a state ω_{ψ} (in the sense of Definition 3.2.12) on the C*-algebra $\mathcal{B}(\mathcal{H})$ by

$$\omega_{\psi}(A) := \langle \psi, A\psi \rangle.$$

Here, $A \in \mathcal{B}(\mathcal{H})$, and $\langle ., . \rangle$ is the inner product of \mathcal{H} . Note that ω_{ψ} is automatically positive, and that

$$\|\omega_{\psi}\| = \omega_{\psi}(I) = \|\psi\|_{\mathcal{H}}^2 = 1.$$

The C*-subalgebra of $\mathcal{B}(\mathcal{H})$ consisting of selfadjoint operators can be seen as the "C*-algebra of observables". However, not all physical observables are bounded, so this is not quite true. Later on, we will see how we can overcome this problem in particular situations.

Example 3.2.16 [33] As an example, we consider the C*-algebra $M_2(\mathbb{C})$ of 2×2 matrices over \mathbb{C} . Using the fact that there is an isomorphism between the elements $B \in M_2(\mathbb{C})$ and the functionals ϕ_B on $M_2(\mathbb{C})$, given by

$$\phi_B(A) = Tr(AB),$$

for all $A \in M_2(\mathbb{C})$ [18], the state space $S(M_2(\mathbb{C}))$ can be identified with the collection of all positive 2×2 matrices ρ with $Tr(\rho) = 1$; in quantum mechanics, these are called **density matrices**. Each $\rho \in S(M_2(\mathbb{C}))$ can be written as

$$\rho = \frac{1}{2} \begin{pmatrix} 1+x & y+iz \\ y-iz & 1-x \end{pmatrix},$$

where $x, y, z \in \mathbb{R}$. Positivity of this matrix corresponds to the constraint $x^2 + y^2 + z^2 \leq 1$ in \mathbb{R}^3 . Thus, $S(M_2(\mathbb{C}))$ can be identified with the closed unit ball in \mathbb{R}^3 . The pure states are precisely the matrices ρ for which $x^2 + y^2 + z^2 = 1$, so $P(M_2(\mathbb{C}))$ may be identified with the sphere S^2 in \mathbb{R}^3 . This example clearly illustrates that the pure states form the boundary of a compact convex state space.

We now turn to the GNS-construction. Given a state $\omega \in S(A)$, define the subspace N_{ω} , called the **null space** of ω , by

$$N_{\omega} := \{ a \in A \mid \omega(a^*a) = 0 \}.$$
(3.13)

It is not hard to see that one can equivalently define N_{ω} as

$$N_{\omega} = \left\{ a \in A \mid \omega(a^*b) = 0 \ \forall b \in A \right\}.$$

So if one multiplies an element $a \in N_{\omega}$ by an arbitrary element $c \in A$, it follows from the second definition of N_{ω} that $ca \in N_{\omega}$, because $\omega((ca)^*d) = \omega(a^*(c^*d)) = 0 \quad \forall d \in A$, since $\omega(a^*b) = 0 \quad \forall b \in A$, in particular for $b = c^*d$. Furthermore, by boundedness of ω (equation (3.11)), ω is continuous, which implies that N_{ω} is closed in A. Thus, we have:

Proposition 3.2.17 N_{ω} is a left ideal of A.

Next, we can define an inner product $\langle ., . \rangle_{\omega}$ on the quotient space A/N_{ω} by

$$\langle [a], [b] \rangle_{\omega} := \omega(a^*b). \tag{3.14}$$

Here, [a] denotes the equivalence class of $a \in A$ with respect to the quotient. By linearity of ω , $\langle ., . \rangle_{\omega}$ is independent of the choice of representative in the equivalence class. Note that $\langle ., . \rangle_{\omega}$ is positive since ω is positive, and that $\langle [a], [a] \rangle_{\omega} = 0$ if and only if [a] = [0], since we take the quotient. Therefore we have an inner product on A/N_{ω} . Next, define \mathcal{H}_{ω} as the completion of A/N_{ω} in the norm defined by the inner product. \mathcal{H}_{ω} is by definition a Hilbert space. Finally, given $\omega \in S(A)$, we define a representation π_{ω} of A on A/N_{ω} by:

$$\pi_{\omega}(a)([b]) := [ab]. \tag{3.15}$$

One can see that $\pi_{\omega}(a) \in \mathcal{B}(A/N_{\omega}) \ \forall a \in A$. Therefore, π_{ω} is continuous, so it can be continuously extended to a map π_{ω} from A to $\mathcal{B}(\mathcal{H}_{\omega})$. Since π_{ω} clearly is a *-homomorphism, π_{ω} indeed is a representation of A on \mathcal{H}_{ω} .

For every state $\omega \in S(A)$, there is a vector $\xi_{\omega} \in \mathcal{H}_{\omega}$ such that

$$\langle \xi_{\omega}, \pi_{\omega}(a)\xi_{\omega} \rangle = \omega(a), \ \forall a \in A.$$
(3.16)

In the unital case, this vector is defined by

$$\xi_{\omega} := [I].$$

Note that $\pi_{\omega}(A)\xi_{\omega} = A/N_{\omega}$ is dense in \mathcal{H}_{ω} . This means that the vector ξ_{ω} is a so called **cyclic** vector for the representation π_{ω} , that is, the closure of $\pi_{\omega}(A)\xi_{\omega}$ is equal to \mathcal{H}_{ω} . A representation π on a Hilbert space \mathcal{H} is called **cyclic** if \mathcal{H} contains a cyclic vector for π .

The following proposition is an easy consequence of the definitions:

Proposition 3.2.18 A representation π of A on \mathcal{H} is irreducible if and only if every nonzero vector $\xi \in \mathcal{H}$ is cyclic for π . \Box

We have seen that for every state $\omega \in S(A)$ a representation π_{ω} on a Hilbert space \mathcal{H}_{ω} can be constructed, with a vector $\xi_{\omega} \in \mathcal{H}_{\omega}$ that is cyclic for π_{ω} . This construction of associating representations to states is called the **GNSconstruction** (GNS stands for Gelfand, Naimark and Segal). The converse can also be realized: every non-degenerate representation π on a Hilbert space \mathcal{H} , together with a vector $\xi \in \mathcal{H}$, defines a state $\omega_{\pi,\xi}$ by

$$\omega_{\pi,\xi}(a) := \langle \xi, \pi(a)\xi \rangle_{\mathcal{H}}.$$
(3.17)

Moreover, every state $\omega \in S(A)$ comes from a representation and a vector by (3.16).

Remark 3.2.19 If we start with a non-degenerate representation π of A on \mathcal{H} and a vector $\xi \in \mathcal{H}$ that is cyclic for π , we can define a state ω by (3.17). Next, we can define π_{ω} and ξ_{ω} via the GNS-construction. Now, we have

$$\langle \xi, \pi(a)\xi \rangle = \omega(a) = \langle \xi_{\omega}, \pi_{\omega}(a)\xi_{\omega} \rangle,$$

for each $a \in A$, and since $\pi(A)\xi$ (respectively $\pi_{\omega}(A)\xi_{\omega}$) is dense in \mathcal{H} (respectively \mathcal{H}_{ω}), it follows that there is an isomorphism U of \mathcal{H} onto \mathcal{H}_{ω} such that $U\pi(a)\xi = \pi_{\omega}(a)\xi_{\omega}$ for any $a \in A$. It easily follows that U makes π and π_{ω} unitary equivalent. In particular, if π is irreducible, every nonzero vector in \mathcal{H} is cyclic for π , so π is defined up to equivalence by any state associated to π .

One can define a universal representation π as the direct sum of all the **GNS**representations π_{ω} , $\omega \in S(A)$; note that π is defined on $\mathcal{H} := \bigoplus_{\omega \in S(A)} \mathcal{H}_{\omega}$. We show that π is injective, and hence, that every C*-algebra A is isomorphic to a subalgebra of $\mathcal{B}(\mathcal{H})$. Hereby we prove the **Gelfand Naimark theorem**, Theorem 3.2.2:

Suppose that $\pi(a) = 0$ for some $a \in A$. This means that $\pi_{\omega}(a) = 0$ for all $\omega \in S(A)$. Hence $\pi_{\omega}(a)\xi_{\omega} = 0$, which gives $\|\pi_{\omega}(a)\xi_{\omega}\|^2 = 0$, or $\omega(a^*a) = 0$ by (3.16), for all $\omega \in S(A)$. Finally, this leads to $\|a^*a\| = 0$, from which it follows that a = 0 by the C*-compatibility condition (3.2). This completes the proof of Theorem 3.2.2. \Box

We already had a correspondence between states and representations via the GNS-construction. It turns out that there is a correspondence between the pure states $\omega \in P(A)$ and the unitary equivalence classes of irreducible representations in \hat{A} . Recall that a **projection** p on a Hilbert space \mathcal{H} is an operator in $\mathcal{B}(\mathcal{H})$ such that $p = p^2 = p^*$.

Proposition 3.2.20 A representation π of a C*-algebra A is irreducible if and only if the only projections that commute with $\pi(A)$ are 0 and 1.

Proof: This is just Schur's lemma, together with the fact that $p = p^2$ for any projection p.

Theorem 3.2.21 The GNS-representation π_{ω} of a state $\omega \in S(A)$ is irreducible if and only if ω is pure.

For a proof, we refer to [33].

So there is a canonical map ϕ from P(A) to \hat{A} , which is surjective by Remark 3.2.19. We can define an equivalence relation \sim on P(A) by

$$\omega_1 \sim \omega_2 \Longleftrightarrow \pi_{\omega_1} \sim_u \pi_{\omega_2}. \tag{3.18}$$

If we denote the graph of this equivalence relation by R, it is clear that R is just the kernel of ϕ , and thus there is a bijective correspondence between P(A)/R(also denoted by $P(A)/\sim$) and \hat{A} .

In our attempt to get a noncommutative analogue of Theorem 3.1.2, we define a noncommutative version of the Gelfand transform (3.4), $\hat{:} A \to \mathcal{B}(\hat{A}, \bigoplus_{\omega \in P(A)} \mathcal{H}_{\omega})$ by

$$\hat{a}(\pi) := \pi(a).$$
 (3.19)

We see that $\hat{a}(\pi_{\omega}) \in \mathcal{H}_{\omega}$ for each $\omega \in P(A)$, so different values of \hat{a} lie in different fibers of the bundle $\bigoplus_{\omega \in P(A)} \mathcal{H}_{\omega}$. Therefore it is hard to see in what way the Gelfand transform can be made continuous. We will not pursue this subject; for more information, see [38, 55].

Chapter 4

Equivalence relations, groupoids and C*-algebras

In this chapter, we will develop the machinery needed to describe the noncommutative topology of non-Hausdorff spaces that are quotient spaces by some equivalence relation. Recall that in a non-Hausdorff space, there are not enough open subsets to separate points. In particular, the C*-algebra of continuous functions is too small to describe every topological aspect of a non-Hausdorff space. We will show that an equivalence relation automatically defines a groupoid, and define a noncommutative C*-algebra associated to this groupoid. This noncommutative C*-algebra will contain the noncommutative topological information about the non-Hausdorff quotient space.

4.1 The groupoid of an equivalence relation

In this section we define groupoids, and we will see in particular in which way every equivalence relation automatically defines a groupoid. This section is largely based on [44]. For a more recent reference, see [37].

A groupoid is a generalization of a group. The crucial difference is that in a groupoid G, not every two elements need to be composable, i.e. the operation (product, summation, composition, etc.) is not defined from $G \times G$ to G, but only on a subset G^2 of $G \times G$. A good example is the **path groupoid** of a space, which is the set G of paths on a topological space X, with composition. Every path is a continuous function $f : [0, 1] \to X$. However, not all paths can be composed with each other. This is only possible if the endpoint of the first path is the starting point of the second path. Thus, we have:

$$G^{2} = \{ (f,g) \in G \times G \mid f(1) = g(0) \}.$$
Every element f of G has an inverse, defined by $f^{-1}(t) = f(1-t)$, and the composition of a path f with its inverse is identified with the constant path on f(0). These constant paths form the unit space G^0 of the groupoid. We can check that the above groupoid is indeed a groupoid according to the following general definition:

Definition 4.1.1 A set G is a groupoid if there is a set $G^2 \subseteq G \times G$, called the set of "composable pairs", a product map $G^2 \to G$, $(x, y) \mapsto xy$, and an inversion map $G \to G$, $x \mapsto x^{-1}$ such that the following relations are satisfied:

- 1. $(x^{-1})^{-1} = x;$
- 2. If $(x, y), (y, z) \in G^2$, then $(xy, z), (x, yz) \in G^2$ and (xy)z = x(yz);
- 3. $(x^{-1},x) \in G^2 \ \forall x \in G \ and \ if \ (x,y), (z,x) \in G^2, \ then \ x^{-1}(xy) = y \ and \ (zx)x^{-1} = z.$

Additionally, we define the **range** of an element $x \in G$ as $R(x) := xx^{-1}$ and its **domain** as $D(x) := x^{-1}x$. We have the following easy consequence:

$$(x,y) \in G^2 \iff R(y) = D(x)$$

Note that for all $x \in G$, xD(x) = R(x)x = x. This leads to the definition of the **unit space** $G^0 \subset G$: $G^0 := D(G) = R(G)$. Here R(G) and D(G) are defined as $R(G) := \{xx^{-1} \mid x \in G\}$ and $D(G) := \{x^{-1}x \mid x \in G\}$ Since for all $x \in G$, $(x^{-1})^{-1} = x$, R(G) and D(G) are equal and G^0 is well defined.

As an alternative definition, one can see a groupoid as a category, in which G^0 serves as the set of "objects". An element $x \in G$ can be seen as a morphism from D(x) to R(x), thus identifying the domain D with the "source" map in the category and the range R with the "target" map in the category. Note that a groupoid is just a special case of a category, because of the existence of an inversion map. For more on categories, see e.g. [28].

Note that in the category formalism, one can see the elements of G as arrows (or paths) from one point in G^0 to another point in G^0 (the "base" points). The product of two elements in G is then the composition of the corresponding arrows. One can compose two arrows if and only if the endpoint of the first arrow is the starting point of the second arrow. Every arrow has an inverse arrow, and the elements of G^0 are identified with the constant arrows. It is easy to see that these arrows satisfy the relations of Definition 4.1.1. Thus we see that the path groupoid defined above is indeed an example of a groupoid. In particular, G^0 may be identified with the topological space X. Note that if we identify homotopic paths with each other, we get the **fundamental groupoid** of X, which is a generalization of the fundamental group $\pi_1(X)$. Let's consider some other examples of groupoids: **Example 4.1.2** A group G itself is of course an example of a groupoid. In this case all elements are composable with each other, i.e. $G^2 = G \times G$. The subset of units, G^0 , is just $\{e\}$, where $e \in G$ is the unit element of the group.

Example 4.1.3 Consider a group S acting on a space X on the right. Denote the image of $x \in X$ under $s \in S$ simply by $x \cdot s$. Then $X \times S$ can be seen as a groupoid, which we denote by $G := X \rtimes S$, if we define the following structure on it: (x, s) and (y, t) are composable if and only if $y = x \cdot s$, the product is defined by

$$(x,s)(x \cdot s,t) = (x,st),$$

and the inverse by

$$(x,s)^{-1} = (x \cdot s, s^{-1}).$$

Then it follows that R(x, s) = (x, e) and $D(x, s) = (x \cdot s, e)$, where e is the unit of the group S. We see that the unit space G^0 can be identified with X under $(x, e) \mapsto x$. $X \rtimes S$ is called a (right) **transformation groupoid**. Similarly, a left action of a group S on a space X defines a left transformation groupoid $S \ltimes X$. Sometimes, we will explicitly denote the action of $s \in S$ by α_s , and in this case, the groupoid is denoted by $X \rtimes_{\alpha} S$.

Definition 4.1.4 A groupoid is called **principal** if the map

$$(R,D): G \to G^0 \times G^0: \quad x \mapsto (xx^{-1}, x^{-1}x),$$

is injective.

Notice that a group with more than one element is certainly not an example of a principal groupoid, as the map $x \mapsto (e, e)$ is not injective, unless $G = \{e\}$. On the positive side, we have

Proposition 4.1.5 A transformation groupoid $X \rtimes S$ is principal if and only if S acts freely (i.e. $x \cdot s = x$ for some x implies s = e).

Proof: The map $(R, D) : X \times S \to X \times X$ is given by $(R, D)(x, s) = (x, x \cdot s)$, where we have identified the unit space with X. Now (R, D) is injective if and only if (R, D)(x, s) = (R, D)(y, t) implies x = y and s = t. The first is automatically satisfied, for the second, we must have that $x \cdot s = x \cdot t$ implies s = t. Multiplying from the right by s^{-1} , we see that s = t if and only if $x = x \cdot ts^{-1}$ means that $ts^{-1} = e$, which is precisely the definition of a free action. \Box

Next, we introduce an example of a principal groupoid, which will play a very important role in the philosophy of noncommutative topology. In fact, this groupoid will be a crucial ingredient in the description of noncommutative spaces. Recall the definition of an equivalence relation \sim on a space X:

Definition 4.1.6 An equivalence relation \sim is a relation on a set X such that the following holds:

- 1. $x \sim x \ \forall x \in X \ (reflexivity);$
- 2. if $x \sim y$ then $y \sim x$ (symmetry);
- 3. if $x \sim y$ and $y \sim z$ then $x \sim z$ (transitivity).

The graph R of an equivalence relation \sim is the subset of $X \times X$ defined by

$$R := \{ (x, y) \in X \times X \mid x \sim y \}$$

Two elements $x, x' \in X$ belong to the same **equivalence class**, denoted by [x], if and only if $x \sim x'$. The set of all equivalence classes is denoted by X/\sim or X/R.

Proposition 4.1.7 The graph R of an equivalence relation \sim on a set X has the structure of a principal groupoid.

Proof: Define the set R^2 of composable pairs by

$$R^{2} := \left\{ ((a, b), (b', c)) \in R \times R \mid b = b' \right\}$$

Define a product map from R^2 to R by (a, b)(b, c) := (a, c), and an inverse map by $(a, b)^{-1} := (b, a)$. Note that product and inverse are well defined due to the transitivity and the symmetry of ~ respectively. Then we have the following:

- 1. $((a,b)^{-1})^{-1} = (b,a)^{-1} = (a,b);$
- 2. If $((a,b),(b,c)),((b,c),(c,d)) \in R^2$, then $((a,c),(c,d)) \in R^2$ and ((a,b)(b,c))(c,d) = (a,d) = (a,b)((b,c)(c,d));
- 3. $((a,b), (a,b)^{-1}) \in \mathbb{R}^2$ and $((a,b)^{-1}, (a,b)) \in \mathbb{R}^2 \ \forall (a,b) \in \mathbb{R}$, because $(a,b)^{-1} = (b,a)$. Moreover, if $((a,b), (b,c)) \in \mathbb{R}^2$ and $((d,a), (a,b)) \in \mathbb{R}^2$, then $(a,b)^{-1}((a,b)(b,c)) = (b,c)$ and $((d,a)(a,b))(a,b)^{-1} = (d,a)$.

So R has the structure of a groupoid.

Now one can see that R(a,b) = (a,a) and D(a,b) = (b,b), so the unit space $R^0 \in R$ is the diagonal in R and can be identified with the set X.

Next we show that R is a principal groupoid: let $(a, b), (c, d) \in R$ such that (R, D)(a, b) = (R, D)(c, d). This means that $((a, a), (b, b)) = ((c, c), (d, d)) \in R^0 \times R^0$, or (a, b) = (c, d) in $X \times X$. This means that (a, b) = (c, d) in R, as R is a subset of $X \times X$. Therefore (R, D) is injective and thus R is a principal groupoid. \Box

Using the fact that $X \times X$ is the graph of the equivalence relation \sim for which $x \sim y$, for all $x, y \in X$, we have the following easy consequence:

Corollary 4.1.8 Let X be a space. Then $X \times X$ is a principal groupoid, with unit space X.

Definition 4.1.9 If G and H are groupoids, a map $\varphi : G \to H$ is called a homomorphism (of groupoids) if $\forall (x,y) \in G^2$, $(\varphi(x),\varphi(y)) \in H^2$ and $\varphi(x)\varphi(y) = \varphi(xy)$.

As a direct consequence of this definition, we have $\varphi(G^0) \subseteq H^0$, that is, $\varphi(u) \in H^0 \quad \forall u \in G^0$. This follows from the fact that every $u \in G^0$ can be written as $u = xx^{-1}$ for some $x \in G$. Therefore, we have $\varphi(u)\varphi(x) = \varphi(xx^{-1}x) = \varphi(x)$, from which it follows that $\varphi(u) \in H^0$.

Definition 4.1.10 Two homomorphisms $\varphi, \psi : G \to H$ are called similar $(\varphi \sim \psi)$ if there is a map $\Theta: G^0 \to H$ such that $\forall x \in G$:

$$(\Theta \circ R)(x)\varphi(x) = \psi(x)(\Theta \circ D)(x).$$

G and H are called similar $(G \sim H)$ if there exist homomorphisms $\varphi : G \to H$ and $\psi : H \to G$ such that $\varphi \circ \psi \sim id_H$ and $\psi \circ \varphi \sim id_G$.

Note that in a general category, the correct notion of a homomorphism is a **func**tor $\varphi : G \to H$, for which the extra condition is necessary that $\varphi(G^0) \subseteq H^0$. The similarity map Θ is just the categorical notion of a **natural transforma**tion [28].

We want to consider groupoids that have the structure of a topological space.

Definition 4.1.11 A topological groupoid is a groupoid G on which a topology is defined that is compatible with the groupoid structure:

- 1. The inverse map $G \to G$; $x \mapsto x^{-1}$ is continuous.
- 2. The product map $G^2 \to G$; $(x, y) \mapsto xy$ is continuous, where G^2 has the induced topology of the product topology on $G \times G$.

We have the following proposition:

Proposition 4.1.12 Let G be a topological groupoid. Then the following hold:

- 1. The inverse map is a homeomorphism.
- 2. The maps $R: G \to G^0$ and $D: G \to G^0$ are continuous.
- 3. If G is Hausdorff, then G^0 is closed in G.

4. If G^0 is Hausdorff, then G^2 is closed in $G \times G$.

Proof: 1. and 2. are easy consequences of the definition.

3. If G is Hausdorff, then the diagonal Δ is closed in $G \times G$. Define a map $\psi: G \to G \times G$ by $\psi(x) := (x, x^{-1})$. Then $\psi^{-1}(\Delta) = \{x \in G \mid x = x^{-1}\}$ is closed in G by continuity of ψ . But $\psi^{-1}(\Delta)$ is just G^0 , so G^0 is closed in G. 4. If G^0 is Hausdorff, then the diagonal Δ^0 is closed in $G^0 \times G^0$. Define the map $\varphi: G \times G \to G^0 \times G^0$ by $\varphi(x, y) := (D(x), R(y))$. Then $\varphi^{-1}(\Delta^0) = \{(x, y) \in G \times G \mid D(x) = R(y)\}$ is closed in $G \times G$ by continuity of φ . But this is just G^2 , so G^2 is closed in $G \times G$. \Box

4.2 Towards the C*-algebra of a groupoid

In this section, we will show how a C*-algebra can be constructed from a topological groupoid, and under which conditions this is possible. Again, this section is largely based on [44].

A topological groupoid can have all sorts of topological features. In particular, a topological groupoid G is **locally compact** if for each $x \in G$, there exists an open set U_x with $x \in U_x$ such that the closure of U_x is compact. On a locally compact groupoid G, one can define the space $C_c(G)$ of continuous functions on G with compact support, that is:

 $C_c(G) := \{ f \in C(G) \mid \exists K \subset G, K \text{ compact, such that } f \equiv 0 \text{ outside } K \}$

Definition 4.2.1 A locally compact groupoid G is called R-discrete if its unit space G^0 is open in G.

Proposition 4.2.2 For an *R*-discrete groupoid G, $R^{-1}(u)$ and $D^{-1}(u)$ are discrete $\forall u \in G^0$.

Proof: Let $x \in R^{-1}(u) \cap D^{-1}(v)$ for $u, v \in G^0$. Such an x defines a homeomorphism $\psi : R^{-1}(v) \to R^{-1}(u); y \mapsto xy$. Since G is R-discrete, G^0 is open in G, and therefore $G^0 \cap R^{-1}(v)$ is open in $R^{-1}(v)$. But $G^0 \cap R^{-1}(v)$ is just $\{v\}$, because if $y \in G^0 \cap R^{-1}(v)$, then y = R(y) and $y \in R^{-1}(v)$, so y = R(y) = v. Now $\{x\} = \psi(\{v\})$ is open in $R^{-1}(u)$, because ψ is a homeomorphism. So $R^{-1}(u)$ is discrete. A similar argument gives that $D^{-1}(u)$ is discrete. \Box

Recall that on a group, we have the notion of a **Haar measure**, which is a left invariant measure. We want to have a similar notion for groupoids.

Definition 4.2.3 Let G be a locally compact groupoid. A left Haar system is a set of measures $\{\lambda^u \mid u \in G^0\}$ such that:

- 1. The support of each measure λ^u is $supp(\lambda^u) = R^{-1}(u)$.
- 2. (continuity) $\forall f \in C_c(G)$, the map $G^0 \to \mathbb{C}$; $u \mapsto \lambda(f)(u) = \int f d\lambda^u$ is continuous.
- 3. (left invariance) $\forall x \in G, \forall f \in C_c(G),$

$$\int f(xy) \, d\lambda^{D(x)}(y) = \int f(y) \, d\lambda^{R(x)}(y)$$

Remark 4.2.4 Note that 1. is necessary for 3. to make sense: f(xy) can only be defined for $(x, y) \in G^2$. Luckily, due to 1., $supp(\lambda^{D(x)}) = R^{-1}(D(x))$. Thus, only for values of y in $R^{-1}(D(x))$ there is a contribution to the integral. For these $y \in G$, R(y) = D(x) holds, which is equivalent to $(x, y) \in G^2$. Therefore the integral is well defined.

The notion of a left Haar system is the extension for groupoids of the group theoretic notion of a Haar measure. Remark 4.2.4 is the reason why in the case of groupoids, one measure is not sufficient. Of course there is also a description in terms of right invariant measures, but one can show that this is in fact equivalent with the description in terms of left invariant measures, since every left Haar system $\{\lambda^u\}$ defines a right Haar system $\{\lambda_u\}$ (where $\lambda_u := (\lambda^u)^{-1}$) under the inverse map $x \mapsto x^{-1}$, and vice versa.

Proposition 4.2.5 If a locally compact groupoid is *R*-discrete and it admits a Haar system, then the latter is the counting measures system (up to scaling with a continuous, positive function).

Proof: Let $\{\lambda^u\}$ be a left Haar system of the *R*-discrete groupoid *G*. For each $u \in G^0$, λ^u has support $R^{-1}(u)$, and by proposition 4.2.2, $R^{-1}(u)$ and $D^{-1}(u)$ are discrete. Thus every point in $R^{-1}(u)$ has positive λ^u -measure. Let $g := \lambda(\chi_{G^0}) = \int \chi_{G^0} d\lambda^u$, where χ_{G^0} is the characteristic function of G^0 . Note that g is a continuous and positive function on G^0 , and replacing λ^u by $g(u)^{-1}\lambda(u)$, we may assume that $\lambda^u(\{u\}) = 1$ for all $u \in G^0$. Then by left invariance, $\lambda^v(\{x\}) = 1$ for any $x \in R^{-1}(v) \cap D^{-1}(u)$.

Basically, an *R*-discrete groupoid *G* can be seen as the union of discrete "fibers", $G = \bigcup_{u \in G^0} R^{-1}(u)$, each with its own counting measure λ^u .

Now if G is a group with a left Haar measure λ , one can define a convolution product on the space $C_c(G)$ by

$$(f * g)(x) := \int f(y)g(y^{-1}x) d\lambda(y).$$
 (4.1)

For example, if G is the abelian group \mathbb{R} , then (4.1) just becomes the usual convolution product:

$$(f * g)(x) = \int f(y)g(x - y) \, dy$$

Next, we will use a similar construction to give $C_c(G)$ a convolution product. Recall from Definition 3.0.2 that a *-algebra is an associative algebra with involution *.

Proposition 4.2.6 Let G be a locally compact groupoid with left Haar system $\{\lambda^u \mid u \in G^0\}$. Define a convolution product * and an involution * on $C_c(G)$ by

$$(f * g)(x) := \int f(xy)g(y^{-1}) \, d\lambda^{D(x)}(y) \tag{4.2}$$

$$f^*(x) := \overline{f(x^{-1})} \tag{4.3}$$

With these operations, $C_c(G)$ becomes a *-algebra.

The proof consists of checking the following $(\forall f, g, h \in C_c(G))$:

- 1. The algebra is closed under multiplication, i.e. $f * g \in C_c(G)$.
- 2. The product is associative, i.e. f * (g * h) = (f * g) * h.
- 3. The involution really is an involution (under which the algebra is closed), that is, all $f, g \in C_c(G)$ satisfy 1., 2. and 3. of Definition 3.0.2.
- 4. the operations * and * are continuous, i.e.: If $f_n \to f$ and $g_m \to g$ in $C_c(G)$, then $f_n * g_m \to f * g$ and $f_n^* \to f^*$ uniformly on a compact subset of G.

We will not do these computations here. For a proof of a more general case, see [44]. Note that a simple computation using the left invariance of the Haar measure, shows that (4.2) reduces to (4.1) in the case that G is a group.

Now recall from Definition 3.0.3 that a C*-algebra A is a *-algebra with norm $\|.\|$ (for which it is complete), such that for all $a, b \in A$ the Banach algebra condition and the C*-condition are satisfied:

$$\|ab\| \le \|a\| . \|b\| \tag{4.4}$$

$$||aa^*|| = ||a||^2. \tag{4.5}$$

So the only thing we need to make the *-algebra $C_c(G)$ into a C*-algebra, is a norm $\|.\|$ in which the algebra is complete, and which satisfies the Banach algebra condition (4.4) and the C*-condition (4.5). This norm is constructed by means of representations of $C_c(G)$ on a Hilbert space (recall that for a Hilbert space \mathcal{H} , the set of bounded operators $\mathcal{B}(\mathcal{H})$ form a C*-algebra).

Now before giving the definition of a representation of $C_c(G)$, we first need to define topologies on $C_c(G)$ and $\mathcal{B}(\mathcal{H})$:

Definition 4.2.7 Let \mathcal{H} be a Hilbert space. Suppose that for each sequence (A_n) in $\mathcal{B}(\mathcal{H})$, $A_n \to A$ if and only if $\langle \psi, A_n \psi \rangle \to \langle \psi, A\psi \rangle \ \forall \psi \in \mathcal{H}$. Then $\mathcal{B}(\mathcal{H})$ has the weak operator topology.

Let K be a compact subset of G. Define a semi-norm on $C_c(G)$ by

$$||f||_K := \sup_{x \in K} |f(x)|$$

Then in the **inductive limit topology**, $f_n \to f$ if and only if $||f - f_n||_K \to 0$ for every compact set K in G.

Remark 4.2.8 The inductive limit topology was originally defined on spaces X that are **inductive limits**, i.e. there is a sequence (X_n) of subsets, such that $X_n \subseteq X_{n+1} \ \forall n \in \mathbb{N}$, and such that $X = \bigcup_{n=1}^{\infty} X_n$. Then a subset V is open in X if and only if $V \cap X_n$ is open in X_n for all $n \in \mathbb{N}$. Since G is a locally compact group, it can be approximated by compact subsets, and therefore it can be seen as an inductive limit.

Using the above definition, we can now give the definition of a representation of $C_c(G)$ on a Hilbert space:

Definition 4.2.9 Let G be a locally compact groupoid with left Haar system $\{\lambda^u\}$. A representation of the *-algebra $C_c(G)$ on a Hilbert space \mathcal{H} is a linear map $\pi : C_c(G) \to \mathcal{B}(\mathcal{H})$ that is continuous if $C_c(G)$ has the inductive limit topology and $\mathcal{B}(\mathcal{H})$ has the weak operator topology. Moreover, π satisfies the following *-homomorphism conditions:

1.
$$\pi(f * g) = \pi(f)\pi(g);$$

2. $\pi(f^*) = \pi(f)^*.$

Now we define a norm on $C_c(G)$ by

$$||f|| := \sup \{ ||\pi(f)||_{op} \mid \pi \text{ is a representation of } C_c(G) \}$$

$$(4.6)$$

Here, $\|\pi(f)\|_{op}$ is the operator norm (3.6) of $\pi(f)$ of $\mathcal{B}(\mathcal{H})$. Note that a priori, the supremum need not exist. However, one can show [44] that we always have $\|\pi(f)\| \leq \|f\|_{I}$, where the *I*-norm is defined as

$$||f||_I := \max\left\{\sup_{u\in G^0}\int |f|d\lambda^u, \sup_{u\in G^0}\int |f|d\lambda_u\right\}.$$

Therefore, the supremum will be finite.

Proposition 4.2.10 The completion of $C_c(G)$ in the above norm (4.6) is a C^* -algebra, called $C^*(G)$.

Proof: We only have to show that the product and involution can be extended from $C_c(G)$ to $C^*(G)$, and that the two conditions (4.4) and (4.5) are satisfied. This follows from the fact that $\mathcal{B}(\mathcal{H})$ is a C*-algebra and the fact that each π is a representation:

$$\|\pi(f * g)\|_{op} = \|\pi(f)\pi(g)\|_{op} \le \|\pi(f)\|_{op} \|\pi(g)\|_{op}$$
$$\|\pi(f^* * f)\|_{op} = \|\pi(f^*)\pi(f)\|_{op} = \|\pi(f)^*\pi(f)\|_{op} = \|\pi(f)\|_{op}^2$$

for all representations π . Since the above is preserved under taking the supremum, it follows that $||f * g|| \le ||f|| \cdot ||g||$ and $||f^* * f|| = ||f||^2$. By definition, $C^*(G)$ is complete in the norm. \Box

There is another norm on $C_c(G)$ that makes it into a different C*-algebra, the so called reduced norm. The definition of this norm has the advantage that it is less abstract then the above one. Let G again be a locally compact groupoid with *-algebra $C_c(G)$ and Haar system $\{\lambda^u\}$. For any $u \in G^0$, we define the Hilbert space $\mathcal{H}_u := L^2(D^{-1}(u), \lambda^u)$, the space of square integrable functions on $D^{-1}(u)$ with respect to the measure λ^u . Next we define the **reduced representation** π_u of $C_c(G)$ on \mathcal{H}_u by

$$(\pi_u(f)\psi)(x) := \int f(xy)\psi(y^{-1}) \, d\lambda^u(y).$$
(4.7)

In this equation, $f \in C_c(G)$, $\psi \in \mathcal{H}_u$, and $x \in D^{-1}(u)$. Note that (4.7) is well defined, since $x \in D^{-1}(u)$ and all $y \in supp(\lambda^u) = R^{-1}(u) \Rightarrow R(y) = u = D(x) \Rightarrow (x, y) \in G^2$. Note that the representation π_u can be equivalently defined by

$$\pi_u(f)\psi \upharpoonright_{D^{-1}(u)} := f * \psi \upharpoonright_{D^{-1}(u)}.$$

In the case that G is an R-discrete groupoid, by Proposition 4.2.5, the Haar system may be taken to be the counting measures system, so the integral in (4.7) can be replaced by a sum:

$$(\pi_u(f)\psi)(x) := \sum_{y \in R^{-1}(u)} f(xy)\psi(y^{-1}).$$
(4.8)

Of course, in this case the Hilbert space \mathcal{H}_u is the space of square summable functions on $D^{-1}(u)$, so $\psi \in \ell^2(D^{-1}(u), \lambda^u)$. We use (4.8) (or, in the more general case, (4.7)) to define the **reduced norm** on the *-algebra $C_c(G)$:

$$||f||_{red} := \sup \{ ||\pi_u(f)||_{op} \mid u \in G^0 \}.$$
(4.9)

Again, $\|\pi_u(f)\|_{op}$ is the operator norm (3.6) of $\pi_u(f)$ of $\mathcal{B}(\mathcal{H}_u)$. Note that since for all $f \in C_c(G)$, we have

$$\|f\|_{red} \le \|f\|,$$

the norm is bounded.

Proposition 4.2.11 The *-algebra $C^*_{red}(G)$, defined as the completion of $C_c(G)$ in the reduced norm (4.9), is a C*-algebra.

Proof: The proof is essentially the same as the proof of Proposition 4.2.10. \Box

Remark 4.2.12 Representation theory is of course not restricted to representations of $C_c(G)$. One can also define groupoid representations and, as a special case, group representations. A representation π of a groupoid G is a collection of maps $\{\pi(x)\}_{x\in G}$ on a collection of Hilbert spaces $\{\mathcal{H}_u\}_{u\in G^0}$ such that

- 1. $\pi(x): \mathcal{H}_{d(x)} \to \mathcal{H}_{r(x)}$ is unitary.
- 2. $\pi(xy) = \pi(x)\pi(y)$ whenever $(x, y) \in G^2$.
- 3. $\pi(x^{-1}) = \pi(x)^*$ for all $x \in G$.

The left regular representation π_L is defined on the collection of Hilbert spaces $\{L^2(r^{-1}(u))\}_{u\in G^0}$ by

$$\pi_L(y)\psi(x) := \psi(y^{-1}x). \tag{4.10}$$

It takes some computations to show that π_L is well defined. In the case that G is a group, only one Hilbert space $\mathcal{H} := \mathcal{H}_e$ needed, and things are a lot easier. For example, the left regular representation of a group G just maps G to $\mathcal{B}(L^2(G))$. The reduced representation of $C_c(G)$ can actually be seen as an integrated version of the left regular representation of G, see e.g. [37, 44]. As a final remark, it should be noted that historically, group representation theory came first, and was later generalized to the groupoid case. For more on this subject, see e.g. [19].

Note that for all $f \in C_c(G)$, we have

$$||f||_{red} \le ||f||.$$

Of course, one wonders if there is a condition for the groupoid G such that $C_{red}^*(G)$ and $C^*(G)$ coincide, i.e. such that $||f||_{red} = ||f||$ for all $f \in C_c(G)$. It turns out that this is the case if G is an **amenable** groupoid [44, 1]. Amenability was originally defined only for groups, and there are several equivalent definitions [22]. We will define this concept in Chapter 7.

Summarizing, we see that the graph R of an equivalence relation can be given a groupoid structure, which can define two different C*-algebras, namely $C^*(R)$ and $C^*_{red}(R)$, if the groupoid has a topology in which it is locally compact and admits a Haar system. If, furthermore, the topology is such that the unit space R^0 is an open subset of R, then R becomes R-discrete and we can use the

summation representation (4.8) instead of the integral representation (4.7) for the construction of the reduced norm. Of course, the topology depends on the nature of the space X on which the equivalence relation is defined, so we cannot say much about the topology of R until the space X and the equivalence relation \sim have been specified. Note however, that the topology on R doesn't have to coincide with the relative topology of the product topology on $X \times X$. For an example of this phenomenon, see Chapter 6.

Chapter 5

Invariants for noncommutative topology

5.1 Possible topological invariants

Recall that to analyze non-Hausdorff spaces, the C*-algebra of continuous functions does not contain enough information, because there are not enough open sets to separate points. For non-Hausdorff spaces that are quotients Y/R it is therefore useful to look at the noncommutative groupoid C*-algebra $C^*(R)$, which will be the true exposer of the topology of Y/R. Therefore, many authors refer to this C*-algebra as the noncommutative space. The fact that C(Y/R)is replaced by $C^*(R)$ in the non-Hausdorff case is motivated by the fact that for Hausdorff quotient spaces, C(Y/R) is "Morita equivalent" with $C^*(R)$, cf. Section 5.2. To look at $C^*(R)$ instead of C(Y/R) is the most important step in the philosophy of noncommutative topology [15].

In topology, it is often useful to define invariants that can be used to characterize certain classes of topological spaces. For example, the fundamental group $\pi_1(X)$ of an arcwise connected space X can be used to distinguish between contractible spaces (with trivial fundamental group) and non-contractible spaces (with nontrivial fundamental group). A deeper example is the classification of knots by the Jones-Conway polynomial [28].

If we want to characterize (noncommutative) topological quotient spaces, we want to distinguish between Hausdorff spaces and non-Hausdorff spaces. For Hausdorff quotient spaces Y/R, the continuous functions already contain all the relevant information, so as a first criterion, a "good" topological invariant should not distinguish between C(Y/R) and $C^*(R)$ in the Hausdorff case. Since in this case C(Y/R) and $C^*(R)$ are actually Morita equivalent (cf. Section 5.2), a good invariant has to label different Morita equivalence classes.

A second criterion for a good invariant is that it has to distinguish between C(Y/R) and $C^*(R)$ in the case that Y/R is not Hausdorff. In particular, if Y/R is trivial from a commutative point of view, i.e., $C(Y/R) = \mathbb{C}$, as will be the case in Chapter 6, our invariant should be nontrivial for the noncommutative C*-algebra $C^*(R)$. Until now, we have seen three possible candidates to serve as a relevant invariant, namely the possible noncommutative structure spaces: the set Prim(A) of primitive ideals of a C*-algebra A, the set \hat{A} of equivalence classes of irreducible representations and the set P(A) of pure states on A. A fourth candidate is K-theory, which will be defined in Section 5.2. Whereas the set of primitive ideals is in general too small to serve as a good invariant, in the next example, we will see that the set of pure states is too large, since it does distinguish between C(Y/R) and $C^*(R)$ in the Hausdorff case.

Example 5.1.1 This simple example of a noncommutative space is treated by Connes in his book [15], where $Y = \{y_1, y_2\}$, with equivalence relation $y_1 \sim y_2$. Then $X := Y/R \cong \{y_1\}$, and $C(X) = \{f \in C(Y) \mid f(y_1) = f(y_2)\} \cong \mathbb{C}$. Now consider a function $f \in C^*(R)$. Note that f has four possible values $f_{ij} := f(y_i, y_j)$, with $i, j \in \{1, 2\}$. Therefore, we have a 2-dimensional representation $\pi_1 : C^*(R) \to M_2(\mathbb{C})$:

$$\pi_1: f \mapsto \left(\begin{array}{cc} f_{11} & f_{12} \\ f_{21} & f_{22} \end{array}\right).$$
 (5.1)

Clearly, this representation is bijective, and thus $C^*(R)$ is isomorphic to $M_2(\mathbb{C})$. Note that π_1 is an irreducible representation, and it can be shown that in fact every irreducible representation is unitarily equivalent to π_1 . Thus, $\widehat{C^*(R)}$, the space of unitary equivalence classes of irreducible representations of $C^*(R)$, consists of one point. In fact, there is a bijection between Y/R and $\widehat{C^*(R)}$: defining the representation π_2 of $C^*(R)$ by

$$\pi_2: f \mapsto \left(\begin{array}{cc} f_{22} & f_{21} \\ f_{12} & f_{11} \end{array}\right), \tag{5.2}$$

and noting that π_2 is just π_1 with the role of y_1 and y_2 interchanged, we see that the unitary equivalence of π_1 and π_2 comes directly from the equivalence $y_1 \sim y_2$ in Y.

However, the pure state space of $C^*(R)$ is larger: it can be identified with S^2 by Example 3.2.16. We see that the bijective correspondence between $P(C^*(R))/\sim$ and $\widehat{C^*(R)}$ yields

$$P(C^*(R)/\sim \widehat{C^*(R)} \cong Y/R.$$

Of course, these spaces consist just of one point; we see that all interesting information is contained in the C*-algebra $C^*(R)$, which describes the noncommutative topology of Y.

In the above trivial example of a Hausdorff quotient space, we see that the pure state space distinguishes between the commutative C*-algebra of continuous

functions and the noncommutative groupoid C*-algebra. Therefore, the pure state space is not a good invariant, since it does not meet our first criterion. This leaves \hat{A} , the set of equivalence classes of irreducible representations and K(A), the K-theory of A. It can be shown that both invariants do not distinguish between $C_0(Y/R)$ and $C^*(R)$ for Hausdorff quotient spaces [15], and therefore they satisfy the first criterion.

As for the second criterion, it is not clear whether the irreducible representations of $C^*(R)$ contain all the relevant information in the non-Hausdorff case. However, when $C^*(R)$ is simple, i.e., it contains no non-trivial ideals, then $\widehat{C^*(R)}$ is non-Hausdorff, and contains no information [15]. Note that this is a purely infinite-dimensional phenomenon. This is one of the reasons that since the eighties, people started to see C*-algebraic K-theory as the relevant invariant instead of the space of equivalence classes of irreducible representations. Another probable reason for this is that K-theory has become increasingly easier to compute, making it convenient to handle. In the next section, we shall define this new invariant, and we will use it in subsequent chapters to analyze noncommutative spaces. In what follows, we will no longer consider the noncommutative structure space, looking only at the C*-algebra and its K-theory.

5.2 *K*-theory

The basic idea of K-theory is to assign abelian groups $K_0(A)$, $K_1(A)$, etc. to a C*-algebra A, in such a way that $K_i(A) \simeq K_i(B)$ when $A \simeq B$. We will mainly use the K_0 -group, but for completeness, we give a description of all K-groups. Our main reference for C*-algebraic K-theory will be [46].

Remark 5.2.1 Originally, K-theory was defined for topological spaces X in terms of complex vector bundles over X. However, the group $K^0(X)$ can also be defined using the continuous functions on X instead of X itself, and in this way, we get an abelian group $K_0(C(X))$, which is equal to the topological group $K^0(X)$. This can then be generalized to noncommutative C*-algebras, yielding the K-theory as we present it. From now on, we will only use C*-algebraic K-theory and not topological K-theory, since we are primarily interested in the C*-algebraic side.

Let A be a C*-algebra with unit. Observe that there are natural embeddings

$$A \subset M_2(A) \subset M_3(A) \subset \dots$$

by identifying $a \in A$ with $\begin{pmatrix} a & 0 \\ 0 & 0 \end{pmatrix} \in M_2(A)$, and, more generally, $(a_{ij}) \in M_n(A)$ with

$$\begin{pmatrix} & & 0 \\ & a_{ij} & \vdots \\ & & 0 \\ 0 & \dots & 0 & 0 \end{pmatrix} \in M_{n+1}(A).$$

Next define $M_{\infty}(A)$ by

$$M_{\infty}(A) := \bigcup_{n=1}^{\infty} M_n(A),$$

respecting the inclusion defined above. Observe that for every element $a \in M_{\infty}(A)$, there is a $k < \infty$ such that $a \in M_k(A)$. We now look at the collection $P_1(A)$ of projections in A, i.e. elements $p \in A$ such that $p^2 = p^* = p$. We define the following three equivalence relations:

- 1. (homotopy equivalence) $p \sim_h q$ if there exists a continuous path $\tilde{p} : [0, 1] \to P_1(A)$ of projections such that $\tilde{p}(0) = p$ and $\tilde{p}(1) = q$.
- 2. (unitary equivalence) $p \sim_u q$ if there is a unitary $u \in A$ such that $q = upu^*$.
- 3. (Murray-von Neumann equivalence) $p \stackrel{MvN}{\sim} q$ if there exists a $v \in A$ such that $p = v^*v$ and $q = vv^*$.

Proposition 5.2.2 Let A be a unital C^* -algebra, and let p, q be projections in A. We have the following implications:

1. $||p - q|| < 1 \Longrightarrow p \sim_h q;$ 2. $p \sim_h q \Longrightarrow p \sim_u q;$ 3. $p \sim_u q \Longrightarrow p \stackrel{MvN}{\sim} q.$

Proof: [46] The proof consists of easy computations. For example, to prove the third implication, suppose that $q = upu^*$, where $u \in A$ is unitary. Now if we define v := up, it is easy to see that $v^*v = p$ and $vv^* = q$.

In particular, we see that if we perturb a projection in a norm continuous way, the perturbed projection is equivalent to the original one. The implications the other way are in general not valid. However, if we look at projections in the matrix algebras $M_n(A)$, we see that all three equivalence relations coincide:

Proposition 5.2.3 Let A be a unital C^* -algebra, and let p, q be projections in A. Then the following holds:

• If
$$p \stackrel{MvN}{\sim} q$$
 in A , then $\begin{pmatrix} p & 0 \\ 0 & 0 \end{pmatrix} \sim_u \begin{pmatrix} q & 0 \\ 0 & 0 \end{pmatrix}$ in $M_2(A)$.
• If $p \sim_u q$ in A , then $\begin{pmatrix} p & 0 \\ 0 & 0 \end{pmatrix} \sim_h \begin{pmatrix} q & 0 \\ 0 & 0 \end{pmatrix}$ in $M_2(A)$.

Proof: The proof is again an easy computation [46]. To prove the first implication, suppose that $p = v^*v$ and $q = vv^*$ for some $v \in A$. Next, define

$$u := \left(\begin{array}{cc} v & 1-q \\ 1-p & v^* \end{array}\right).$$

One can show that u is unitary (i.e. $u^*u = 1$), and

$$u\left(\begin{array}{cc}p&0\\0&0\end{array}\right)u^*=\left(\begin{array}{cc}q&0\\0&0\end{array}\right).$$

For the second implication, suppose that there is a unitary $u \in A$ such that $p = uqu^*$. One must first verify that

$$\left(\begin{array}{cc} u & 0 \\ 0 & u^* \end{array}\right) \sim_h \left(\begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array}\right),$$

i.e. there is a continuous path of unitaries w(t) such that

$$w(0) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, w(1) = \begin{pmatrix} u & 0 \\ 0 & u^* \end{pmatrix}.$$

Next, define a path $\tilde{p}(t) := w(t) \begin{pmatrix} p & 0 \\ 0 & 0 \end{pmatrix} w(t)^*$. Then one can show that $\tilde{p}(t)$ is a projection for all t, and that $\tilde{p}(0) = \begin{pmatrix} p & 0 \\ 0 & 0 \end{pmatrix}$ and $\tilde{p}(1) = \begin{pmatrix} q & 0 \\ 0 & 0 \end{pmatrix}$. \Box .

Now if we define

$$P_n(A) := P(M_n(A)), \text{ and } P_{\infty}(A) := \bigcup_{n=1}^{\infty} P_n(A),$$

we have

Corollary 5.2.4 The equivalence relations \sim_h , \sim_u and $\overset{MvN}{\sim}$ coincide on $P_{\infty}(A)$.

This is an immediate consequence of Proposition 5.2.2 combined with Proposition 5.2.3. As a result, we can denote the equivalence relation on $P_{\infty}(A)$ by \sim . In particular, we have equivalence classes of projections $[p] \in P_{\infty}(A)/\sim$.

Remark 5.2.5 For a C*-algebra without a unit, it is of course impossible to define unitary equivalence. Therefore, Murray-von Neumann equivalence is necessary to extend the construction of the K_0 -group to the non-unital case.

Next, we consider again a unital C*-algebra A. Note that for $p \in P_n(A)$ and $q \in P_m(A)$,

$$p \oplus q := \left(\begin{array}{cc} p & 0\\ 0 & q \end{array}\right)$$

is again a projection, i.e. $p \oplus q \in P_{n+m}(A)$. Observe the following facts: let $p, q, r \in P_{\infty}(A)$ (note that $p \in P_{\infty}(A)$ means that $p \in P_n(A)$ for some $n \in \mathbb{N}$). Then we have:

- 1. $p \oplus 0 \sim p;$
- 2. $p \oplus q \sim q \oplus p$;
- 3. $(p \oplus q) \oplus r = p \oplus (q \oplus r);$
- 4. if $p \sim p'$ and $q \sim q'$, then $p \oplus q \sim p' \oplus q'$;
- 5. if pq = 0, then $p + q \sim p \oplus q$.

Now we can define an operation + on $P_{\infty}(A)/\sim$ by

$$[p] + [q] := [p \oplus q], \tag{5.3}$$

and by the above facts, this is a well defined, abelian operation. So we have an abelian semigroup (i.e. a group without inverses)

$$S(A) := (P_{\infty}(A)/\sim, +),$$
 (5.4)

To get the abelian group $K_0(A)$, we use the so called "Grothendieck construction". Given an abelian semigroup (S, +), consider the equivalence relation \sim_G on $S \times S$ defined by

$$(x,y) \sim_G (x',y') \iff \exists z \in S \text{ such that } x+y'+z = x'+y+z.$$
 (5.5)

Define

$$G(S) := S \times S / \sim_G,$$

and write $\langle x, y \rangle_G$ for the equivalence class of (x, y) under \sim_G . The operation +, defined by

$$\langle x, y \rangle_G + \langle x', y' \rangle_G = \langle x + x', y + y' \rangle_G,$$

is well defined, and turns G(S) into an Abelian group. Observe that the inverse of an element $\langle x, y \rangle_G$ is given by $-\langle x, y \rangle_G = \langle y, x \rangle$, and that the unit element is given by $0 = \langle x, x \rangle_G$. G(S) is called the **Grothendieck group** of S.

Remark 5.2.6 The Grothendieck construction is a generalization of the construction of the group \mathbb{Z} from the semigroup \mathbb{N} . \mathbb{Z} is constructed as $\mathbb{N} \times \mathbb{N} / \sim$, where $(n,m) \sim (n',m')$ if n + m' = n' + m. Note that this is a simplification of the Grothendieck construction, because there is no extra z needed for the equivalence relation. In other words, \mathbb{N} has the **cancellation property**, i.e. if x,y,z are elements in \mathbb{N} with x + z = y + z, then it follows that x = y. It is important to notice that in general a semigroup (S, +) does not have the cancellation property. In particular, if we define the **Grothendieck map** by

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

which is additive and independent of $y \in S$, then it is easy to show that γ_S is injective if and only if S has the cancellation property.

Definition 5.2.7 Let A be a unital C*-algebra. Then $K_0(A)$ is defined to be the Grothendieck group of S(A) (defined in (5.4)), i.e.

$$K_0(A) := G(S(A)).$$
 (5.6)

Define $[\cdot]_0 : P_\infty(A) \to K_0(A)$ by

$$[p]_0 := \gamma([p]), \quad p \in P_\infty(A), \tag{5.7}$$

where $\gamma : S(A) \to K_0(A)$ is the Grothendieck map. Then we have the following alternative description of the K_0 -group in terms of formal differences [46]:

Proposition 5.2.8 Let A be a unital C^* -algebra. Then

$$K_0(A) = \{ [p]_0 - [q]_0 \mid p, q \in P_{\infty}(A) \} = \{ [p]_0 - [q]_0 \mid p, q \in P_n(A), n \in \mathbb{N} \}.$$
(5.8)

Moreover,

- 1. $[p \oplus q]_0 = [p]_0 + [q]_0;$
- 2. $[0_A]_0 = 0;$
- 3. if $p \sim_h q$ in $P_n(A)$ for some n, then $[p]_0 = [q]_0$.

Proof: Each element in $K_0(A)$ has the form $\langle [p], [q] \rangle_G$ for some $[p], [q] \in S(A)$. Recall that $[p]_0 = \gamma([p]) = \langle [p] + [r], [r] \rangle_G$ for any $[r] \in S(A)$. Then we have

$$\langle [p], [q] \rangle_G = \langle [p] + [q], [q] \rangle_G - \langle [q] + [p], [p] \rangle_G = \gamma([p]) - \gamma([q]) = [p]_0 - [q]_0.$$

Moreover, $p \in P_k(A)$ and $q \in P_l(A)$, for some k, l, so if we choose n larger than k and l, then $p \sim p \oplus 0_{n-k} =: p'$ and $q \sim q \oplus 0_{n-l} =: q'$, and we have $[p]_0 - [q]_0 = [p']_0 - [q']_0$, and $p, q \in P_n(A)$. 1.,2. and 3. are then easy computations. \Box

The semigroup S(A) appears in $K_0(A)$ as

$$K_0(A)^+ = \{ [p]_0 - [0_A]_0 \mid p \in P_\infty(A) \},$$
(5.9)

and is called the **positive cone** of $K_0(A)$. It is clear that it satisfies

$$K_0(A)^+ + K_0(A)^+ \subseteq K_0(A)^+$$
 and $K_0(A) = K_0(A)^+ - K_0(A)^+$

If moreover, $K_0(A)^+ \cap (-K_0(A)^+) = \{0\}$, then we can define an order on $K_0(A)$ by

$$y \le x \Longleftrightarrow x - y \in K_0(A)^+, \tag{5.10}$$

leading to the **ordered** K_0 -group $(K_0(A), K_0(A)^+, \leq)$.

Before we give some examples of the computation of K_0 -groups, let us state that K_0 can be extended to a functor from the category of unital C*-algebras and *-homomorphisms to the category of abelian groups and group homomorphisms in the following way: given unital C*-algebras A and B, and a *-homomorphism $\varphi : A \to B, \varphi$ can be extended to a map $\varphi_n : M_n(A) \to M_n(B)$ defined by $\varphi_n(a_{ij}) := (\varphi(a_{ij}))$. Since a *-homomorphism maps projections to projections, φ can be extended to a map $\mathcal{P}_{\infty}(A)$ to $\mathcal{P}_{\infty}(B)$, which will also be called φ . Then we can define $K_0(\varphi) : K_0(A) \to K_0(B)$ by

$$K_0(\varphi)([p]_0) := [\varphi(p)]_0, \tag{5.11}$$

for $p \in P_{\infty}(A)$, and one can show that this leads to the following commutative diagram:

Proposition 5.2.9 Let A, B, C be unital C^* -algebras, and let $\varphi : A \to B$ and $\psi : B \to C^*$ -homomorphisms. We have

- 1. $K_0(id_A) = id_{K_0(A)};$
- 2. $K_0(\psi \circ \varphi) = K_0(\psi) \circ K_0(\varphi);$
- 3. $K_0(\{0\}) = \{0\}.$

The proof consists again of easy computations, see [46]. Summarizing, we have:

Corollary 5.2.10 K_0 is a functor from the category of unital C*-algebras and *-homomorphisms to the category of abelian groups and group homomorphisms. In particular, isomorphic C*-algebras have isomorphic K_0 -groups.

Note that so far, we have always assumed that our C*-algebra is unital. However, K-theory can also be defined for C*-algebras without a unit. Consider the **split exact sequence**

$$0 \longrightarrow A \xrightarrow{i} \tilde{A} \xrightarrow{\pi} \mathbb{C} \longrightarrow 0, \qquad (5.13)$$

where \tilde{A} is the unitization of A, i is the natural injection of A into \tilde{A} , π is the natural projection from \tilde{A} onto \mathbb{C} , and λ is defined by $\lambda(\alpha) := \alpha \mathbb{I}$ for all $\alpha \in \mathbb{C}$. **Exactness** of the sequence means that Ker(i) = 0, $Ker(\pi) = Im(i)$ and $Im(\pi) = 0$. This is clearly fulfilled in this case. Moreover, the sequence is **split**, because $\pi \circ \lambda = id_{\mathbb{C}}$. Now $K_0(\tilde{A})$ has already been defined, since \tilde{A} is a unital C*-algebra. Then, $K_0(A)$ is defined as

$$K_0(A) := Ker(K_0(\pi)), \tag{5.14}$$

where $K_0(\pi) : K_0(\bar{A}) \to K_0(\mathbb{C})$ is the map induced by π . Note however, that not everything that is true for K_0 -groups of unital C*-algebras is also true for K_0 -groups of non-unital C*-algebras. So non-unital C*-algebras have to be handled with extra care.

Next, we compute the K_0 -group of the matrix algebras $M_n(\mathbb{C})$. But first, we need the following definition:

Definition 5.2.11 Let A be a C*-algebra. A (positive) trace on A is a bounded linear map $\tau : A \to \mathbb{C}$ such that, for all $a, b \in A$,

$$\tau(ab) = \tau(ba). \tag{5.15}$$

Moreover, we assume positivity of τ , i.e., for all $a \in A$,

$$\tau(a^*a) \ge 0. \tag{5.16}$$

If A is unital, then $\tau(\mathbb{I}_A) = 1$.

It follows directly from (5.15) that $\tau(p) = \tau(q)$ for Murray-von Neumann equivalent projections p and q. Every trace τ on A can be extended in an obvious way to a trace τ_n (usually also denoted by τ), defined by

$$\tau_n \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{pmatrix} := \sum_{i=1}^n \tau(a_{ii}).$$

In this way, τ can be extended to a function $\tau : P_{\infty}(A) \to \mathbb{C}$, and this function has the following properties: $\tau(p \oplus q) = \tau(p) + \tau(q)$ for all $p, q \in P_{\infty}(A)$, $\tau(0_A) = 0$ and $\tau(p) = \tau(q)$ for equivalent projections. Thus, τ induces a map $\tau_* : K_0(A) \to \mathbb{R}$, satisfying

$$\tau_*([p]_0) := K_0(\tau)([p]_0) = \tau(p), \tag{5.17}$$

for all $p \in P_{\infty}(A)$. Note that due to the positivity of a trace τ , τ_* is real valued, because of the property $p = p^* = p^2$ for every projection p, together with the fact that $\tau(p^*p) \ge 0$. In particular, $\tau_*(K_0(A)^+) \subseteq [0, \infty)$.

Now we can compute $K_0(M_n(\mathbb{C}))$:

Example 5.2.12 We show that the K_0 -group of $M_n(\mathbb{C})$ is isomorphic to \mathbb{Z} for all $n \in \mathbb{N}$. Recall that an element in $K_0(M_n(\mathbb{C}))$ can always be written as $[p]_0 - [q]_0$, where p and q are projections in $M_k(M_n(\mathbb{C})) = M_{kn}(\mathbb{C})$ for some $k \in \mathbb{N}$. Define the trace $Tr(a_{ij})$ of an m-dimensional matrix (a_{ij}) by $Tr(a_{ij}) := \sum_{i=1}^m a_{ii}$, and observe that Tr(p) = Tr(q) if and only if the rank of p is equal to the rank of q, i.e. $dim(p\mathbb{C}^m) = dim(q\mathbb{C}^m)$. Moreover, equivalent projections have equal rank and trace. Then we have

$$Tr_*([p]_0 - [q]_0) = Tr(p) - Tr(q) = dim(p\mathbb{C}^{kn}) - dim(q\mathbb{C}^{kn}),$$

so the induced trace Tr_* maps $K_0(M_n(\mathbb{C}))$ to \mathbb{Z} . It is easy to show that Tr_* is an isomorphism, so we have, for all $n \in \mathbb{N}$,

$$K_0(M_n(\mathbb{C})) \simeq \mathbb{Z}.$$
 (5.18)

In particular, $K_0(\mathbb{C}) = \mathbb{Z}$. Since Tr is positive, we have $Tr_*(K_0(\mathbb{C})^+) = \mathbb{N}$. Moreover, $K_0(\mathbb{C})^+ \cap (-K_0(\mathbb{C})^+) = \{0\}$, so Tr_* is an order preserving isomorphism between the ordered K_0 -group $(K_0(\mathbb{C}), K_0(\mathbb{C})^+, \leq)$ and the ordered abelian group $(\mathbb{Z}, \mathbb{N}, \leq)$.

We can now replace \mathbb{C} by an arbitrary C*-algebra A, and observe that $P_{\infty}(A) = P_{\infty}(M_n(A))$ for all $n \in \mathbb{N}$. In particular, using the identification between $M_n(A)$ and $A \otimes M_n(\mathbb{C})$, we have

Proposition 5.2.13 Let A be a C*-algebra. Then $K_0(A)$ is isomorphic to $K_0(A \otimes M_n(\mathbb{C}))$ for all $n \in \mathbb{N}$. \Box

The above proposition can even be generalized to the **stabilization** $A \otimes \mathcal{K}$ of a C*-algebra A, where $\mathcal{K} := \bigcup_{n=1}^{\infty} M_n(\mathbb{C})$ is the algebra of compact operators on a separable Hilbert space (i.e. with a countable basis); recall that $\mathcal{K}(\mathcal{H}) \simeq \mathcal{K}(\mathcal{H}')$ for all separable Hilbert spaces \mathcal{H} and \mathcal{H}' , so we can omit the reference to the Hilbert space:

Proposition 5.2.14 Let A be a C*-algebra. Then A and its stabilization have isomorphic K_0 -groups, i.e.

$$K_0(A \otimes \mathcal{K}) \simeq K_0(A).$$

For a proof, we refer to [46]. However, observe that $A \otimes \mathcal{K}$ can be identified with $\mathcal{K}(A) := \overline{\bigcup_{n=1}^{\infty} M_n(A)}$. In this way, we see that $P_{\infty}(A)$ lies densely in $P(A \otimes \mathcal{K})$.

In particular, we see that $K_0(\mathcal{K}) = K_0(\mathbb{C}) = \mathbb{Z}$, because the stabilization of \mathbb{C} , i.e., $\mathbb{C} \otimes \mathcal{K}$, can be identified with \mathcal{K} .

Definition 5.2.15 Two C^* -algebras A and B are called stably isomorphic if

$$A \otimes \mathcal{K} \simeq B \otimes \mathcal{K}.$$

Remark 5.2.16 There is a natural notion of equivalence of C*-algebras, called **Morita equivalence**, which is used a lot in literature. We will not define this here, because it can be proved, that for separable C*-algebras (even more generally for C*-algebras with countable approximate identities), two C*-algebras are Morita equivalent if and only if they are stably isomorphic (moreover, K-theory is an invariant for Morita equivalence for general C*-algebras).

We now state a direct consequence of Proposition 5.2.14:

Corollary 5.2.17 If C*-algebras are stably isomorphic, they have isomorphic K_0 -groups. \Box

Remark 5.2.18 The C*-algebras $C(Y/R) = \mathbb{C}$ and $C^*(R) = M_2(\mathbb{C})$ of Example 5.1.1 are Morita equivalent, and have the same K_0 -group Z. In general, for compact Hausdorff spaces X = Y/R, C(X) is Morita equivalent with $C^*(R)$ [15]. So in this case, the K_0 -group does not distinguish between the commutative C*-algebra C(X) and the noncommutative C*-algebra $C^*(R)$. The fact that C(X) and $C^*(R)$ are Morita equivalent in the Hausdorff case is one of the main motivations for the the replacement of C(X) by $C^*(R)$ in the non-Hausdorff case. An important example will be treated in Chapter 6. In this case, the K_0 -group will be the relevant invariant to distinguish between commutative and noncommutative topology. In fact, $K_0(C^*(R))$ contains all interesting information about the underlying space.

In the examples we have seen so far, we see that the K_0 -group is countable. This is in fact true for a large class of C^{*}-algebras. Recall that a C^{*}-algebra is **separable** if it has a countable dense subset.

Proposition 5.2.19 Let A be a separable C^* -algebra. Then $K_0(A)$ is countable.

Proof: Recall from Proposition 5.2.2 that if ||p - q|| < 1, then p and q are equivalent. Now since A is separable, it has a countable dense subset. Combining these two facts, leads to the fact that there are at most countably many equivalence classes of projections. \Box

Since many C*-algebras are in fact separable - for example the C*-algebra of compact operators on a separable Hilbert space, and the so called AF-algebras that we define in Chapter 6 - this is a very useful proposition.

It turns out that K-theory is a powerful invariant. In Chapter 6, we will see that for a certain class of C*-algebras, the so called AF-algebras, K-theory provides a complete classification. Moreover, we will compute the K_0 -group of the C*-algebra of Penrose tilings. K_0 -theory will also play an important role in the gap labelling of Schrödinger operators on quasicrystals. To conclude this chapter, let's say a few things about higher K-groups for completion. For more information, see [46]. We stress however that we will only use the K_0 -group in subsequent chapters.

We define $K_1(A)$ by

$$K_1(A) := K_0(SA),$$

where SA is the suspension of the C*-algebra A, defined by

$$SA := \left\{ f \in C([0,1],A) \mid f(0) = f(1) = 0 \right\} = C_0((0,1),A).$$

Now we can define higher K-groups by

$$K_n(A) := K_1(S^{n-1}A) \simeq K_0(S^nA),$$
 (5.19)

where $S^n A$ is the suspension of $S^{n-1}A$ for all n, and one can show that every K_n is a functor, and that $K_n(A)$ is abelian for all n. Then every short exact sequence of C*-algebras,

$$0 \longrightarrow I \xrightarrow{\varphi} A \xrightarrow{\psi} B \longrightarrow 0$$

induces a long exact sequence of K-groups

$$\cdots \xrightarrow{K_{n+1}(\psi)} K_{n+1}(B) \xrightarrow{\delta_{n+1}} K_n(I) \xrightarrow{K_n(\varphi)} K_n(A) \xrightarrow{K_n(\psi)} K_n(B) \xrightarrow{\delta_n} \cdots$$
$$\cdots \xrightarrow{\delta_1} K_0(I) \xrightarrow{K_0(\varphi)} K_0(A) \xrightarrow{K_0(\psi)} K_0(B),$$

where the δ_n are called index maps. The main result in K-theory is then

Theorem 5.2.20 (Bott periodicity) $K_0(A)$ is isomorphic to $K_2(A)$.

In particular, the above long exact sequence reduces to the six term exact sequence

This is a short summary of C*-algebraic K-theory. In the following chapters, we will use the K_0 -group of tiling C*-algebras to describe properties of the underlying tiling.

Chapter 6

Connes's space of Penrose tilings

Figure 6.1: A patch of a Penrose tiling

We will now review an important example of a non-Hausdorff quotient space that can be described using noncommutative topology. In his book [15], Connes uses the description of Penrose tilings given by Robinson (see, e.g. [24]), to construct the non-Hausdorff space X of Penrose tilings. Using the substitution properties of the Penrose tiling, one can assign an indexing sequence to a tiling, and it can be shown that there is a bijective correspondence between X and a quotient of the Cantor set. C(X) contains no information, i.e. $C(X) = \mathbb{C}$, and from that point of view, X can therefore not be distinguished from a single point. However, by constructing the (noncommutative) C*-algebra $C^*_{red}(R)$, which contains C(X), Connes shows that X is actually a very rich space in the noncommutative sense. The C*-algebra of Connes is an example of the groupoid C*-algebra of an equivalence relation, as constructed in Chapter 4. See also [37].

6.1 Penrose tilings and index sequences

Figure 6.2: Elementary tiles

Penrose tilings are normally generated by kites and darts. However, following Robinson (see e.g. [24]), we can cut the kite and the dart along their symmetry axis into two halves, and thus a tiling by triangles, called L_A and S_A respectively,

is obtained. The edges of the triangles have length 1 or τ , where $\tau = \frac{1+\sqrt{5}}{2}$ is the famous golden number, cf. Section 2.4. The angles are all $\pi/5$ or $2\pi/5$, exhibiting a fivefold symmetry. To ensure that with these triangles we cannot form tilings different from the ones we get using the kites and darts, we have to impose matching conditions on L_A and S_A . Tiles are equipped with vertices with or without dot, and the edges between two vertices of the same type is oriented. For a Penrose tiling, common vertices must all be with or all be without a dot to match, and common edges must have the same orientation. We can form a Penrose tiling by starting with a tile S_A , inflating it by a factor τ to get L_B , cutting it into a patch of L_A and $S_{\tau A'}$, and cutting these again. Repeating the process of cutting and inflating gives a Penrose tiling, a patch of which is shown in Figure 6.1. From Figure 6.2, it is clear that going down one level (i.e. going from type A to type B, from type B to type $\tau A'$, etc.), corresponds to a substitution

$$L \mapsto L + S; \quad S \mapsto L,$$
 (6.1)

with corresponding substitution matrix given by

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

Note that this is precisely the same substitution as the one generating the one dimensional Fibonacci chain. The important thing is that the process of cutting and inflating is invertible: starting with a Penrose tiling T_1 by triangles L_A and S_A , we can cut every edge between the short edge of L_A and a long edge of S_A . In this way, we get a tiling T_2 by tiles L_B and S_B . Cutting again leads to a tiling T_3 by $L_{\tau A'}$ and $S_{\tau A'}$. This procedure can be iterated, leading to sequence (T_n) of tilings by triangles L_n and S_n . Now, suppose α is a triangle in a Penrose tiling T_1 . Following [24, 15], we assign the value 1 to α if it is small (i.e. isometric to S_A) and 0 if it is large (i.e. isometric to L_A). Then we cut edges to obtain a tiling T_2 by tiles L_B and S_B , and again we assign a value 1 to α if it lies in a tile isometric to S_B , and 0 if it lies in a tile isometric to L_B . We can again iterate this procedure, and in this way, an index sequence (x_n) consisting of 0's and 1's is assigned to α . Note that since each S_n is only contained in L_{n+1} and not in $S_{n+1} = L_n$, every 1 in a sequence is necessarily followed by a 0. Let K denote the set of such sequences, i.e. K is the set of sequences (x_n) with values 0 or 1, obeying

$$x_n = 1 \Longrightarrow x_{n+1} = 0. \tag{6.2}$$

Every element of K is the index sequence for some triangle α in some Penrose tiling T. Observe that K is a closed subset of the Cantor set, and therefore it is a compact Hausdorff space. In fact, we even have:

Proposition 6.1.1 There is a bijective correspondence between K and the Cantor "middle third" set.

Proof: Recall that the Cantor "middle third" set is obtained by first removing the middle third $(\frac{1}{3}, \frac{2}{3})$ from the interval [0, 1], then removing the middle thirds $(\frac{1}{9}, \frac{2}{9})$ and $\frac{7}{9}, \frac{8}{9}$, etc. An element x of the Cantor set can be described by requiring that in its ternary expansion,

$$x=\frac{c_1}{3}+\ldots+\frac{c_n}{3^n}+\ldots,$$

each c_n is equal to 0 or 2. Now if we regard an element of K as a sequence in 0's and 10's (in this way it automatically obeys condition (6.2)), this is precisely in a bijective correspondence to a sequence of ternary expansion coefficients (c_n) of an element of the Cantor set, where 0 corresponds to 0 and 2 corresponds to its binary equivalent 10.

In this way, the topology of the Cantor set, which is just the relative topology inherited from \mathbb{R} , can be transferred to K. We see that two index sequences (i.e. elements of K) are "close" to each other if they coincide on their first entries.

Next, we return to the Penrose tiling T. It is clear that if we choose a triangle β in T that is different from the triangle α that led to a index sequence (x_n) in K, then the index sequence assigned to β will eventually coincide with (x_n) , since at some stage, α and β will lie in the same tile. Thus, it seems natural to define an equivalence relation R (or, strictly speaking, the graph of an equivalence relation) on K by

$$R := \{ (x, y) \in K \times K \mid \exists N \text{ such that } \forall n \ge N \ x_n = y_n \}.$$
(6.3)

So two sequences are equivalent if they coincide eventually. Note that this is certainly not the same as two sequences lying in the same neighbourhood, which is the case if there is an N such that $x_n = y_n$ for all n smaller than N. If we take the quotient of K by R, we see that this corresponds to the fact that it is irrelevant which triangle in a tiling T we choose, and in this way, we can assign an equivalence class of an index sequence (i.e. an element of K/R) to each Penrose tiling T. However, it is clear that if a tiling T' is isometric to T, their (equivalence class of) sequence is the same. So identical (i.e. isometric) tilings are mapped to the same element of K/R. Conversely, every element of K/R defines a Penrose tiling T, which is unique up to isometry. We thus have the following:

Proposition 6.1.2 Let X be the space of Penrose tilings, where isometric tilings are identified with each other. Then we have a bijective correspondence between X and K/R.

Now, recall that K is a Cantor set, and is therefore an uncountable, compact Hausdorff space. In particular, K/R is a topological space, and this topology can be transferred to X by the bijective correspondence between the two sets. It is known that any two Penrose tilings are locally the same, that is, every finite patch P of a Penrose tiling T occurs in every other Penrose tiling, and moreover, it occurs infinitely many times (for a proof of this fact, see [24]). Thus, a Penrose tiling has a pattern that repeats itself over and over again, although it is not periodic, because its fivefold symmetry is incompatible with periodicity by the crystallographic restriction (see Proposition 2.1.5). From this, we can show that essentially, there is only one Penrose tiling, or:

Proposition 6.1.3 The space X of Penrose tilings can not be distinguished from a single point, i.e. the C^{*}-algebra of continuous functions on X is equal to \mathbb{C} .

Proof: Note that for every $z \in K$,

$$\overline{\{z' \in K \mid z' \sim z\}} = K,$$

which means that each equivalence class for R lies densely in K. Thus, the only closed sets in K/R are \emptyset and K/R itself. Therefore, the only continuous functions on X are the constant functions, which means that $C(X) = \mathbb{C}$. It follows that X is trivial as a topological space. \Box

In particular, we see that points in X cannot be separated by open sets, so X is a non-Hausdorff space. Nevertheless, the topology of the space of Penrose tilings is very rich, but this cannot be detected by commutative topological instruments. However, it can in fact be detected by using noncommutative topology. Instead of looking at C(X) = C(K/R), we look at the C*-algebra of the groupoid R. Thus, the information is contained in the pair (K, R) and its noncommutative C*-algebra.

6.2 The groupoid R

Of course, by Proposition 4.1.7, the equivalence relation R is a groupoid. To give it a topology, it might seem natural to look at the relative topology of the product topology on $K \times K$. However, this topology has a major disadvantage [37]:

Proposition 6.2.1 *R* is not locally compact Hausdorff in the relative topology of the product topology on $K \times K$.

Proof: $K \times K$ is compact Hausdorff, as a product of compact Hausdorff spaces. Now, for $x \in K$, consider $(x, x) \in R$. Every open neighbourhood $U_x \subseteq R$ of (x, x) (in the relative topology) contains a set of the form

$$\{(y, z) \in R \mid y_n = z_n = x_n \text{ for } 1 \le n \le N\},\$$

for some $N \in \mathbb{N}$, since elements x and y are close to each other if there is an N such that $x_n = y_n$ for all $n \leq N$. In fact, the larger N, the closer x and y are.

But the above set has a limit point that is not an element of R. Therefore, R is not closed, which also means that it is not compact, by the Hausdorff property of $K \times K$. It follows that the closure of U_x in the relative topology, i.e. $\overline{U_x} \cap R$, is not compact in this topology. Because U_x was an arbitrary neighbourhood of $(x, x) \in R$, it follows that R is not locally compact. \Box

So we need a different topology on R. For $n \in \mathbb{N}$, define $R^{(n)}$ by:

$$R^{(n)} := \{ (x, y) \in R \mid x_i = y_i \ \forall i \ge n \}.$$

Each $R^{(n)}$ is a closed subspace of $K \times K$ and is therefore compact and Hausdorff. It is clear that $R^{(n)} \subseteq R^{(n+1)} \forall n$, and that $R = \bigcup_{n=1}^{\infty} R^{(n)}$. So R is an inductive limit, and can therefore be equipped with the inductive limit topology, in which a subset V is open in R if and only if $V \cap R^{(n)}$ is open in $R^{(n)}$ for all n (see Remark 4.2.8).

Proposition 6.2.2 For each $R^{(n)}$, the relative inductive limit topology inherited from R coincides with the relative product topology inherited from $K \times K$. Furthermore, each $R^{(n)}$ is a compact, open subset of R.

Proof: In the relative topology inherited from the inductive limit topology on $R, V \subseteq R^{(n)}$ is open in $R^{(n)}$, if and only if there exists an open subset W of R, such that $V = R^{(n)} \cap W$. But W is open in R in the inductive limit topology if and only if $W \cap R^{(m)}$ is open in $R^{(m)} \forall m \in \mathbb{N}$, in the relative topology inherited from the product topology on $K \times K$. Thus, the two topologies coincide. Since each $R^{(n)}$ is compact in the relative product topology, and by the above also in the inductive limit topology of R, it only needs to be proved that each $R^{(n)}$ is an open subset of R. But this is immediately clear in the inductive limit topology. \Box

We now have the following important result:

Proposition 6.2.3 With the inductive limit topology, R is a locally compact, R-discrete groupoid.

Proof: R is the inductive limit of the compact sets $R^{(n)}$. Now let $(x, y) \in R$. By definition of R, there is an m such that $x_n = y_n$ for all $n \ge m$. Thus, for this $m, (x, y) \in R^{(m)}$. Then $R^{(m)}$ is the open neighbourhood of (x, y) whose closure, $\overline{R^{(m)}}$, is compact. So R is a locally compact groupoid. Now, the unit space R^0 of R is just the diagonal in R:

$$R^{0} = \{ (x, y) \mid x_{i} = y_{i} \; \forall i \ge 1 \}.$$

But this is exactly $R^{(1)}$, which is open in R. So the unit space R^0 is open in R, which by definition means that R is an R-discrete groupoid. \Box

Note that R is not Hausdorff (by Proposition 4.1.12, the unit space $R^{(0)}$ has to be closed for R to be Hausdorff, which is not the case). However, the compact, open subsets $R^{(n)}$ of R, which cover R, are all Hausdorff.

6.3 The groupoid C*-algebra of R

As in Section 4.2, there are two possibilities to make a C*-algebra out of R, $C^*(R)$ and the "reduced" $C^*_{red}(R)$. The first case is treated by Paterson in [37], the second case is treated by Connes himself in [15]. Both algebras turn out to be AF-algebras, and this fact can be used to compute their K-theory. Since the reduced C*-algebra has a norm that is more easily accessible, we follow Connes, and compute only $C^*_{red}(R)$.

As in Section 4.2, we start with the space of continuous functions on R with compact support, $C_c(R)$. Recall that if R has a left Haar system, by R-discreteness, it will be the counting measures system (see Proposition 4.2.5). With this measure system, we can equip $C_c(R)$ with a convolution product *. Compared with (4.2), the integral is replaced by a sum. Recalling that for $(x, y), (y, z) \in R$, the product is defined by (x, y)(y, z) = (x, z), and the inverse by $(x, y)^{-1} = (y, x)$, we get:

$$(f * g)(x, x'') = \sum_{x' \sim x''} f(x, x')g(x', x'')$$
(6.4)

This equation should remind one of matrix multiplication: if x, x' and x'' were integers i, j and k, the equation would read

$$(fg)_{ik} = \sum_{j} f_{ij}g_{jk}$$

However, we have to keep in mind that the variables x are in fact elements of K, that is, sequences in 0's and 1's. Nevertheless, it is clear that, since K is a countable set, we can see (6.4) as a matrix product of infinite dimensional matrices. The involution on $C_c(R)$ is just the same as in (4.3):

$$f^*(x,x') := \overline{f(x',x)} \tag{6.5}$$

This should remind one of hermitian conjugation of a matrix, $(A^{\dagger})_{ij} = \overline{A_{ji}}$.

It is clear that this product and involution give $C_c(R)$ a noncommutative algebraic structure, just as the matrix algebras $M_n(\mathbb{C})$ are noncommutative.

Equipping $C_c(R)$ with a norm $\|.\|$ (respectively $\|.\|_{red}$), we get the C*-algebra $C^*(R)$ (respectively $C^*_{red}(R)$). In the reduced case, we have the analogue of (4.8). Recalling the fact that R(x,y) = (x,x) and D(x,y) = (y,y), we can label an element $(y,y) \in R^0$ by $y \in K$. Since $(z,w) \in supp\lambda^{D(x,y)}$ if and only if w = y, we get:

$$(\pi_y(f)\psi)(x,y) = \sum_{z \sim x \sim y} f(x,z)\psi(z,y).$$
(6.6)

Since $\psi \in \ell^2(D^{-1}(y))$, the argument of ψ will always be of the form (x, y) for some $x \in K$. Therefore we can drop the y, and just write x instead of (x, y). Then (6.6) becomes:

$$(\pi_y(f)\psi)(x) = \sum_{z \sim x \sim y} f(x, z)\psi(z).$$
(6.7)

This should remind one of the action of a matrix on a vector-space:

$$(Ae)_i = \sum_j A_{ij} e_j$$

Again, (6.7) defines a norm on $C_c(G)$:

$$||f||_{red} := \sup_{y \in K} ||\pi_y(f)||_{op}, \tag{6.8}$$

where $\|\pi_y(f)\|_{op}$ denotes the operator norm (3.6) of $\mathcal{B}(\ell^2(D^{-1}(y)))$. The resulting algebra $C^*_{red}(R)$ is a C*-algebra by Proposition 4.2.11. Note that it is in fact a unital C*-algebra, with unit I given by

$$\mathbb{I}(x, x') := \delta_{x, x'}.$$

Next, we will show that this C*-algebra is an AF-algebra, in the following sense:

Definition 6.3.1 An approximately finite algebra (or AF-algebra) A is a C^* -algebra that contains an increasing sequence $\{A_n\}$ of finite-dimensional C^* -algebras such that $\bigcup_{i=1}^{\infty} A_i$ is dense in A.

In other words, an AF-algebra is the inductive limit of finite dimensional C*algebras. Note that if A is the inductive limit of a sequence

$$A_1 \xrightarrow{\varphi_1} A_2 \xrightarrow{\varphi_2} A_3 \xrightarrow{\varphi_3} \cdots$$

and $\mu_n: A_n \to A$ are *-homomorphisms, then by definition the diagram



commutes for every n. It follows that $A = \overline{\bigcup_{n=1}^{\infty} \mu_n(A_n)}$. For the case of AFalgebras, where every φ_n and every μ_n is an inclusion, so that every A_n can be identified with a subalgebra of A, it follows that $A = \overline{\bigcup_{n=1}^{\infty} A_n}$. One can actually show that every finite dimensional C*-algebra A_n is isomorphic to $M_{k_1}(\mathbb{C}) \oplus$ $\dots \oplus M_{k_n}(\mathbb{C})$, where k_1, \dots, k_n are integers [46]. Note that every AF-algebra is a separable C*-algebra. In particular, by Proposition 5.2.19, the K_0 -group of an AF-algebra is countable.

Example 6.3.2 The easiest example of an AF-algebra is of course the C*algebra of compact operators on a separable Hilbert space, $\mathcal{K} = \bigcup_{n=1}^{\infty} M_n(\mathbb{C})$. We will now show that our C*-algebra associated to the equivalence relation on the space of Penrose tilings is indeed an AF-algebra. Consider the finite sets K_m , consisting of finite sequences $x \equiv (x_n)_{n=1,2,\dots,m}$, of 0's and 1's obeying the rule (6.2). There is a natural projection $K_{m+1} \to K_m$, that simply "forgets" the final x_{m+1} . By construction, our Cantor set K is the projective limit $\varprojlim K_m$ of the sequence of finite sets K_m . On each K_m , we have an equivalence relation R_m defined by

$$R_m := \{ (x, x') \in K_m \times K_m \mid x_m = x'_m \}.$$

These equivalence relations are all finite groupoids. We can define the C*algebras $A_m := C^*_{red}(R_m)$ in the same way as above. In particular, elements $f \in A_m$ can be seen as finite matrices $(f_{x,x'})$. If the number of sequences in K_m with $x_m = 0$ is denoted by k_m , and the number of sequences with $x_m = 1$ is denoted by l_m , we see that A_m is isomorphic to $M_{k_m}(\mathbb{C}) \oplus M_{l_m}(\mathbb{C})$, and in what follows, we will identify these algebras with each other. Note that by (6.2), we have

$$k_{m+1} = k_m + l_m; \quad l_{m+1} = k_m.$$
(6.9)

In this way, there are inclusions $i_m: A_m \hookrightarrow A_{m+1}$, defined by

$$i_m(a \oplus b) := (a \oplus b) \oplus a, \tag{6.10}$$

where a is a $k_m \times k_m$ matrix and b is a $l_m \times l_m$ matrix. Observe that $(a \oplus b) \oplus a$ is indeed an element of $M_{k_{m+1}}(\mathbb{C}) \oplus M_{l_{m+1}}(\mathbb{C})$ because of the equalities (6.9). It is now easy to see that $C^*_{red}(R)$ is equal to the inductive limit $\varinjlim A_m$ of the finite-dimensional C*-algebras A_m . Thus, we have:

Proposition 6.3.3 $C^*_{red}(R)$ is a unital AF-algebra.

Remark 6.3.4 Note that since the substitution rule (6.1) is the same as in the case of Fibonacci chains, these will yield the same groupoid and thus the same C*-algebra. This is also apparent in (6.9): we can combine the two equalities in (6.9) to get precisely the Fibonacci recursion formula,

$$f_{n+1} = f_n + f_{n-1}.$$

6.4 The scaled ordered K_0 -group

Next, we will compute the scaled ordered K_0 -group of $C^*_{red}(R)$ [16]. We will do this using the K-theory of the finite dimensional C*-algebras that approximate $C^*_{red}(R)$. Since $K_0(M_n(\mathbb{C})) = \mathbb{Z}$ for all $n \in \mathbb{N}$, and since the K_0 -group of a direct sum is the direct sum of K_0 -groups, it follows that, for all $m \in \mathbb{N}$,

$$K_0(A_m) = K_0(M_{k_m}(\mathbb{C}) \oplus M_{l_m}(\mathbb{C})) = \mathbb{Z} \oplus \mathbb{Z} = \mathbb{Z}^2.$$

Next, we use the fact that the K_0 -group of an inductive limit is isomorphic to the inductive limit of K_0 -groups [46], i.e.

$$K_0(\varinjlim A_m) \simeq \varinjlim K_0(A_m)$$

In fact, if all the finite C*-algebras A_m have an ordered K_0 -group, the above isomorphism is order preserving. The ordered K_0 -group of an AF-algebra is called a **dimension group**. From the above, it is clear that the dimension group of an AF-algebra $A = \bigcup_{m=1}^{\infty} A_m$ is equal to the inductive limit of a sequence of ordered abelian groups

$$\mathbb{Z}^{n_1} \to \mathbb{Z}^{n_2} \to \dots$$

for some positive integers n_i , and with the usual order on each \mathbb{Z}^n defined by

$$(\mathbb{Z}^n)^+ = \{ (x_1, x_2, ..., x_n) \in \mathbb{Z}^n \mid x_j \ge 0 \text{ for all } j \}.$$

To compute the dimension group of our C*-algebra $C_{red}^*(R)$, we use the inclusions $i_m : A_m \to A_{m+1}$ defined by (6.10). The corresponding induced maps $K_0(i_m) : \mathbb{Z}^2 \to \mathbb{Z}^2$ are then given by

$$K_0(i_m)\binom{n}{k} = \binom{n+k}{n},$$

or, equivalently, by the matrix $M = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}$. Note that this is the same matrix as the one that describes the substitution

$$L \mapsto L + S; \quad S \mapsto L.$$

For the finite-dimensional C*-algebras A_m , it is clear that the scaled ordered K_0 -groups are given by

$$K_0(A_m) = \left(\mathbb{Z}^2, (\mathbb{Z}^+)^2, \binom{k_m}{l_m}\right).$$
(6.11)

The maps $K_0(i_m)$ are clearly all bijections of \mathbb{Z}^2 onto \mathbb{Z}^2 , since the matrix M is invertible in $M_2(\mathbb{Z})$. It follows that $K_0(C^*_{red}(R)) = \varinjlim K_0(A_m) = \mathbb{Z}^2$, by checking that the diagram

$$K_0(A_m) = \mathbb{Z}^2 \xrightarrow{M^{n-m}} K_0(A_n) = \mathbb{Z}^2$$

$$K_0(A) = \mathbb{Z}^2$$
(6.12)

is commutative for all $m \leq n$. In the same way, we see that the order unit u of $K_0(A)$ is

$$u = M^{-m} \begin{pmatrix} k_m \\ l_m \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

One would expect that $K_0(C^*_{red}(R))^+ = \mathbb{Z}^+ \oplus \mathbb{Z}^+ = (\mathbb{Z}^+)^2$. However, the matrix M is not invertible in $M_2(\mathbb{Z}^+)$, and thus, the map $K_0(i_m)$ is not a bijection from $(\mathbb{Z}^+)^2$ onto $(\mathbb{Z}^+)^2$. By requiring the commutativity of a diagram similar to (6.12), we see that the positive cone is given by

$$K_0(C^*_{red}(R))^+ = \bigcup_{m=1}^{\infty} M^{-m} (\mathbb{Z}^+)^2.$$
(6.13)

Using induction, we can show that

$$M^{-m} = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}^{-m} = \begin{pmatrix} (-1)^m f_{m-1} & (-1)^{m-1} f_m \\ (-1)^{m-1} f_m & (-1)^m f_{m+1} \end{pmatrix},$$

where f_m are the Fibonacci numbers given by

$$f_{m+1} = f_m + f_{m-1};$$
 $f_0 = 0;$ $f_1 = 1.$

The image of $(\mathbb{Z}^+)^2$ under M^{-m} is the positive cone generated by the vectors

$$\alpha_m := \begin{pmatrix} (-1)^m f_{m-1} \\ (-1)^{m-1} f_m \end{pmatrix} \quad \text{and} \quad \beta_m := \begin{pmatrix} (-1)^{m-1} f_m \\ (-1)^m f_{m+1} \end{pmatrix}.$$

Now one can show that

$$\lim_{m \to \infty} \frac{f_{2m+1}}{f_{2m}} = \tau_+ \quad \text{and} \quad \lim_{m \to \infty} \frac{f_{2m}}{f_{2m-1}} = \tau_- = -\frac{1}{\tau_+},$$

where $\tau_{\pm} := \frac{1 \pm \sqrt{5}}{2}$ are the two eigenvalues of the matrix M. In the end, we find that

$$K_0(C^*_{red}(R))^+ = \varinjlim K_0(A_m)^+ = \left\{ \binom{k}{l} \in \mathbb{Z}^2 \mid k + \tau l \ge 0 \right\},$$
$$= \tau_{k-1} = \frac{1+\sqrt{5}}{2}$$

where $\tau = \tau_{+} = \frac{1+\sqrt{5}}{2}$.

Proposition 6.4.1 The scaled ordered K_0 -group of $C^*_{red}(R)$ is isomorphic to

$$(\mathbb{Z} + \tau \mathbb{Z}, (\mathbb{Z} + \tau \mathbb{Z}) \cap \mathbb{R}^+, 1).$$

Proof: Define the map $\psi: K_0(C^*_{red}(R)) \to \mathbb{R}$ by

$$\psi\begin{pmatrix}k\\l\end{pmatrix} := k + \tau l.$$

It is clear that ψ is a bijection between \mathbb{Z}^2 and $\mathbb{Z} + \tau^{-1}\mathbb{Z}$. Furthermore, ψ is positive (i.e. $\psi(K_0(C_{red}^*(R))^+) \subseteq \mathbb{R}^+)$ and order unit preserving $(\psi \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 1)$, which proves the proposition. \Box

The map ψ can actually be seen as a state on $K_0(C^*_{red}(R))$, i.e., a normalized positive homomorphism from $K_0(C^*_{red}(R))$ to \mathbb{R} . Now we can use the following basic fact for unital AF-algebras [18]:

Proposition 6.4.2 If A is a unital AF-algebra, and ψ is a state on $K_0(A)$, then there exists a unique trace τ on A such that $\psi = \tau_*$.

Proof: [18] We'll first prove this for arbitrary finite dimensional algebras $A_n = \bigoplus_{i=1}^n M_{k_i}(\mathbb{C})$, where $\{k_i\}$ are integers. We have $K_0(A_n) = \mathbb{Z}^n$, and a homomorphism $\psi : \mathbb{Z}^n \to \mathbb{R}$ is given by $\psi(k_i) := \sum_{i=1}^n \lambda_i k_i$, where $(\lambda_i)_{i=1}^n$ is a real-valued sequence. For ψ to be positive on $K_0(A_n)^+ = (\mathbb{Z}^+)^n$, we must have $\lambda_i \ge 0$. Define τ on A_n by

$$\tau(\oplus_{i=1}^n m_i) := \sum_{i=1}^n \lambda_i Tr(m_i),$$

where $m_i \in M_{k_i}(\mathbb{C})$, and Tr is the usual matrix trace. Then τ is a trace on A_n , and if p_i is a projection in $M_{k_i}(\mathbb{C})$, we get $\psi([p_i]) = \lambda_i = \tau_*([p_i])$. It follows that $\tau_* = \psi$, and τ is uniquely determined by this condition.

Now suppose A is a unital AF-algebra, i.e., $A = \overline{\bigcup_{n=1}^{\infty} \mu_n(A_n)}$ for some increasing sequence of finite dimensional C*-algebras $\{A_n\}$, where μ_n denotes the inclusion of A_n into A, and let φ_n denote the inclusion of A_n into A_{n+1} ; cf. Definition 6.3.1. Then the commuting diagram of algebras yields a commuting diagram of K_0 -groups:



Here, $\varphi_{n*} = K_0(\varphi_n)$ and likewise for μ_{n*} . Now let ψ be a state on $K_0(A)$. Then $\psi_n := \psi \circ \mu_{n*}$ is a state on $K_0(A_n)$, so by the finite dimensional case, treated above, there exists a unique trace τ_n on A_n such that $\tau_{n*} = \psi \circ \mu_{n*}$. Since the above diagram commutes, we get:

$$\tau_{n*} = \psi \circ \mu_{n*} = \psi \mu_{n+1*} \varphi_{n*} = \tau_{n+1*} \circ \varphi_{n*}$$

It follows that $\tau_{n*} = (\tau_{n+1}\varphi_n)_*$, so by uniqueness in the finite dimensional case, we get $\tau_n = \tau_{n+1} \circ \varphi_n$. Since ψ is normalized, we $\tau_n(\mathbb{I}) = 1$, and the direct limit of the sequence τ_n is a normalized trace τ on A. Then if p_n is a projection in A_n , we get

$$\tau_* \circ \mu_{n*}([p_n]) = \tau_n(p_n) = \tau_{n*}([p_n]) = \psi \circ \mu_{n*}([p_n]),$$

Since this holds for every n, we have $\tau_* = \psi$, and uniqueness follows from the finite dimensional case. \Box

Corollary 6.4.3 The isomorphism $\psi : K_0(C^*_{red}(R)) \to \mathbb{Z} + \tau\mathbb{Z}$ comes from a unique normalized trace τ on $C^*_{red}(R)$. \Box

Note that although both the trace and the golden number are denoted by τ , the meaning will be clear from the context. Now the trace τ defines a measure μ on K by

$$\tau(f) = \int_K f(x, x) d\mu(x). \tag{6.14}$$

Positivity of this measure follows from the following: observe that each positive $f \in C^*_{red}(R)$ can be written as $f = g^* * g$ for some $g \in C^*_{red}(R)$. We have to show that such f is pointwise positive on the diagonal $K \times K$ in R, such that it defines a positive element \tilde{f} of C(K). This follows from

$$f(x,x) = \sum_{z \sim x} g^*(x,z) g(z,x) = \sum_{z \sim x} |g(z,x)|^2 \ge 0,$$

so the positivity of τ on $C^*_{red}(R)$ indeed implies the positivity of the measure μ on K. Moreover, μ is a probability measure on K, i.e., $\mu(K) = 1$, by normalization of τ . Observe that μ is uniquely determined by the condition $\tau(f * g) = \tau(g * f)$. In Section 9.1, the situation is the other way round, i.e. we have a unique measure on a space Ω_T of tilings, which defines a trace on $C^*(R_T)$, where R_T is an equivalence relation on Ω_T .

Actually, the trace on $C^*_{red}(R)$ can be seen as a continuous dimension in the sense of Murray and von Neumann [15], and in this sense, the numbers in $\mathbb{Z} + \tau \mathbb{Z}$ can be interpreted as measures for the density of tiles. In the same way, the measure μ on the space Ω_T of tilings will be a measure for the occurrence of finite patches in the tiling T.

Remark 6.4.4 There is an important theorem by Elliott, stating that two unital AF-algebras A and B are isomorphic if and only if the dimension groups $K_0(A), K_0(A)^+$ and $(K_0(B), K_0(B)^+)$ are isomorphic in an order unit preserving way, i.e. there is a group isomorphism $\phi : K_0(A) \to K_0(B)$ such that $\phi(K_0(A)^+) = K_0(B)^+$ and $\phi([\mathbb{I}_A]) = [\mathbb{I}_B]$, and there is a *-isomorphism $\rho : A \to B$ such that $K_0(\rho) = \phi$ [46]. This theorem provides a complete classification of (isomorphism classes of) AF-algebras by their scaled dimension groups (actually, the theorem of Elliott is also true for non-unital AF-algebras, but then there are some difficulties with the order unit). In fact, recently, it has been shown that a much larger class of C*-algebras can be classified by K-theory, see [47]. This shows that K-theory is indeed a very powerful invariant.

By the above remark, it is clear that the scaled ordered K_0 -group of $C^*_{red}(R)$, which is isomorphic to $\mathbb{Z} + \tau \mathbb{Z}$, completely characterizes the noncommutative topology of the space of Penrose tilings. In particular, we see that this noncommutative topology, in contrast to the ordinary commutative topology, is by no means trivial.

Remark 6.4.5 Since the Fibonacci strings are constructed using the same substitution as for the Penrose tilings, they yield the same equivalence relation and the same C^* -algebra, cf. Remark 6.3.4. Therefore, their K-theory is the same.

Chapter 7

Electronic transport in periodic media

The most important features of a material are its electronic transport properties: whether it is a good conductor, such as a metal, or a semiconductor, or an insulator. In this chapter, we will define the spectrum of Schrödinger operators Next we will give a description of electronic motion in crystals, known as Bloch theory, which uses explicitly the periodicity of the crystal, and of the tiling by unit cells associated to it. Then we rephrase this theory to a more general, noncommutative setting of arbitrary tilings. In the subsequent chapters, we will see that in this setting, quasicrystals can be described as the noncommutative analogue of crystals.

7.1 The spectrum of Schrödinger operators

To describe electronic transport properties of a crystal, one usually begins with a Hamiltonian describing the motion of one electron in the crystal. This Hamiltonian is a self-adjoint **Schrödinger operator** H on the Hilbert space $L^2(\mathbb{R}^d, d^dx)$, defined by

$$H := -\nabla^2 + V, \tag{7.1}$$

where the domain of H is given by

$$\mathcal{D}(H) := \{ \psi \in L^2(\mathbb{R}^d \mid \nabla^2 \psi \in L^2(\mathbb{R}^d) \}.$$

Here, $\nabla^2 \psi$ is meant in the weak sense, see [42]. In (7.1), V is a potential that depends on the structure of the material. In general, it depends on the interaction the electron has with ions and with other electrons. The potential due to ion-electron interaction will be a superposition of Coulomb potentials,
and this potential will be a periodic function of $x \in \mathbb{R}^d$, with periods in the lattice Γ of the crystal. We use the "independent electron approximation" [2], in which it is assumed that the electron-electron interactions have a screening effect, such that the effective potential is flattened off in the regions between the ions. In this way V becomes a continuous function. Note, however, that we assume that the electron-electron interactions do not affect the periodicity of the effective potential, so we have

$$V(x+a) = V(x), \text{ for all } a \in \Gamma.$$
(7.2)

Note that if the temperature is nonzero, the ions in the crystal will vibrate around their equilibrium position, which will affect the periodicity of the potential by a small modulation. This can be described by **phonons** [2]. In general, we will ignore electron-phonon interactions. Also, we will only describe the situation in the absence of an external magnetic field, and we will ignore spin interactions.

Remark 7.1.1 Basically, phonons are just the harmonic approximation of the atomic motion ("oscillation") around their equilibrium positions. Electron-phonon interactions would thus make things a lot more complicated. However, the differential equation associated to phonons can be treated separately of the electronic motion, and this is a problem of roughly the same level of difficulty as the problem of electronic motion. Just as electronic motion can be used to derive conductivity properties of the medium, phononic motion can be used to derive its elastic properties. We will not discuss this subject, neither in the periodic case nor in the aperiodic case. For investigations in this direction, see [9].

Now let's return to the description of electronic motion in a crystal. Note that, due to the periodicity of V, H commutes with all translation operators T(a)(for $a \in \Gamma$) on $L^2(\mathbb{R}^d)$, defined by

$$T(a)\psi(x) := \psi(x+a). \tag{7.3}$$

Of course, T can be extended from Γ to \mathbb{R}^d . So we have, for all $a \in \Gamma$,

$$HT(a) = T(a)H\tag{7.4}$$

Now, if one wants to describe electronic motion in a crystal, it is useful to compute the spectrum of H. Recall that for an $n \times n$ -matrix A, the spectrum $\sigma(A)$ is defined as the set of eigenvalues of A, i.e. the set of all $\lambda \in \mathbb{C}$ such that

$$A\psi = \lambda\psi,$$

for some $\psi \in \mathbb{C}^n$. Eigenvalues of A can be computed by requiring $\det(A - \lambda \mathbb{I}) = 0$, where \mathbb{I} is the identity in $M_n(\mathbb{C})$. So the spectrum consists of precisely those

 $\lambda \in \mathbb{C}$ for which $A - \lambda \mathbb{I}$ is not invertible. This can be generalized to arbitrary operators on a Hilbert space \mathcal{H} . Therefore, we define the spectrum of H to be

$$\sigma(H) := \{ \lambda \in \mathbb{C} \mid H - \lambda \mathbb{I} \text{ is not invertible in } \mathcal{B}(\mathcal{H}) \}.$$
(7.5)

One can prove that since H is self-adjoint, $\sigma(H) \subseteq \mathbb{R}$. If the spectrum of H is a "point" spectrum, it consists of the energy eigenvalues of H. In general, the spectrum can consist of three different types [41, 36]:

Proposition 7.1.2 The spectrum $\sigma(A)$ of an operator A can be decomposed as

$$\sigma(A) = \sigma_{ac}(A) \cup \sigma_{sc}(A) \cup \overline{\sigma_p(A)}.$$

Here, $\overline{\sigma_p(A)}$ denotes the **point spectrum** (consisting of the eigenvalues of A) and its limit points, and $\sigma_{ac}(A)$ and $\sigma_{sc}(A)$ denote the **absolutely continuous** and the **singular continuous** part of the spectrum, respectively. The absolutely continuous spectrum is defined as the support of the spectral measure μ_{ac} that is absolutely continuous with respect to the Lebesgue measure (i.e., $\int_A dE = 0$ implies $\int_A dN = 0$), whereas the singular continuous spectrum has zero Lebesgue measure (it is the support of the singular continuous measure μ_{sc} , which is characterized by the fact that $\mu_{sc}(S) = 0$ for some set S with $\lambda(\mathbb{R}\backslash S) = 0$). Typically, the a point part consists of isolated points, the absolutely continuous part consists of intervals or bands, and the singular part is what remains. Note that the different types of spectrum can overlap.

Example 7.1.3 Let's give an example of a singular continuous measure [41]. Recall that the Cantor "middle-third" set C has zero Lebesgue measure. Define the **Cantor function** α on $[0,1] \subset \mathbb{R}$ as follows: set $\alpha(x) := \frac{1}{2}$ on the open interval $(\frac{1}{3}, \frac{2}{3})$; $\alpha(x) := \frac{1}{4}$ on $(\frac{1}{9}, \frac{2}{9}) \alpha(x) := \frac{3}{4}$ on $(\frac{7}{9}, \frac{8}{9})$, etc. Next, extend α (uniquely) to a continuous, nondecreasing function on [0,1]. This function is called the **Cantor function** (see Figure 7.1). Note that α has the property that its derivative $\alpha'(x)$ exists Lebesgue-almost everywhere (namely, on $[0,1]\setminus C$) and is zero almost everywhere, i.e., α is almost everywhere constant. Construct the measure μ_{α} on [0,1] by defining it on open intervals (a, b) as

$$\mu_{\alpha}(a,b) := \lim_{\epsilon \to 0} \alpha(b - |\epsilon|) - \lim_{\epsilon \to 0} \alpha(a + |\epsilon|).$$

By continuity of α , we have $\mu_{\alpha}(\{p\}) = 0$ for any point $\{p\}$, so μ_{α} is not a point measure. On the other hand, μ_{α} is not absolutely continuous with respect to the Lebesgue measure, since $\mu_{\alpha}([0,1]\backslash C) = 0$, where $\lambda([0,1]\backslash C) = 1$ and vice versa. Hence, μ_{α} must be a singular continuous measure. In particular, we see that if the spectrum is homeomorphic with the Cantor set C, the spectrum is purely singular continuous.

Remark 7.1.4 In spectral theory, the spectrum is often called a "Cantor set" if it is a closed, nowhere dense subset of \mathbb{R} without isolated points. Note however that this admits a nonzero Lebesgue measure, so in this case, a Cantor spectrum doesn't have to be purely singular continuous. To avoid confusion, we will call these spectra "Cantor-like", reserving the name "Cantor set" for sets that are homeomorphic with the "middle-third" set, such as the unit space K of the groupoid R in Chapter 6.

Until the eighties, it was thought that singular continuous spectrum was unphysical, and an important issue in spectral theory was to show that σ_{sc} is empty for physically realistic Hamiltonians [41, 43]. We will see that for a crystal, the spectrum of the Hamiltonian is purely absolutely continuous, exhibiting a typical "band structure". On the other hand, the spectrum of quasiperiodic Hamiltonians may contain a singular continuous part, which makes them an important counterexample to what was believed until the eighties. However, this also makes quasiperiodic Hamiltonians particularly difficult to handle.

7.2 Bloch theory

Now let's first show how the spectrum of a periodic Hamiltonian can be computed. Since it is difficult to do this directly, it is useful to decompose H into a so called direct integral of Hamiltonians, each with discrete spectrum. The idea is as follows: first of all, note that the translation operator T defined by (7.3) can be seen as representation of the discrete, abelian group Γ on the Hilbert space $L^2(\mathbb{R}^d)$. In fact, T coincides with the right regular representation π_L of Γ . Note that T is a unitary representation, since $T(x)^* = T(-x) = T(x)^{-1}$. Furthermore, observe that Γ is a locally compact, discrete subgroup of \mathbb{R}^d . We want to decompose T into a direct integral of irreducible representations. Recall that every irreducible representation of an abelian group is one-dimensional (this is the group-theoretic analogue of Proposition 3.2.5). Therefore, analogous to the C^* -algebraic case, every irreducible representation is just a character, and the "structure space" of an abelian group itself, which is called the **character group** (or dual group) \hat{G} .

Example 7.2.1 We want to compute the character group $\hat{\Gamma}$ of the lattice Γ , seen as a sa an abelian, locally compact group. Recall that a character of a group G is a group homomorphism $\chi : G \to \mathbb{C}$ such that $|\chi(g)| = 1$ for all

 $g \in G$. The easiest case to compute is the lattice $\Gamma = \mathbb{Z}$. Recall that the reciprocal lattice Γ^* is defined as the set of all b such that, for all $a \in \Gamma$,

$$e^{ib \cdot a} = 1.$$

In this case we see that the reciprocal lattice Γ^* is equal to $2\pi\mathbb{Z}$. Now, the character group of \mathbb{Z} consists of the maps $T_{\theta}: \mathbb{Z} \to \mathbb{C}$ defined by

$$T_{\theta}(n) := e^{in\theta},$$

and since θ can take values between 0 and 2π , it is easy to see that \mathbb{Z} is isomorphic to S^1 , which is precisely \mathbb{R}/Γ^* . Now, if Γ is an arbitrary lattice in \mathbb{R}^d , the above can be easily generalized to see that $\hat{\Gamma}$ is equal to \mathbb{R}^d/Γ^* , which is identified with the Brillouin zone \mathcal{B} .

We can decompose the representation T, using the concept of direct integrals [5, 17, 43], which are generalizations of direct sums:

Definition 7.2.2 Let (Λ, μ) be a measure space, and let $\{\mathcal{H}_{\lambda}\}_{\lambda \in \Lambda}$ be a family of Hilbert spaces, each with inner product $\langle \cdot, \cdot \rangle_{\lambda}$. The **direct integral** \mathcal{H} of this family is defined as the Hilbert space of all measurable families ψ over Λ (see [43]) such that $\psi(\lambda) \in \mathcal{H}_{\lambda}$, with inner product

$$\langle \psi, \phi \rangle := \int_{\Lambda} \langle \psi(\lambda), \phi(\lambda) \rangle_{\lambda} d\mu(\lambda) < \infty.$$

 $\psi: \Lambda \to \{\mathcal{H}_{\lambda}\}$ is called a section of the field $\{\mathcal{H}_{\lambda}\}$. We will write

$$\mathcal{H} = \int_{\Lambda}^{\oplus} \mathcal{H}_{\lambda} d\mu(\lambda).$$

An operator A on \mathcal{H} is **decomposable** if there exists a section of operators $A(\cdot) : \lambda \in \Lambda \mapsto A(\lambda) \in \mathcal{B}(\mathcal{H}_{\lambda})$ such that

$$(A\psi)(\lambda) = A(\lambda)\psi(\lambda),$$

for all $\psi \in \mathcal{H}$, $\lambda \in \Lambda$. We will write

$$A = \int_{\Lambda}^{\oplus} A(\lambda) d\mu(\lambda).$$

One can show that the space \mathcal{H} is indeed a Hilbert space. Note that if Λ is a finite or countable set and μ is the counting measure, then the direct integral reduces to the familiar direct sum of Hilbert spaces.

Theorem 7.2.3 Let Γ be a lattice in \mathbb{R}^d , seen as a discrete abelian subgroup of \mathbb{R}^d . Let T be the representation of Γ on $L^2(\mathbb{R}^d)$ defined by (7.3). Then T can be decomposed such that, for every $a \in \Gamma$,

$$T(a) = \int_{\hat{\Gamma}}^{\oplus} \chi(a) d\mu(\chi), \qquad (7.6)$$

where every χ is a character of G, and $L^2(\mathbb{R}^d)$ decomposes as

$$L^2(\mathbb{R}^d) = \int_{\hat{\Gamma}}^{\oplus} \mathcal{H}_{\chi} d\mu(\chi)$$

This theorem is a special case of a theorem concerning representations of abelian locally compact groups, called the SNAG Theorem (Stone, Naimark, Ambrose, Godement). For a proof, see [5]. By the above Example 7.2.1, the decomposition may alternatively be written as

$$T(a) = \int_{\mathcal{B}}^{\oplus} e^{ik \cdot a} d^d k, \qquad (7.7)$$

and the Hilbert space $L^2(\mathbb{R}^d)$ on which each T(a) acts is decomposed into the direct integral

$$L^{2}(\mathbb{R}^{d}) \simeq \int_{\mathcal{B}}^{\oplus} \mathcal{H}_{k} d^{d}k.$$
(7.8)

Elements $\psi \in L^2(\mathbb{R}^d)$ can thus be seen as sections $\psi : \mathcal{B} \to {\mathcal{H}_k}$ such that $\psi_k \in \mathcal{H}_k$. By (7.7), we have for every $\psi_k \in \mathcal{H}_k$:

$$\psi_k(x+a) = T(a)\psi_k(x) = e^{ik \cdot a}\psi_k(x), \tag{7.9}$$

for all $x \in \mathbb{R}^d$, $a \in \Gamma$. A norm on each \mathcal{H}_k is given by

$$\|\psi_k\|^2 = \int_{\mathcal{V}} |\psi_k(x)|^2 d^d x < \infty,$$
(7.10)

where $\mathcal{V} = \mathbb{R}^d / \Gamma$ is the Voronoi unit cell. Note that \mathcal{H}_k is not a subspace of $L^2(\mathbb{R}^d)$, since the L^2 -norm of an element $\psi_k \in \mathcal{H}_k$ is in general infinite.

Now we can decompose the Hamiltonian H using the decomposition (7.8) and the fact that H commutes with all T(a)'s. This yields

$$H = \int_{\mathcal{B}}^{\oplus} H_k d^d k, \tag{7.11}$$

where, for fixed k, each wave function ψ_k in the domain $\mathcal{D}(H_k)$ of H_k is an element in \mathcal{H}_k that obeys (7.9) and (7.10), and for which $\partial^2 \psi_k / \partial x_i^2 \in \mathcal{H}_k$ for i = 1, 2, ..., d, where again the derivative is meant in the weak sense [42].

Each H_k acts on $\psi_k \in \mathcal{H}_k$ by

$$H_k \psi_k(x) = -\nabla^2 \psi_k(x) + (V_k \psi_k)(x), \qquad (7.12)$$

where V_k is the operator on \mathcal{H}_k defined by

$$(V_k\psi)(x) := V(x)\psi(x).$$

Note that V_k is independent of k, that is, each V_k acts in the same way on its own Hilbert space \mathcal{H}_k .

We have now reduced the problem of finding the spectrum of H acting on $L^2(\mathbb{R}^d)$ to the case of H_k acting on \mathcal{H}_k , which is simpler, because we can use the "boundary conditions" (7.9) for each ψ_k . For fixed $k \in \mathcal{B}$, we can solve the equation

$$H_k\psi_k(x) = E(k)\psi_k(x),$$

and one can show [43] that this leads to a discrete spectrum $\{E_n(k) \mid n \in \mathbb{N}\}$ that is bounded from below, with corresponding eigenfunctions $\psi_{k,n}$. Next, letting k run through all the values in \mathcal{B} , we find the spectrum of the Hamiltonian H, i.e.

$$\sigma(H) = \bigcup_{k \in \mathcal{B}} \sigma(H_k).$$

The above is a mathematically precise description of Bloch theory. In particular, we have the following famous theorem (see, for example, [2]):

Theorem 7.2.4 (Bloch's theorem) The "improper" eigenstates ψ of the oneelectron Hamiltonian $H := -\nabla^2 + V$, where V(x + a) = V(x) for all $a \in \Gamma$, obey

$$\psi_{n,k}(x+a) = e^{ik \cdot a} \psi_{n,k}(x).$$
(7.13)

Note that an eigenstate $\psi_{n,k}$ of H_k is not an eigenstate of H, since \mathcal{H}_k is not a proper subspace of $L^2(\mathbb{R}^d)$. This is the reason that we call $\psi_{n,k}$ improper eigenstates of H. Another, equivalent way of formulating Bloch's theorem is that every improper eigenstate ψ of H is of the form

$$\psi_{n,k}(x) = e^{ik \cdot x} u_{n,k}(x), \tag{7.14}$$

where $u_{n,k}$ obeys

$$u_{n,k}(x+a) = u_{n,k}(x), (7.15)$$

for all $a \in \Gamma$. We see that the improper eigenfunctions of H are plane waves modified by a Γ -periodic function, so they are extended wave functions.

Remark 7.2.5 Observe that T represents Γ onto $L^2(\mathbb{R}^d)$, and in this way the family of operators $\{T(a) \mid a \in \Gamma\}$ generates a sub-C*-algebra $C^*(T(\Gamma))$ of the C*-algebra $\mathcal{B}(L^2(\mathbb{R}^d))$, defined by

$$C^*(T(\Gamma)) := \left\{ \sum_{a \in \Gamma} f(a)T(a) \mid f \in \ell^1(\Gamma) \right\}.$$

By commutativity of Γ , this C*-algebra is commutative, so it is equal to the C*algebra of continuous functions on its character space by Theorem 3.1.2. Since T(a) acts as multiplication by $e^{ik \cdot a}$ on each fiber \mathcal{H}_k , where $k \in \mathcal{B}$, it is clear that the C*-algebra $C^*(T(\Gamma))$ is nothing but the algebra $C(\hat{\Gamma}) = C(\mathcal{B})$ acting by multiplication on $L^2(\mathbb{R}^d)$. See [38] for more information. We also refer to Remark 7.4.2. We will show that the stabilized version of $C(\mathcal{B})$ can actually be seen as the C*-algebra generated by the Hamiltonian, see Section 7.4 below.

7.3 Band spectrum, the IDS and conductivity

One can show [43] that the spectrum of the periodic Hamiltonian H is absolutely continuous with respect to k, whereas for fixed k, it is discrete. Observe that, for fixed n, $E_n(k)$ assumes a minimum $E_{n,min}$ and a maximum $E_{n,max}$ on \mathcal{B} , because E_n is a continuous function of k and \mathcal{B} is compact. If we index the wave functions $\psi_{n,k}$ in such a way that $E_{0,min} \leq E_{1,min} \leq \dots$, then one sees that the spectrum just consists of intervals $E_n(\mathcal{B}) = [E_{n,min}, E_{n,max}]$ in \mathbb{R} , labeled by the index n:

$$\sigma(H) = \bigcup_{n=0}^{\infty} E_n(\mathcal{B}).$$

These intervals are the bands in the familiar **band spectrum** of periodic Hamiltonians. Note however, that the bands may overlap, i.e., the gaps between the bands can close. We will now show how the analysis of the spectrum can be used to deduce conductivity properties of the crystal.

Recall that in atomic physics the spectrum of a Hamiltonian is discrete and bounded from below. In the atomic model, the ground state is the eigenstate ψ_0 of the Hamiltonian with the lowest energy eigenvalue E_0 . Subsequently, we have excited eigenstates ψ_1, ψ_2, \dots corresponding to energies $E_1 \leq E_2 \leq \dots$ which are possibly degenerate. Recall that according to the Pauli principle, it is not possible that two electrons are in the same state. If we ignore spin (which would give an extra factor 2), this means that every energy eigenstate is only occupied by one electron. Thus, the electrons have to be distributed over the possible eigenstates, beginning with the lowest energy. However, in the case of a crystal, the problem is that the spectrum is absolutely continuous. In particular, the Hamiltonian has no proper eigenstates, and the electrons have to be distributed over a continuum of energies. We can overcome this problem by restricting the Hamiltonian to a unit cell \mathcal{V} , subject to periodic boundary conditions. Then the restriction $H_{\mathcal{V}}$ has a discrete spectrum that is bounded from below. In particular, for each energy E, one can compute the number $N_{\mathcal{V}}(E)$ of eigenvalues of $H_{\mathcal{V}}$ smaller than or equal to E, i.e.

$$N_{\mathcal{V}}(E) := \sharp \{ E' \in \sigma(H_{\mathcal{V}}) \mid E' \le E \},\$$

where $\sharp X$ denotes the number of elements of a countable set X. Again, ignoring spin (which would give an unimportant extra factor 2), this is equal to the number of eigenstates of $H_{\mathcal{V}}$ with eigenvalue less than or equal to E. Next, define $\mathcal{V}^{(m)}$ to be the set of volume $m^d |\mathcal{V}|$ obtained by stacking up $m \times m \times \ldots \times m$ unit cells. Now we can define the **integrated density of states (IDS)** N(E)by

$$N(E) := \lim_{m \to \infty} \frac{1}{m^d |\mathcal{V}|} N_{\mathcal{V}^{(m)}}(E).$$
(7.16)

The IDS can be seen as the number of states per unit volume with energy up to an energy E. One can show that the limit exists [36], so the IDS is well defined. It is clear that it is a nonnegative, nondecreasing function on \mathbb{R} . It defines a so called **Stieltjes-Lebesgue measure** dN on \mathbb{R} by

$$dN(E', E] := N(E) - N(E'),$$

which is a generalization of the Lebesgue measure $d\lambda(E', E] := E - E'$. Note that dN is absolutely continuous with respect to the Lebesgue measure dE (i.e., $\int_A dE = 0$ implies $\int_A dN = 0$) [41]. Therefore, by the Radon-Nikodym theorem, we can define the **density of states** to be the derivative $\frac{dN}{dE}$ of the IDS [43]. This density of states is a well known quantity in solid state physics, which is in fact accessible by scattering experiments [7].

For the band spectrum of H, it is clear that the IDS is constant on the gaps between the bands. Thus, a gap \mathfrak{g} can be labeled by the value N(E) for $E \in \mathfrak{g}$, where the choice of E in \mathfrak{g} is not relevant. This gap labelling is very robust under perturbations of the Hamiltonian. Mathematically, the arbitrariness of the choice of $E \in \mathfrak{g}$ is not very satisfactory. Therefore, we will try to find invariants that can be mapped to the set of gap labels in a canonical way. In Chapter 9, we will see that actually, the K_0 -group of a certain C*-algebra, called the C*-algebra of observables, can serve as the set of invariants we are looking for.

To deduce conductivity properties of the crystal from the spectrum of the Hamiltonian, suppose that the number of electrons per unit volume is l. In the ground state, we fill up the lowest l energy levels of $H_{\mathcal{V}}$. Then we define the **Fermi energy** E_F is the lowest energy for which the IDS is precisely l, i.e.

$$E_F := \inf\{E \in \mathbb{R} \mid N(E) = l\}.$$

The space of all $k \in \mathcal{B}$ such that

$$E_n(k) = E_F,$$

for some band index n is called the **Fermi surface**. Note that if E_F lies in a gap, the Fermi surface is empty.

To set up a current in a crystal, electrons have to be excited from the ground state to a state with higher energy, i.e., a state with energy above the Fermi level E_F . Now if E_F lies in a band $E_n(\mathcal{B})$ for some n, electrons can be excited by an arbitrary small amount of energy, so not much effort (energy) is needed to set up a current. In this case, the crystal is a good conductor. However, if E_F lies in a gap \mathfrak{g} , there is a forbidden region $(E_F, E_F + \epsilon) \subseteq \mathfrak{g}$, for which no states are possible. In particular, a finite amount of energy is needed to excite an electron above the Fermi level, because the gap has to be crossed. So in this case, a certain amount of energy is needed to set up a current, which typically means that the crystal is not a good conductor. If the band gap is large compared to k_BT , where T is the temperature and k_B is Boltzmann's constant, the crystal is an insulator. If the band gap is of the order of k_BT , the crystal is a semiconductor [2]. We see that basically, the difference between Figure 7.2: Energy bands in conductors and insulators

insulator and conductor lies in the fact whether the Fermi energy lies in a gap of the spectrum or not (see Figure 7.2).

From the above, it is clear that the conductivity properties of a crystal can largely be deduced from the band spectrum of the one-electron Hamiltonian. In particular, the (integrated) density of states is an important tool. Therefore, we want to analyze the spectrum of quasiperiodic Hamiltonians in order to obtain electronic properties of quasicrystals. It is clear that in the aperiodic case we cannot use Bloch theory to obtain the spectrum, because of its crucial dependence on the periodicity of the crystal. Therefore, we have to find a different method. Numerical computations using Bloch theory in periodic approximants of quasicrystals show that the density of states, which is the derivative of the IDS, consists of locally dense sets of sharp spikes (see Figure 7.3), indicating that it consists of δ -functions in the idealized situation without perturbations (see the contribution of Fujiwara in [54]). Therefore, it is believed that in contrast to crystals, quasicrystals have a singular continuous spectrum, or at least a large singular continuous part. As mentioned before, in this sense the spectrum of the Schrödinger operator describing electronic motion in quasicrystals is an important example that singular continuous spectrum can in fact be physical, in contrast to what people believed until the eighties [41, 43].

Figure 7.3: IDS (non-decreasing function) and DOS ("spiky function") of a one-dimensional quasicrystal (arbitrary scale)

The spectrum appears to be generically **Cantor-like**, in the sense that it is a closed nowhere dense subset of \mathbb{R} without isolated points, cf. Remark 7.1.4. Note that this does not imply that it is singularly continuous, cf. Section 9.3. Observe that if the spectrum is equal to the Cantor "middle third" set, its IDS is exactly given by the Cantor function of Figure 7.1.

By observing that amorphous materials have pure point spectrum and exponentially localized wave functions, whereas crystals have absolutely continuous spectrum and extended wave functions, it seems natural to hope that quasicrystals lie in between, with (partly) singular continuous spectrum and critical (i.e. neither extended nor exponentially localized) wave functions. Note that these spectral properties can also account for the observed low conductance of quasicrystals.

In the following, we will develop an operator-algebraic approach to analyze the spectrum of Schrödinger operators, which can be generalized to the aperiodic

7.4 The C*-algebra of observables

In this section, we mainly use results from [8]. Recall from Definition 3.2.10 that for a unital C*-algebra A, the spectrum of an element $a \in A$ is defined as

$$\sigma(a) := \{ \lambda \in \mathbb{C} \mid \lambda \mathbb{I} - a \text{ is not invertible in } A \}.$$
(7.17)

Of course, if H is a bounded operator on $L^2(\mathbb{R}^d)$, i.e. $H \in \mathcal{B}(L^2(\mathbb{R}^d))$, this is a generalization of (7.5). Note however, that the Hamiltonian H is in general not a bounded operator, so any *-algebra that contains H cannot be a C*-algebra. However, we can still form a C*-algebra using the resolvent of H in the following way. Recall that the resolvent $\rho(H)$ is the complement of $\sigma(H)$. Alternatively, $\rho(H)$ can be defined by

$$\rho(H) = \{\lambda \in \mathbb{C} \mid (\lambda \mathbb{I} - H)^{-1} \in \mathcal{B}(L^2(\mathbb{R}^d))\}.$$

Now for all $\lambda \in \rho(H)$, we can define the operator $R(\lambda)$ on $L^2(\mathbb{R}^d)$ by

$$R(\lambda) := (\lambda \mathbb{I} - H)^{-1}.$$

This operator is called the **resolvent operator** (also called a Green's function). For a periodic Hamiltonian H, we can decompose $R(\lambda)$ using the direct integral decomposition of H over the Brillouin zone \mathcal{B} : observe that since $\sigma(H_k) \subset \sigma(H)$ for all $k \in \mathcal{B}$, we get the converse inclusion for the resolvents, i.e. $\rho(H) \subset \rho(H_k)$ for all $k \in \mathcal{B}$. Therefore, we have for fixed $\lambda \in \rho(H)$:

$$R(\lambda) = \int_{\mathcal{B}}^{\oplus} R_k(\lambda) d^d k,$$

where $R_k(\lambda)$ is defined as

$$R_k(\lambda) = (\lambda \mathbb{I} - H_k)^{-1}.$$

Recall that H_k has discrete spectrum. Now one can show [43] that for an operator with discrete spectrum, the resolvent operators are compact operators. So every $R_k(\lambda)$ is a compact operator. In particular, it is a bounded operator for all $k \in \mathcal{B}$. These bounded operators can be seen as elements of a C*-algebra, called the **C*-algebra of observables** [8]. Note that normally, the algebra of observables is generated by the momentum and position operators. It is in general the real part of a C*-algebra, since observables have a real spectrum. However, in general we will look at the full C*-algebra, and not just at its real part. In Section 8.4, we will actually identify the momentum and position operators in a discrete version of the C*-algebra of observables in aperiodic media.

case.

To actually construct the C*-algebra of observables, note that, since the crystal is a homogeneous medium, there is no natural choice of an origin in an infinitely large crystal. In particular, for every $x \in \mathbb{R}^d$, $T(x)HT(x)^{-1}$ describes the same physics as H. This means that the C*-algebra of observables should not only contain the resolvent operator, but also all its translates. Therefore, we simply define the C*-algebra of observables to be the C*-algebra generated by the resolvent operator and all its translates. In particular, viewing $R(\lambda)$ as a function on \mathcal{B} , i.e.

$$R(\lambda): k \in \mathcal{B} \mapsto R_k(\lambda) \in \mathcal{K}(\mathcal{H}_k),$$

we see that the C*-algebra must be generated by the family $\{T(x)R(\lambda)T(x)^{-1} \mid x \in \mathbb{R}^d\}$. Actually, by the simple equality

$$R(\lambda) = (\mathbb{I} + (\lambda - \lambda')R(\lambda'))^{-1}R(\lambda'),$$

which holds for all $\lambda, \lambda' \in \rho(H)$, we see that the C*-algebra that is generated by the above family of operators is independent of $\lambda \in \rho(H)$.

We will now show that this C*-algebra of observables is actually isomorphic to $C(\mathcal{B}) \otimes \mathcal{K}$, the stabilized version of the algebra of the Brillouin zone. First, we decompose the representation T of \mathbb{R}^d into representations of Γ and \mathbb{R}^d/Γ , using the decomposition

$$\mathbb{R}^d \simeq (\mathbb{R}^d / \Gamma) \times \Gamma; \quad x \mapsto (\overline{x}, a),$$

where $\overline{x} := x \mod \Gamma$ and $a \in \Gamma$ is such that $a = x - \overline{x}$. Recall from Remark 7.2.5 that the T(a)'s form the C*-algebra $C(\mathcal{B})$, acting by multiplication on $L^2(\mathbb{R}^d)$. We can now use an abstract Fourier transformation to transform the remaining factor $T(\overline{x})R(\lambda)T(\overline{x})^{-1}$. Recall that Fourier transformation of a function in $L^2(G)$, where G is a (locally compact) abelian group, yields an element in $L^2(\hat{G})$, where \hat{G} is the character group of G. Now we can use the fact that for our lattice Γ , we have $\hat{\Gamma} = \mathbb{R}^d/\Gamma^* = \mathcal{B}$ and $\widehat{\Gamma^*} = \mathbb{R}^d/\Gamma = \mathcal{V}$, and vice versa. The Fourier transform of a function f on \mathcal{V} is then the function \tilde{f} on Γ^* defined by

$$\tilde{f}(b) = \frac{1}{|\mathcal{V}|} \int_{\mathcal{V}} f(\overline{x}) e^{-ib \cdot \overline{x}} d^d \overline{x}.$$
(7.18)

In this way, for $\overline{x} \in \mathbb{R}^d/\Gamma$, the operator $T(\overline{x})R_k(\lambda)T(\overline{x})^{-1}$ is transformed to $T(b)\tilde{R}_k(\lambda)T(b)^{-1}$, where $b \in \Gamma^*$. Here, $\tilde{R}_k(\lambda)$, acting on $\ell^2(\Gamma^*)$, denotes the Fourier transform of $R_k(z)$, acting on \mathcal{H}_k . If we denote by $\{u_k(b) \mid b \in \Gamma^*\}$ an orthonormal basis of the fiber $\ell^2(\Gamma^*)$ (where k is fixed), the compact operator $\tilde{R}_k(\lambda)$ has matrix elements

$$(\hat{R}_k(\lambda))_{bb'} := \langle u_k(b), \hat{R}_k(\lambda)u_k(b') \rangle,$$

labeled by $b, b' \in \Gamma^*$. The map $\tilde{R}(\lambda)$, defined by

$$\tilde{R}(\lambda): k \in \mathcal{B} \mapsto \tilde{R}_k(\lambda) \in \mathcal{K}(\ell^2(\Gamma^*)),$$

is norm continuous. Therefore, we see that every element of the C*-algebra generated by $\{T(x)R(\lambda)T(x)^{-1} \mid x \in \mathbb{R}^d\}$ defines an element of $C(\mathcal{B}, \mathcal{K})$. Note that we use the fact that $\mathcal{K}(\ell^2(\underline{\Gamma^*}))$, the C*-algebra of compact operators on $\ell^2(\Gamma^*)$, can be replaced by $\mathcal{K} := \bigcup_{n=1}^{\infty} M_n(\mathbb{C})$, because the C*-algebra of compact operators on a separable Hilbert space is always isomorphic to \mathcal{K} . We now have [8, 6]:

Theorem 7.4.1 Let $H = -\nabla^2 + V$ be a Schrödinger operator, where V is a potential chosen in such a way that:

- 1. V has the periodicity of the lattice Γ ;
- 2. Each band function E_n is smooth;
- 3. the bands $E_n(k)$ are non-degenerate in the sense that for all $k \in \mathcal{B}$, we have $E_n(k) \neq E_m(k)$ if $n \neq m$, and for fixed k, each $E_n(k)$ is a non-degenerate eigenvalue of H_k .

Then the C*-algebra generated by the family $\{T(x)R(\lambda)T(x)^{-1} \mid x \in \mathbb{R}^d\}$ of translated of the resolvent of H is isomorphic to $C(\mathcal{B}) \otimes \mathcal{K}$.

Actually, in [8], J. Bellissard stated the theorem without the second and third condition, but this is in fact not true [6] (for example, if $V \equiv 0$, obviously the C*-algebra generated will be commutative, so that the theorem does not hold in this case).

Sketch of the proof: We have already shown that one may equivalently look at the C*-algebra generated by the family

$$\{T(b)\tilde{R}(\lambda)T(b)^{-1} \mid b \in \Gamma^*\}.$$

Noting that $C(\mathcal{B},\mathcal{K})$ is isomorphic to $C(\mathcal{B}) \otimes \mathcal{K}$, which is in turn isomorphic to $\overline{\bigcup_{n=1}^{\infty} M_n(C(\mathcal{B}))}$, we see that every continuous function of elements $T(b)\tilde{R}(\lambda)T(b)^{-1}$ defines an element of $C(\mathcal{B})\otimes\mathcal{K}$. To show that in fact every element of $C(\mathcal{B}) \otimes \mathcal{K}$ can be obtained in this way, we want to indicate that we can generate any finite rank matrix by considering continuous functions of $\{T(b)\tilde{R}_k(\lambda)T(b)^{-1} \mid b \in \Gamma^*\}$. Now observe that for fixed $k \in \mathcal{B}$, H_k has discrete spectrum $\bigcup_{n=1}^{\infty} E_n(k)$. Moreover, the same holds for the Fourier transform H_k , acting on $\ell^2(\Gamma^*)$, and if we diagonalize H_k , we see that the bands $E_n(k)$ can actually be labeled by $n \in \Gamma^*$. Now any continuous function of $T(b)R_k(\lambda)T(b)^{-1}$ can be written as a continuous bounded function of the band functions $E_b(k)$. Using the non-degeneracy of the $E_b(k)$'s, each spectral projection $P_b(k)$ of H_k associated to $E_b(k)$ belongs to the C*-algebra generated by $T(b)R_k(\lambda)T(b)^{-1}$'s, and in this way, all rank one matrices over $C(\mathcal{B})$ can be generated. Since T(b'')acts as a shift operator on the matrix elements $(\tilde{R}_k(\lambda))_{bb'}$, we can generate any finite rank matrix over $C(\mathcal{B})$. \square

The C*-algebra $C(\mathcal{B}) \otimes \mathcal{K}$ is called the algebra of the Brillouin zone. Note that this formulation is different from the one in Chapter 3, where $C(\mathcal{B})$ is regarded as the natural C*-algebra associated to a compact space. However, the

two C*-algebras are stably equivalent, so neither main invariant we are using, namely K-theory, nor the structure space, will not distinguish between the two of them. Note that in the present formulation, \mathcal{K} is the algebra of a point, since $C(\{p\}) \simeq \mathbb{C}$, and $\mathbb{C} \otimes \mathcal{K} \simeq \mathcal{K}$. The remarkable thing is that the C*-algebra of observables does not depend on the shape of the potential, apart from its periodicity and the other moderate conditions of the theorem: indeed, any potential Vwith periodicity of the lattice, yielding smooth band functions $E_n(k)$ satisfying the non-degeneracy condition, gives the same algebra. Although $C(\mathcal{B}) \otimes \mathcal{K}$ is noncommutative, its noncommutativity is entirely contained in the stabilizing factor \mathcal{K} . We will show that in the general (not necessarily periodic) case we can form a certain groupoid C*-algebra, the "noncommutative C*-algebra of the hull", which reduces to $C(\mathcal{B}) \otimes \mathcal{K}$ in the periodic case. Therefore, it can be seen as the "noncommutative C*-algebra of observables", or the "noncommutative Brillouin zone", and we will see that, just as in the periodic case, its construction doesn't depend on the form of the Hamiltonian, but only depends on the shape of the material and of the tiling that serves as a model for the material.

Remark 7.4.2 There is a different approach, due to Gruber [23], using the concept of Hilbert C*-modules. Note that by identifying the Brillouin zone \mathcal{B} with the character group $\hat{\Gamma}$ of the lattice Γ , one can establish an isomorphism between $C(\mathcal{B}) = C(\hat{\Gamma})$ and $C^*_{red}(\Gamma)$, the reduced group C*-algebra of Γ , in the following way: for $f \in C^*_{red}(\Gamma)$, we define its generalized Fourier transform $\hat{f} \in C(\mathcal{B})$ by

$$\hat{f}(k) = \sum_{a \in \Gamma} f_a e^{ik \cdot a},$$

cf. (7.18). Just as in the ordinary case, the Fourier transform of the convolution product is precisely the pointwise product of the Fourier transforms, i.e.

$$\widehat{f \ast g} = \widehat{f}\widehat{g},$$

and also, $\widehat{f^*} = \widehat{f}^*$. Thus, $C^*_{red}(\Gamma)$ is mapped into $C(\mathcal{B})$. Since one can prove the existence of an inverse Fourier transform, this map is an isomorphism. Now if Γ is no longer abelian, although it is still a discrete group (for example if a magnetic field is applied to a crystal, in which case translations are replaced by "magnetic translations", which do not commute), $C(\widehat{\Gamma})$ has lost its meaning. However, we can still define $C^*_{red}(\Gamma)$ for non-abelian groups. According to [23], this algebra is then the noncommutative C*-algebra of the Brillouin zone.

However, for quasicrystals, this method doesn't seem to be applicable, since we cannot form a translation group that maps the Delone set of atomic positions into itself, not even if we try it with a non-abelian group. This is due to the fact that if a translation over x maps one point of a Delone set into another, it does not necessarily map every point of the Delone set into another point of the Delone set. This reminds us of the concept of a groupoid G, where not all pairs in $G \times G$ were composable. So if we can find a groupoid G that reflects the local

symmetry properties of the quasicrystal, the groupoid C*-algebra $C^*_{red}(G)$ will be a good candidate for the role of noncommutative C*-algebra of observables.

The question now arises how the C*-algebra of observables can be used to compute the spectrum of the Hamiltonian. Recall that for Hamiltonians describing electronic motion in aperiodic media such as quasicrystals, it is in general impossible to compute their spectrum, because without periodicity, Bloch's theorem no longer holds, so we cannot decompose the Hamiltonian to compute the spectrum. However, the interesting thing is that the K-theory of the noncommutative C*-algebra of observables can be used to obtain properties of the spectrum of the Hamiltonian, such as the value of the integrated density of states on gaps of the spectrum, which can serve as a labelling for these gaps. But first, let us construct this noncommutative C*-algebra of observables, using the concept of the hull of a tiling.

Remark 7.4.3 One may wonder why we don't just generalize the above computation of the C*-algebra of observables, generated by all translates of the resolvent of the Hamiltonian, to the aperiodic case. We won't do this, because this C*-algebra is in general very difficult to compute, since we cannot use a direct integral decomposition of the Hamiltonian over the Brillouin zone. Another obvious choice for a C*-algebra would be to consider the C*-algebra $\mathcal{B}(L^2(\mathbb{R}^d))$ of bounded operators on $L^2(\mathbb{R}^d)$, but this algebra is obviously much too large to reflect any properties of the medium we are looking at, since it is totally independent of the material. It turns out that the noncommutative C*-algebra of the hull is relatively easy to compute, and that it sufficiently reflects the properties of the medium, although it is larger than the C*-algebra generated by the Hamiltonian. Of course, we must find a criterion for a Schrödinger operator to be "affiliated to" a C*-algebra, otherwise it would be impossible to say anything about the spectrum of the operator by just examining the K-theory of the C*-algebra.

Chapter 8

The aperiodic case

In this chapter, we will define the hull of arbitrary tilings, define an equivalence relation on it and construct its groupoid C*-algebra. We will show that this C*-algebra reduces to $C(\mathcal{B}) \otimes \mathcal{K}$ in the periodic case of a tiling by unit cells. Therefore, the C*-algebra of the hull may be viewed as the noncommutative C*-algebra of observables.

We will define two hulls, the continuous one and the discrete one, and show that their C*-algebras are stably equivalent, which means that they have the same K-theory. This can be used to obtain properties of the spectrum of quasiperiodic Schrödinger operators, which is the subject of the next chapters. In the last section, we will compare the construction of the hull and its noncommutative C*-algebra with the construction of the noncommutative space of Penrose tilings by Connes, cf. Chapter 6.

8.1 The hull

Let T_0 be a *d*-dimensional tiling, which models a not necessarily periodic medium. If a self-adjoint operator H describes the motion of an electron in this tiling, this motion can also be described by an electron that is at rest in the origin of \mathbb{R}^d , while the tiling is moving. In other words, we consider the frame of reference where the electron is at rest. Thus, instead of considering one tiling T_0 and a moving electron in it, we consider the collection $\{T_0 + x \mid x \in \mathbb{R}^d\}$ of all translates of the tiling. The Hamiltonian H will then be replaced by a family of selfadjoint operators $\{H_T\}$, satisfying the **covariance condition**

$$T(x)H_TT(x)^{-1} = H_{T+x},$$
 (8.1)

where we set $H_{T_0} := H$. The idea is now to look at the set of translates of the tiling, and define a topology on it.

For an arbitrary tiling T of \mathbb{R}^d , consider the set of tilings

$$T + \mathbb{R}^d := \{T + x \mid x \in \mathbb{R}^d\}$$

Following [31], we define a metric d on $T + \mathbb{R}^d$ as

$$d(T_1, T_2) := \min\{1, d(T_1, T_2)\},\$$

where

$$\widetilde{d}(T_1, T_2) := \inf \left\{ \epsilon \mid \exists x_1, x_2 \in B(0, \epsilon) \text{ s.t. } (T_1 + x_1) \upharpoonright_{B(0, \frac{1}{\epsilon})} = (T_2 + x_2) \upharpoonright_{B(0, \frac{1}{\epsilon})} \right\}.$$

In other words, we define d in the following way: for $0 < \epsilon < 1$, we say that the distance $d(T_1, T_2)$ between two tilings in $T + \mathbb{R}^d$ is less than ϵ if there are $x_1, x_2 \in B(0, \epsilon)$ such that the tilings $T_1 + x_1$ and $T_2 + x_2$ coincide on $B(0, \frac{1}{\epsilon})$. If there are no such x_1, x_2 for any $\epsilon < 1$, then we set $d(T_1, T_2) = 1$. It is easy to show that d is indeed a metric. Now we have the following definition:

Definition 8.1.1 Given a tiling T, the hull Ω_T of T is defined as the completion of the metric space $(T + \mathbb{R}^d, d)$.

Proposition 8.1.2 In the case that T is a periodic tiling by unit cells \mathcal{V} , with lattice Γ , the hull Ω_T is homeomorphic to the unit cell \mathcal{V} .

Proof: Note that when T is periodic, with lattice Γ , one has T + a = T for all $a \in \Gamma$, so it is clear that by the above, as a set, $T + \mathbb{R}^d$ is just $\mathcal{V} = \mathbb{R}^d/\Gamma$, described in a difficult way. If we can prove that in the periodic case the metric d is equivalent to the Euclidean metric on \mathbb{R}^d/Γ , we have proved the proposition. Now, suppose that T_1, T_2 are two elements of $(T + \mathbb{R}^d, d)$. Then it follows that $T_1 = T_2 + x$ for some $x \in \mathbb{R}^d$, and by periodicity there is an $x' \in \mathbb{R}^d/\Gamma$ and a $\gamma \in \Gamma$ such that $x = x' + \gamma$. If we assume that the unit cell $\mathbb{R}^d/\Gamma = \mathcal{V}$ is contained in a ball of radius 1 (otherwise, we can scale the unit cell such that this condition is satisfied, which can be done since \mathcal{V} is compact), then $x' \in B(0, |x'|) \subset B(0, 1)$, so $d(T_1, T_2) = |x'|$. So the metric d is a scalar multiple of the Euclidean metric. This means that the closure Ω_T of $(T + \mathbb{R}^d, d)$ is homeomorphic to the closure of \mathcal{V} , which is just \mathcal{V} . \Box

An important property of the hull in the periodic case is that it is a compact space. This follows immediately from Proposition 8.1.2, because \mathcal{V} is compact. It turns out that the periodicity condition can be relaxed [40, 31]:

Theorem 8.1.3 Let T be a tiling. Suppose that, for any R > 0, there are, up to translation, only finitely many patches in T (i.e. subsets of T) that fit into a ball of radius R. Then Ω_T is compact.

Proof: We give a proof different from the original one in [40]. Our proof resembles the proof in [29], but the conditions are slightly different. Recall that

for a complete metric space X, to prove compactness, it is enough to prove pre-compactness (also called total boundedness), i.e. for every $\epsilon > 0$ there is N > 0 such that X is covered by a union of $N \epsilon$ -balls. Now let $\epsilon > 0$. Choose an $R > \frac{1}{\epsilon}$. Then consider the covering of Ω_T by $\{B(T', \epsilon) \mid T' \in \Omega_T\}$. Since there are finitely many patches $\{P_i\}_{i=1}^n$ that fit in an R-ball around the origin, we choose tilings $T_i \in \Omega_T$ such that

$$T_i \upharpoonright_{B(0,R)} = P_i.$$

Now let $T' \in \Omega_T$. Then T' has a patch P_i or a small translate of it around the origin, so $d(T', T_i) < \epsilon$ for some T_i . We thus have

$$\Omega_T = \bigcup_{i=1}^n B(T_i, \epsilon),$$

which proves pre-compactness and therefore compactness of Ω_T .

The condition in the theorem is called the **finite pattern condition**. Note that this condition automatically implies that there is a finite number of prototiles (i.e., finitely many tiles, up to translation). Many interesting tilings obey the finite pattern condition, including periodic tilings and Penrose tilings. In what follows, we will always assume that a given tiling T satisfies the finite pattern condition. In particular, we will always assume that Ω is compact.

In the periodic case, another property of the hull is that every element T' of the hull Ω_T defines the same hull, i.e.

$$\Omega_{T'} = \Omega_T \text{ for all } T' \in \Omega_T.$$
(8.2)

This is due to the fact that for every $T' \in \Omega_T$, the orbit $T' + \mathbb{R}^d$ under the group action of \mathbb{R}^d on Ω_T is dense in Ω_T (note that in this construction, there is always a dense orbit in Ω_T , namely that of T itself). An arbitrary hull Ω_T for which every orbit is dense is called **minimal**. Note that for a minimal hull Ω_T , due to (8.2) we can drop the subscript T. In particular, we see that for a minimal hull, there is no natural choice for an origin in the medium that is modeled by a tiling $T \in \Omega$.

Definition 8.1.4 A tiling T is said to be **repetitive** if for every finite patch P in T, there is an R > 0, such that for every $x \in \mathbb{R}^d$ there is a translate of P contained in T and in B(x, R).

In particular, this means that translates of any patch in T, no matter how large, can be found infinitely many times in T, so T repeats itself locally. Note that this does not imply that T repeats itself globally, i.e., that T is periodic. A Penrose tiling is again the basic example of an aperiodic tiling that satisfies the repetitivity condition. The following proposition is standard (see e.g. [31, 53]):

Proposition 8.1.5 Ω_T is minimal if and only if T is repetitive.

We are mainly interested in aperiodic tilings. Note however, that in principle, for an aperiodic tiling T, the space Ω_T can contain periodic tilings (consider tiling the plane by unit squares, and remove a finite number of edges; the hull of this tiling will contain the original periodic tiling by unit squares). To avoid this situation, we will say that T is **strongly aperiodic** if Ω_T contains no periodic tilings. Note that in the converse situation it is clear that the hull of a periodic tiling cannot contain aperiodic tilings, since every limit point of a sequence of periodic tilings (all necessarily with the same period) is itself a periodic tiling. Hence we have [31]:

Proposition 8.1.6 If T is aperiodic and Ω_T is minimal, then T is strongly aperiodic.

Proof: Suppose there is a $T' \in \Omega_T$ such that T' = T' + x for some $x \in \mathbb{R}^d$. Since Ω_T is minimal, $\Omega_{T'} = \Omega_T$. In particular, $T \in \Omega_{T'}$. But T is aperiodic, so this contradicts the fact that the hull of a periodic tiling does not contain aperiodic tilings. \Box

In what follows, unless otherwise stated we will always assume that a given tiling T is aperiodic, repetitive and satisfies the finite pattern condition. In particular, this means that the hull is minimal and compact, and that T is strongly aperiodic. It is important to notice that given two tilings in the hull Ω , we cannot distinguish them locally, i.e. by looking at finite patches. Finally, we will define an equivalence relation R_T on the hull Ω by

$$R_T := \{ (T', T'') \in \Omega \times \Omega \mid T' \text{ is a translate of } T'' \}.$$

$$(8.3)$$

Viewing this equivalence relation as a groupoid (cf. Chapter 4), we are now in the position to define the (truly) noncommutative analogue of the C*-algebra $C(\mathcal{B}) \otimes \mathcal{K}$.

Remark 8.1.7 The construction of the hull Ω by Kellendonk in fact resembles the construction of the space of Penrose tilings X = K/R of Chapter 6. We will comment on this in Section 8.5.

8.2 The noncommutative C*-algebra of observables

In aperiodic media, such as quasicrystals, Bloch's theorem no longer holds. Hence we need to find an alternative description of electronic motion. Bellissard [8] has suggested to use noncommutative geometry to describe the aperiodic case. To this effect he developed a method based on measures. We use the topological approach of Kellendonk [29, 31], based on the hull of tilings as defined above. Recall that we can associate a C*-algebra to a topological groupoid when the latter is locally compact and admits a (left) Haar system. For our groupoid R_T as defined in (8.3), an obvious choice for a topology would be the relative topology of the product topology on $\Omega \times \Omega$. However, although $\Omega \times \Omega$ is compact, as a product of compact spaces, R_T is not locally compact in this topology, since Ω lacks the Hausdorff property, just as in the Penrose case, where the groupoid R is not locally compact in the relative topology of $K \times K$ although K itself is compact.

We define a topology on R_T as follows: Consider the space $\Omega \times \mathbb{R}^d$, with the product topology, where Ω is equipped with the metric topology induced by the metric d, and \mathbb{R}^d is equipped with the usual Euclidean topology. Consider the map

$$\varphi: \Omega \times \mathbb{R}^d \to R_T; \ (T, x) \mapsto (T, T - x).$$

Clearly, φ is surjective. Moreover, φ is injective if and only if Ω contains no periodic tilings. In that case, we can equip R_T with the topology, called \mathcal{T} , for which φ is a homeomorphism.

Lemma 8.2.1 R_T is locally compact in the topology \mathcal{T} inherited from $\Omega \times \mathbb{R}^d$ via φ .

Proof: Since $\Omega \times \mathbb{R}^d$ is locally compact, each element (T, x) of $\Omega \times \mathbb{R}^d$ has an open neighbourhood $U_{T,x}$ such that $\overline{U_{T,x}}$ is compact. Next, consider an element (T_1, T_2) of R_T . By definition of the equivalence relation, there is an $x \in \mathbb{R}^d$ such that $T_2 = T_1 - x$. Thus, $(T_1, T_2) = \varphi(T_1, x)$. Now by continuity of $\frac{\varphi^{-1}}{\varphi(U_{T_1,x})}$ is an open neighbourhood of (T_1, T_2) , and by continuity of φ , $\varphi(\overline{U_{T_1,x}})$ is a compact neighbourhood of (T_1, T_2) . So R_T is locally compact in the topology \mathcal{T} . \Box

We have equipped the groupoid R_T with a topology in which it is locally compact. Next, we need a left Haar system on R_T . This can be constructed by observing that the topological space $\Omega \times \mathbb{R}^d$ can be given the structure of a transformation groupoid, denoted by $\Omega \rtimes \mathbb{R}^d$, where $x \in \mathbb{R}^d$ acts on Ω by $T \mapsto T - x$, and using the homeomorphism φ to transfer the Haar system of $\Omega \rtimes \mathbb{R}^d$ to R_T . Recall from Example 4.1.3 that the groupoid structure on $\Omega \rtimes \mathbb{R}^d$ is defined as follows:

$$(T,x)(T-x,y) := (T,x+y);$$
 $(T,x)^{-1} := (T-x,-x);$
 $R(T,x) = T;$ $D(T,x) = T-x,$ (8.4)

for all $T \in \Omega$, $x, y \in \mathbb{R}^d$, where the unit space of the groupoid is identified with Ω . Checking the conditions of Definition 4.1.9 of a groupoid homomorphism, it is easy to see that φ is also a groupoid isomorphism between $\Omega \rtimes \mathbb{R}^d$ and R_T . Summarizing, we have two locally compact groupoids, which are isomorphic and homeomorphic if and only if Ω contains no periodic tilings. R_T is a principal groupoid, and from Proposition 4.1.5, it can be seen that $\Omega \rtimes \mathbb{R}^d$ is principal if

and only if Ω contains no periodic tilings. In what follows, we assume that this is the case. So we are describing the true aperiodic case.

Now, to construct the C*-algebras associated to these groupoids, we need left Haar systems. Note that for the transformation groupoid, each fiber $R^{-1}(T) = \{(T, x) \in \Omega \rtimes \mathbb{R}^d \mid x \in \mathbb{R}^d\}$ is homeomorphic to \mathbb{R}^d , so we have a left Haar system consisting of Lebesgue measures λ on all fibers $R^{-1}(T)$. If we define a product on $C_c(\Omega \rtimes \mathbb{R}^d)$ by

$$f * g(T, x) = \int_{\mathbb{R}^d} f(T, y) g(T - y, x - y) d\lambda(y),$$

and involution by

$$f^*(T,x) = \overline{f(T-x,-x)},$$

it is easy to show that the usual definitions of a (matrix like) product and involution on $C_c(R_T)$, defined by

$$f * g(T,T') = \int_{T'' \sim T} f(T,T'')g(T'',T')d\tilde{\lambda}(T''),$$

and

$$f^*(T,T') = \overline{f(T',T)},$$

are mapped bijectively to the product and involution on $C_c(\Omega \rtimes \mathbb{R}^d)$ under the pullback φ^* of φ , if we set T' = T - x and T'' = T - y. This pullback $\varphi^* : C_c(R_T) \to C_c(\Omega \rtimes \mathbb{R}^d)$ is defined by

$$\varphi^*(f)(T,x) := f(\varphi(T,x)) = f(T,T-x).$$

Note that the Haar system of R_T , consisting of measures $d\tilde{\lambda}(T'') = d\tilde{\lambda}(T-y)$, comes directly from the Haar system of $\Omega \rtimes \mathbb{R}^d$, consisting of Lebesgue measures $d\lambda(y)$. Just as in Chapter 4, we define reduced representations of $C_c(\Omega \rtimes \mathbb{R}^d)$ on the Hilbert spaces $L^2(R^{-1}(T))$ by

$$\pi_T(f)\psi(x) := \int_{\mathbb{R}^d} f(T-x, y-x)\psi(y)d\lambda(y).$$
(8.5)

Note that since $R^{-1}(T) = \{(T, x) \mid \mathbb{R}^d\}$ is homeomorphic to \mathbb{R}^d , the reference to T has been omitted, and ψ is seen as an element of $L^2(\mathbb{R}^d)$.

Proposition 8.2.2 If Ω is minimal, then every π_T is faithful.

Proof: Suppose that Ω is minimal, and assume that $\pi_T(f) = 0$ for some $f \in C_c(\Omega \rtimes \mathbb{R}^d)$. Then by definition of π_T ,

$$\int f(T-x, y-x)\psi(y)d\lambda(y) = 0 \text{ for all } \psi \in L^2(\mathbb{R}^d).$$

Since the above holds for all $x \in \mathbb{R}^d$ and f is continuous, we get f(T-x, y-x) = 0for all $x, y \in \mathbb{R}^d$. Moreover, since $\{T - x \mid x \in \mathbb{R}^d\}$ is dense in Ω , we get f(T, y) = 0 for all $y \in \mathbb{R}^d$, and for all T in a dense subset of Ω , so by continuity of f, we get $f \equiv 0$. It follows that π_T is faithful. \Box

So to each element of $C^*(\Omega \rtimes \mathbb{R}^d)$, an operator on $L^2(\mathbb{R}^d)$ is associated via π_T . A simple computation shows that π_T satisfies the following covariance condition:

$$\pi_{T+x} = T(x)\pi_T T(x)^{-1}.$$
(8.6)

In particular, we can try to find an element h of $C_c(\Omega \rtimes \mathbb{R}^d)$ such that $H_T := \pi_T(h)$ is the Hamiltonian of an electron moving in the aperiodic medium modeled by the tiling T. Since the Hamiltonian is not bounded, this is of course not possible. However, in the discrete case, it will be possible to find elements that correspond to the "tight binding" Hamiltonian on the discrete Hilbert space $\ell^2(\mathbb{Z}^d)$. In the same way as π_T is defined, we have reduced representations $\tilde{\pi}_T$ of $C_c(R_T)$ defined by

$$\tilde{\pi}_T(f)\psi(T') := \int_{T''\sim T} f(T', T'')\psi(T'')d\tilde{\lambda}(T''), \qquad (8.7)$$

which satisfy a covariance condition similar to (8.6). The definition of $\tilde{\pi}_T$ is analogous to (6.7), except that in this case, the groupoid R_T is not *R*-discrete. Equipping $C_c(\Omega \rtimes \mathbb{R}^d)$ and $C_c(R_T)$ with norms in the usual way by defining

$$\|f\|_{C^*(\Omega \rtimes \mathbb{R}^d)} := \sup_{T \in \Omega} \pi_T(f),$$

$$\|f\|_{C^*(R_T)} := \sup_{T \in \Omega} \tilde{\pi}_T(f),$$

(8.8)

we get the C*-algebras $C^*(\Omega \rtimes \mathbb{R}^d)$ and $C^*(R_T)$. Observe that these C*-algebras are the reduced versions. However, in both cases, the reduced and the full groupoid C*-algebra coincide, because of the amenability of the groupoids.

To define this concept [22], recall from Definition 3.2.12 that a state is a positive normalized linear functional.

Definition 8.2.3 Let G be a locally compact group. A left invariant mean is a state M on $C_b(G)$, the algebra of continuous bounded functions on G, such that

$$M(T_x f) = M(f)$$
 for all $x \in G$,

where $T_x f$ is defined as $T_x f(y) = f(yx^{-1})$. G is **amenable** if there exists a left invariant mean on $C_b(G)$.

It can be shown that abelian groups are amenable, so \mathbb{R}^d is amenable. There is a similar notion of amenability for groupoids [44, 1], which we will not define here. Let us simply state that if a group G is amenable, and X admits an action of G, the transformation groupoid $X \rtimes G$ is an amenable groupoid [44]. So $\Omega \rtimes \mathbb{R}^d$ is amenable. Similarly, R_T is amenable, since it is homeomorphic and isomorphic to $\Omega \rtimes \mathbb{R}^d$. The main result for amenable groupoids G is that their full and reduced C*-algebra coincide, i.e. $||f|| = ||f||_{red}$ for all $f \in C_c(G)$ [44, 1]. This applies to both $\Omega \rtimes \mathbb{R}^d$ and R_T . Moreover, we have: **Proposition 8.2.4** If Ω contains no periodic tilings, $C^*(\Omega \rtimes \mathbb{R}^d)$ and $C^*(R_T)$ are isomorphic under the continuous extension of the pullback $\varphi_* : C^*(R_T) \to C^*(\Omega \rtimes \mathbb{R}^d)$.

Apart from trivial algebraic verifications, the proof consists of checking that φ_* is continuous, i.e.

$$\|\varphi_*(f)\|_{C^*(\Omega \rtimes \mathbb{R}^d)} = \|f\|_{C^*(R_T)}.$$
(8.9)

This can be done by checking that

$$\pi_T(\varphi_*(f))\tilde{\varphi}(\psi)(x) = \tilde{\pi}_T(f)\psi(T-x), \qquad (8.10)$$

for all $T \in \Omega$, $f \in C_c(R_T)$, $\psi \in L^2(R^{-1}(T))$ and $x \in \mathbb{R}^d$. Here,

$$\tilde{\varphi}: L^2(R^{-1}(T)) \to L^2(\mathbb{R}^d); \quad \tilde{\varphi}(\psi)(x) = \psi((T-x),$$

is also a map induced by φ . Since (8.10) holds for all $T \in \Omega$, we can take the supremum over Ω on both sides, and (8.9) holds, which proves the proposition. These are all easy computations, and we will not do them here. \Box

Remark 8.2.5 Actually, if a group G acts on a space X, the C*-algebra $C^*(X \rtimes G)$ is isomorphic to the **crossed product algebra** $C_0(X) \rtimes G$. In our case, this means that the C*-algebra $C^*(\Omega \rtimes \mathbb{R}^d)$ is isomorphic to $C(\Omega) \rtimes_{\alpha} \mathbb{R}^d$, where the action α of \mathbb{R}^d on the algebra $C(\Omega)$ is given through homeomorphisms on Ω , i.e. for all $(f, x) \in C(\Omega) \rtimes_{\alpha} \mathbb{R}^d$, we have

$$\alpha_x(f)(T) = f(T - x).$$

For more on crossed products, see [38]. Many authors in fact identify the transformation groupoid C*-algebra with the crossed product algebra, but we will stick with $C^*(\Omega \rtimes \mathbb{R}^d)$ for clarity.

Next, we will show that in the periodic case, $C^*(\Omega \rtimes \mathbb{R}^d)$ is isomorphic to $C(\mathcal{B}) \otimes \mathcal{K}$. In particular, this will show that $C^*(R_T)$, which is isomorphic to $C^*(\Omega \rtimes \mathbb{R}^d)$ in the aperiodic case, is the generalization of the crystallographic C*-algebra of observables $C(\mathcal{B}) \otimes \mathcal{K}$ to the non-crystallographic case. This leads to the following diagram:



Note however, that in the periodic case, $\varphi_* : C^*(R_T) \to C^*(\Omega \rtimes \mathbb{R}^d)$ is not injective, since $\varphi : \Omega \rtimes \mathbb{R}^d \to R_T$ is not injective.

Proposition 8.2.6 The C*-algebra $C^*(\Omega \rtimes \mathbb{R}^d)$ is isomorphic to $C(\mathcal{B}) \otimes \mathcal{K}$ if Ω consists of periodic tilings by unit cells.

Proof: This proposition is due to Bellissard, and can be found in, e.g., [9]. The proof uses the fact that in this case, $\Omega \simeq \mathbb{R}^d / \Gamma = \mathcal{V}$, where Γ is the lattice of the crystal. Then we can use the following theorem by Green, which can be found in different versions in [33] and [35]:

Theorem 8.2.7 Let $(G/H) \rtimes G$ be a transformation groupoid, where G acts on G/H. Then $C^*((G/H) \rtimes G)$ is isomorphic to $C^*(H) \otimes \mathcal{K}(L^2(G/H))$.

Here, $C^*(H)$ is the group C*-algebra of the group H. Specializing to our case, where $G = \mathbb{R}^d$, $H = \Gamma$, $G/H = \mathbb{R}^d/\Gamma \simeq \Omega$, we get the isomorphism

$$C^*((\mathbb{R}^d/\Gamma) \rtimes \mathbb{R}^d) \simeq C^*(\Gamma) \otimes \mathcal{K},$$

where the reference to the Hilbert space on which the compact operators act is omitted. Recall from Remark 7.2.5 the isomorphism $C^*(\Gamma) \simeq C(\mathcal{B})$, where we use that $C^*_{red}(\Gamma) = C^*(\Gamma)$ by amenability of Γ . Proposition 8.2.6 then follows directly from this theorem. \Box

Summarizing, we have:

Theorem 8.2.8 In the periodic case, the algebra $C^*(\Omega \rtimes \mathbb{R}^d)$ is isomorphic to the C^* -algebra of observables $C(\mathcal{B}) \otimes \mathcal{K}$. In the aperiodic case, $C^*(\Omega \rtimes \mathbb{R}^d)$ is isomorphic to $C^*(R_T)$, the noncommutative analogue of $C(\Omega/R_T)$. \Box So this is where physics and the philosophy of Connes come together: following the lines of noncommutative topology [15], Ω/R_T is non-Hausdorff and useless as an ordinary topological space, i.e. $C(\Omega/R_T) \simeq \mathbb{C}$, hence Ω/R_T can be seen as a point. This means that from a commutative point of view, there is essentially only one tiling. However, Ω/R_T is actually a very rich space, and this is exhibited in the noncommutative C*-algebra $C^*(R_T)$, which is far from trivial. As a matter of fact, this noncommutative C*-algebra turns out to be precisely the aperiodic analogue of the C*-algebra of observables! We thus have

commutative topology
$$\longleftrightarrow$$
 noncommutative topology
periodic media \longleftrightarrow aperiodic media. (8.12)

A comparison between the construction of the hull by Kellendonk and the construction of the space of Penrose tilings by Connes will be given in Section 8.5.

We stress that Proposition 8.2.6 states the fact that the C*-algebra of observable, generated by the (resolvent of the) Hamiltonian, can be computed without precise knowledge of the Hamiltonian. It is the hull that contains the information about the structure of the tilings representing the crystal, although it doesn't contain any information about the precise form of the potential V, except for its (quasi-)periodicity. We will see that apparently this is enough to obtain certain properties of the spectrum of the Hamiltonian.

The question arises how we can show that a self-adjoint operator H describes the physics that is modeled by a tiling T. Bellissard has stated a useful criterion. Recall that a Hamiltonian $H = H_{T_0}$ can be replaced by a family $\{H_T\}$ of selfadjoint operators satisfying the covariance condition (8.1):

$$T(x)H_TT(x)^{-1} = H_{T+x}.$$

Definition 8.2.9 [9] A covariant family $\{H_T \mid T \in \Omega\}$ of selfadjoint operators is affiliated to a C*-algebra A if, for all $f \in C_0(\mathbb{R})$, the bounded operator $f(H_T)$ can be represented as $\pi_T(h_f)$ for some $h_f \in A$ such that the map $h : C_0(\mathbb{R}) \to$ A; $f \mapsto h_f$ is a bounded *-homomorphism.

In particular, in the periodic case, we see that the covariant family $\{H_T \mid T \in \Omega\}$ of Hamiltonians, where $\Omega = \mathcal{V}$ is the unit cell by Proposition 8.1.2, is affiliated to the C*-algebra $C^*(\Omega \rtimes \mathbb{R}^d) \simeq C(\mathcal{B}) \otimes \mathcal{K}$ in this sense. The compact operator R(z) is given by $r_z(H_{T_0})$, where for all $z \in \rho(H_{T_0})$ the function $r_z \in C_0(\mathbb{R})$ is given by $r_z(t) := \frac{1}{z-t}$. Next, we define $h_{r_z} \in C^*(\Omega \rtimes \mathbb{R}^d)$ by

$$h_{r_z}(T, y) := r_z(H_T)\delta(y)$$

Using the definition of the representation π_T given by (8.5), we see that the resolvent $R(z) = r_z(H_{T_0})$ can be represented as $\pi_T(h_{r_z})$.

8.3 The discrete hull

The computation of the C*-algebra of observables can actually be simplified by discretizing the motion of electrons. A physical motivation for discretization is the so-called tight binding approximation, which will be discussed below. Mathematically, discretization is motivated by the fact that the discrete hull, called Ω_{punc} , is an "abstract transversal" to the action of \mathbb{R}^d on Ω , which means that Ω_{punc} is a closed subset of the unit space Ω of the transformation groupoid $\Omega \rtimes \mathbb{R}^d$ meeting every orbit (under the \mathbb{R}^d -action) in Ω . A similar concept is known in foliation theory [15]. The main result is that the discrete analogue of the groupoid C*-algebra of observables is stably equivalent to the continuous C*-algebra of observables, cf. Theorem 8.3.8. Therefore, they have the same K-theory, and all K-theoretic results can be obtained in the discrete model, which is often simpler to handle than the continuous case. Moreover, we will explicitly identify the discrete momentum and the position operators in the discrete groupoid C*-algebra. This is an extra justification for the name "C*algebra of observables".

Every solid can be modeled by a Delone set, with an atom placed at each point. An electron moving in the solid is subject to a Schrödinger operator H with potential V, and this potential is mainly a superposition of the Coulomb potentials of the ions. In particular, in a mono-atomic crystal, we have

$$V(x) = \sum_{a \in \Gamma} v(x-a), \qquad (8.13)$$

where Γ is the lattice, and v(x) can be approximated by the Coulomb potential of a single atom at the origin, modified by the screening effect of other electrons. Now let ϕ_{at} be an eigenfunction of the single atom Hamiltonian $H_{at} := -\nabla^2 +$ v_{at} , with energy E. The Coulomb potential v_{at} tends to zero at infinity, leading to exponentially localized wave functions ϕ_{at} and a discrete spectrum, bounded from below. Next, for all $a \in \Gamma$, we define the function ϕ_a by $\phi_a(x) := \phi(x - \phi_a)$ a), where ϕ is derived from the single atom wave function ϕ_{at} . Then in the neighbourhood of the position $a \in \Gamma$, the wave function of H with energy E will look like ϕ_a , provided the overlap between the Coulomb potentials of different ions is small, which is, for example, the case when the interatomic distance is large. The idea of the "tight binding approximation" [2] is that only local effects are important in order to obtain the spectrum of H, because of the negligible influence on an electron of the potential of atoms that are far away. In particular, in the sum in (8.13), only a few atoms have to be considered, for example only the nearest neighbours of the atom whose unit cell contains the position x of the electron. This means that if we orthonormalize the system $\{\phi_a \mid a \in \Gamma\}$, the matrices $V_{aa'}$, defined by

$$V_{aa'} := \langle \phi_a | V \phi_{a'} \rangle,$$

only have nonzero entries near the diagonal. Now $(\phi_a)_{a\in\Gamma}$ can be seen as an element of $\ell^2(\Gamma)$, so we may replace the Hamiltonian H on $L^2(\mathbb{R}^d)$ by its discrete

tight-binding version H_{TB} on $\ell^2(\Gamma)$. In the simplest case, namely the onedimensional lattice $\Gamma = \mathbb{Z}$, where the potential $V_{nn'}$ is diagonal and only hopping to nearest neighbours is considered, we get

$$H_{TB}\psi(n) = -t\psi(n+1) - t\psi(n-1) + V(n)\psi(n),$$

where t is the hopping amplitude (typically, $0 \le |t| \le 1$), and $V(n) := V_{nn}$. We see that the matrix corresponding to the operator H_{TB} is tridiagonal, i.e.,

$$(H_{TB})_{nm} = \begin{cases} V(n) & \text{if } n = m, \\ -t & \text{if } |n - m| = 1, \\ 0 & \text{otherwise.} \end{cases}$$

The motion of an electron then consists of "hopping" from one lattice point to a neighbouring one. We see that in general, by looking only at local effects, the Schrödinger operator H on $L^2(\mathbb{R}^d)$, which is in general unbounded, is replaced by its discrete version H_{TB} on $\ell^2(\mathbb{Z}^d)$, which is a bounded operator. We will now reformulate this tight binding approximation for arbitrary aperiodic solids in d dimensions. For this, we will need the notion of a discrete hull.

Figure 8.1: A punctured tiling

Recall that given a Delone set, we can form a corresponding tiling (for example by the Voronoi construction), and vice versa. Indeed, to construct a Delone set from a d-dimensional tiling T, we use so-called punctured tiles [29, 31]. For each tile type (or "prototile") of a tiling T, we choose points x(t) in the interior of the tiles t, which are called **punctures**, in such a way that if t_1 and t_2 are two copies of the same prototile (that is, they are translates of each other by some $x \in \mathbb{R}^d$), then their punctures are also translates of each other by x, i.e.,

$$t_1 = t_2 + x \text{ for some } x \in \mathbb{R}^d \implies x(t_1) = x(t_2) + x.$$
 (8.14)

Note that we use a slightly different definition of prototile: instead of defining a prototile as an equivalence class under congruence, we now define it as an equivalence class under translation. In the above way, we'll puncture all tiles in all tilings in the hull Ω_T . Note that in the periodic case of a tiling by translates of the Voronoi unit cell \mathcal{V} , the obvious choice would be to assign a puncture in such a way that the Voronoi cell of the puncture gives the original unit cell again, i.e.

$$\mathcal{V}(x(\mathcal{V})) = \mathcal{V}.$$

In general, if we can recover the positions of the atoms from the structure of the tiling, it is obvious to place the punctures precisely at the locations of the atoms, although in principal any point in the tile will suffice, as long as it lies in the interior of the tile and satisfies (8.14).

Definition 8.3.1 Let T be a tiling. The **discrete hull** Ω_{punc} of T is the subset of Ω_T consisting of tilings that have a puncture of a tile in the origin, i.e.,

$$\Omega_{punc} := \{ T' \in \Omega_T \mid x(t) = 0 \text{ for some } t \in T' \}$$

Moreover, for each tiling T we define T^{punc} to be the subset of \mathbb{R}^d consisting of all the punctures of T.

Example 8.3.2 In the periodic case of a tiling by unit cells Ω_{punc} is just the point set of atomic positions in the unit cell, just as Ω is the unit cell itself (see Figure 8.2). Furthermore, in the periodic case T^{punc} is a point lattice. In the general case, T^{punc} is a Delone set, which is the generalization of a point lattice to the aperiodic case.

Figure 8.2: For a periodic tiling, the discrete hull consists of the atomic positions in the unit cell

To justify the name "discrete hull", we observe that Ω_{punc} is indeed discrete: note that for every tiling $T' \in \Omega_{punc}$, there is an $\epsilon > 0$ such that T' + x is not in Ω_{punc} , for all x with $0 < |x| < \epsilon$. Furthermore, Ω_{punc} is a closed subset of Ω : let $(T_n) \in \Omega_{punc}$ converge to $T \in \Omega$, then $\forall \epsilon > 0$, $\exists N$ such that $\forall n \ge N$, there are vectors $x, y \in B(0, \epsilon)$ such that

$$(T_n+x)\upharpoonright_{B(0,\frac{1}{2})}=(T+y)\upharpoonright_{B(0,\frac{1}{2})}.$$

But since ϵ goes to 0, |x| and |y| both tend to zero, so for the tile $t \in T$ covering the origin, we get x(t) = 0, because $x(t_n) = 0$ for every n, where t_n is the tile covering the origin in T_n . Therefore, $T \in \Omega_{punc}$, and Ω_{punc} is closed.

Proposition 8.3.3 If T is repetitive and satisfies the finite pattern condition, then its discrete hull Ω_{punc} is a Cantor set.

Proof: Ω_{punc} is compact as a closed subset of Ω_T (which is compact because T satisfies the finite pattern condition). Next, we show that Ω_{punc} is totally disconnected. Let P be a patch in T, and $t \in P$ a tile. Then P - x(t) is a patch with a puncture in the origin. Define

$$U(P,t) := \{ T' \in \Omega \mid P - x(t) \subset T' \}.$$
(8.15)

Observe that $U(P,t) \subset \Omega_{punc}$. We will show that the sets U(P,t) are both open and closed, and that they generate the relative topology of Ω_{punc} , thereby establishing total disconnectedness. Let (T_n) be a sequence in U(P,t), with $\lim_{n\to\infty} T_n = T \in \Omega_{punc}$. Now $\forall \epsilon > 0$ there is an N such that $\forall n \ge N$ there are $x, y \in B(0, \epsilon)$ such that

$$(T_n+x)\upharpoonright_{B(0,\frac{1}{\epsilon})} = (T+y)\upharpoonright_{B(0,\frac{1}{\epsilon})}$$

But for ϵ small enough, $T_n + x$ and T + x are not elements of Ω_{punc} unless x = 0. So we have

$$T_n \upharpoonright_{B(0,\frac{1}{\epsilon})} = T \upharpoonright_{B(0,\frac{1}{\epsilon})}.$$

Now for ϵ small enough, P - x(t) fits in $B(0, \frac{1}{\epsilon})$, so $T \in U(P, t)$, and U(P, t) is closed. A same argument for $\Omega_{punc} \setminus U(P, t)$ shows that U(P, t) is open. Moreover, the sets U(P, t) generate the same topology as the open balls $B(T, \epsilon)$ that generate the relative topology induced by the metric d. This can easily be shown easily by checking that for every $T \in \Omega_{punc}$, and every set $U(P, t) \ni T$, there is an $\epsilon > 0$ such that $T \in B(T, \epsilon) \subset U(P, t)$, and that for every $B(T, \epsilon)$, there is are P and t in T such that $T \in U(P, t) \subset B(T, \epsilon)$.

Finally, we have to show that Ω_{punc} consists entirely of limit points, or equivalently, that Ω_{punc} has no isolated points, i.e. for any $T' \in \Omega_{punc}$, for all $\epsilon > 0$, there is a tiling $T'' \in \Omega_{punc}$ such that $d(T', T'') < \epsilon$. Now let $T' \in \Omega_{punc}$, and $\epsilon > 0$. Observe that since T is repetitive, Ω_T is minimal, and every element of Ω is repetitive, in particular T'. Let $P \subset T$ be a patch around the origin such that $T' \upharpoonright_{B(0,\frac{1}{\epsilon})} = P \upharpoonright_{B(0,\frac{1}{\epsilon})}$. Since T' is repetitive, there is an R > 0 such that for every $x \in \mathbb{R}^d$, there is a translate P + x' of P in T' such that P + x' lies in $T' \cap B(x, R)$. Evidently, P covers the origin in T' - x', P, and in particular, $T' - x' \in \Omega_{punc}$. Now we have

$$(T'-x')\upharpoonright_{B(0,\frac{1}{\epsilon})} = T'\upharpoonright_{B(0,\frac{1}{\epsilon})},$$

which means that $d(T', T' - x') < \epsilon$, and this proves the proposition. \Box

Remark 8.3.4 In [29], Kellendonk works with the set T^{punc} of one tiling T, whereas in [31], he uses the discrete hull Ω_{punc} , which is the space of tilings with a puncture at the origin. These two approaches correspond to different frames of reference: in the first case, the electron is moving, while the tiling (i.e. the solid) is at rest. In the second case, the electron is at rest in the origin, while the tiling gets (discretely) translated.

On the discrete hull Ω_{punc} , we define the obvious equivalence relation

$$R_{punc} := \{ (T', T'') \in \Omega_{punc} \times \Omega_{punc} \mid T'' \text{ is a translate of } T' \}.$$
(8.16)

It is clear that R_{punc} is just the discrete version of R_T , i.e.,

$$R_{punc} = R_T \cap (\Omega_{punc} \times \Omega_{punc}).$$

In particular, R_{punc} is a topological groupoid with the induced topology of R_T , inherited from $\Omega \times \mathbb{R}^d$. In practice, this means that a sequence $(T_n, T_n - x_n)$

in R_{punc} converges to (T, T - x) if and only if both $d(T_n, T)$ and $|x_n - x|$ tend to zero. Here the metric d on Ω_{punc} is the one induced from the metric on Ω . Note that R_{punc} is locally compact and R-discrete. Hence, we can form the C*-algebra $C^*(R_{punc})$ by defining product and involution on $C_c(R_{punc})$ in the usual way (compare to the Penrose case in Chapter 6):

$$f * g(T, T'') := \sum_{T' \sim T''} f(T, T') g(T', T''),$$
 (8.17)

$$f^*(T,T') := \overline{f(T',T)}.$$
 (8.18)

Again, we have reduced representations $\pi_T : C_c(R_{punc}) \to \ell^2(R^{-1}(T))$, labeled by elements T in the unit space Ω_{punc} , defined by

$$\pi_T(f)\psi(T') := \sum_{T'' \sim T'} f(T', T'')\psi(T'').$$
(8.19)

Of course, π_T satisfies the covariance condition (8.6). We proceed to define a C*-norm by

$$||f||_{C^*(R_{punc})} := \sup_{T \in \Omega_{punc}} ||\pi_T(f)||,$$

yielding the C*-algebra $C^*(R_{punc})$. This construction is the same as the construction of $C^*_{red}(R)$ of Chapter 6. We can identify $C^*(R_{punc})$ as the discrete version of the C*-algebra of observables. Note that $C^*(R_{punc})$ is a unital C*algebra, with unit I defined by

$$\mathbb{I}(T, T+x) := \delta_{x,0}.$$

This is well defined since x can only have discrete values, i.e. there is always an $\epsilon > 0$ such that $(T, T + x) \notin R_{punc}$ for all x such that $0 < |x| < \epsilon$. Note that the continuous version $C^*(R_T)$ has no unit.

Of course, we can also define the discrete version of the transformation groupoid $\Omega \rtimes \mathbb{R}^d$, and its corresponding C*-algebra, which are isomorphic to R_{punc} and $C^*(R_{punc})$ respectively, as long as Ω contains no periodic tilings. Note however that only pairs (T, x) for which $x \in T^{punc}$ are elements of this discrete transformation groupoid G_{punc} , where we have identified the set T^{punc} of punctures of a tiling with the discrete subgroup of \mathbb{R}^d that generates T^{punc} as the orbit of the origin under the group action (in the periodic case, this identification corresponds to the identification of the lattice Γ with the orbit, i.e. the point lattice). Equivalently, G_{punc} can be defined as

$$G_{punc} := \{ (T, x) \in \Omega_{punc} \times \mathbb{R}^d \mid T - x \in \Omega_{punc} \}.$$
(8.20)

Typically, the discrete transformation groupoid G_{punc} will look like $\Omega_{punc} \rtimes \mathbb{Z}^d$. A tiling is called a **decoration of** \mathbb{Z}^d [29] if the following holds: suppose that F is the (finite) set of pattern classes in T made of a tile t_0 together with all the tiles that touch t_0 at a common hypersurface (this is sometimes called "the first corona" of t_0), and define $x_0 := x(t_0)$. Then T is a decoration of \mathbb{Z}^d if there is an action α of \mathbb{Z}^d on Ω_{punc} such that for all $P \in F$, the following holds:

$$\forall x \in P^{punc} \setminus \{x_0\} \exists s \in \{\pm e_i\}_{i=1}^d \text{ such that } \forall T \in U(P, t_0) : \alpha_s(T) = T - x.$$
(8.21)

Here $\{e_i\}_i$ denotes the standard basis of \mathbb{Z}^d .

Example 8.3.5 Of course, the periodic case, of a tiling T consisting of unit hypercubes, is a trivial example of a decoration of \mathbb{Z}^d . In this case, α just acts as a translation, i.e. $\alpha_s(T) = T - s$.

In general, the action α of \mathbb{Z}^d on T depends only on a finite patch around the origin, and consists of next-neighbour shifts. α_s is continuous, and we have $\alpha_s(U(T, x_0)) = U(T, x)$ for x and x_0 as in (8.21). Therefore, the map $\varphi : \Omega_{punc} \times \mathbb{Z}^d \to R_{punc}; (T, s) \mapsto (T, \alpha_s(T))$ is continuous with respect to the product topology. Moreover, it is surjective, since $\varphi(\{T\} \times \mathbb{Z}^d) = R^{-1}(T)$. Again, φ is a homeomorphism if and only if Ω_{punc} contains no periodic tilings.

Now, recall that by projecting a higher dimensional periodic lattice onto an irrational cut, quasiperiodic tilings can be obtained cf. Section 2.4.

Proposition 8.3.6 If T is a quasiperiodic tiling obtained via the projection method, then it is a decoration of \mathbb{Z}^d .

Proof: Let π_{\parallel} (π_{\perp} respectively) define the projection from $\mathbb{R}^d \times \mathbb{R}^n$ to the physical space \mathbb{R}^d (respectively the internal space \mathbb{R}^n), let Γ be a lattice in $\mathbb{R}^d \times \mathbb{R}^n$, and let M denote the acceptance domain in \mathbb{R}^n . For simplicity we assume $\Gamma = \mathbb{Z}^{d+n}$, but the argument is valid for every lattice Γ in $\mathbb{R}^d \times \mathbb{R}^n$. Then T is a tiling with $T^{punc} = \Lambda(M)$, where $\Lambda(M)$ is defined as

$$\Lambda(M) := \{ \pi_{\parallel}(a) \mid a \in \Gamma \text{ such that } \pi_{\perp}(a) \in M \}.$$

Now let t_0 be a tile in T with puncture x_0 , and let F be the set of pattern classes consisting of first coronas of t_0 , and let $P \in F$. Next, we have an action S of \mathbb{Z}^d on the set $U(P, t_0)$ by defining S_{s_d} for every standard basis-vector $s_d \in \mathbb{Z}^d$ as

$$\alpha_{s_d}(T) = \pi_{\parallel}(\pi_{\parallel}^{-1}(T) - s_{d+n}),$$

where s_{d+n} denotes the standard basis-vector in \mathbb{Z}^{d+n} such that $s_d = \pi_{\parallel}(s_{d+n})$. Since π_{\parallel} restricted to \mathbb{Z}^{d+n} is injective, this action is well defined. Moreover, it satisfies (8.21). \Box

Example 8.3.7 By the above proposition, the Fibonacci chain, which can be obtained via the projection method (see Figure 8.3), is a decoration of \mathbb{Z} . We will discuss electronic motion on a Fibonacci chain in Section 9.3.

Figure 8.3: The Fibonacci chain, obtained via the projection method, is a decoration of $\mathbb Z$

Actually, also many of the quasiperiodic tilings obtained via the substitution method, among which the Penrose tilings, can be seen as decorations of \mathbb{Z}^d [30]. In all these cases, the transformation groupoid G_{punc} is given by $\Omega_{punc} \rtimes_{\alpha} \mathbb{Z}^d$, where α denotes the action of \mathbb{Z}^d on Ω_{punc} . However, an important difference with the continuous transformation groupoid lies in the fact that since for every tiling $T \in \Omega_{punc}$ the fiber $R^{-1}(T)$ can be identified with T^{punc} , all fibers are different, which is in contrast with the continuous case, where $R^{-1}(T) = \mathbb{R}^d$ for all $T \in \Omega$. As mentioned at the beginning of this section, Ω_{punc} is an **abstract transversal** to the \mathbb{R}^d -action [35, 31], which means that it is a closed subset of the unit space Ω of the transformation groupoid $\Omega \rtimes \mathbb{R}^d$ meeting every orbit in Ω . Using a theorem of [35], we have the following important fact [11]:

Theorem 8.3.8 $C^*(R_{punc})$ is stably equivalent to $C^*(R_T)$.

Actually, the main theorem in [35] states that if there is a (G, H)-equivalence between two groupoids (which is the notion of Morita equivalence for groupoids, see [34]), their C*-algebras are Morita equivalent. Moreover, in [35], it is shown that for an abstract transversal $N \subset G^0$ for a groupoid G, there is a (G, G_N^N) equivalence, where $G_N^N = R^{-1}(N) \cap D^{-1}(N)$. Specializing to our case, where $G = \Omega \rtimes \mathbb{R}^d$, $G^0 = \Omega$, $N = \Omega_{punc}$, we see that

$$G_N^N = R^{-1}(\Omega_{punc}) \cap D^{-1}(\Omega_{punc}) = G_{punc}$$

so $\Omega \rtimes \mathbb{R}^d$ is groupoid-Morita equivalent with G_{punc} , and from the theorem in [35], it then follows that $C^*(\Omega \rtimes \mathbb{R}^d)$ and $C^*(G_{punc})$ are Morita equivalent, hence stably equivalent. Using the isomorphisms between R_T and $\Omega \rtimes \mathbb{R}^d$ and between R_{punc} and G_{punc} , the theorem follows.

Corollary 8.3.9 $K_0(C^*(R_{punc})) = K_0(C^*(R_T)).$

This is immediate from the above theorem and Corollary 5.2.17. \Box

This corollary will play an important role in the gap labelling of Schrödinger operators. In general, it follows from the above theorem that the discrete hull yields as much information about the spectrum of the Hamiltonian as the continuous hull, as long as this information is contained in the stabilized versions of the C*-algebras. Since the discrete version is often easier to compute, this is a very useful fact. In what follows, sometimes we will only prove certain properties in the discrete case, using the above Morita equivalence to apply them to the continuous case.

8.4 The discrete C*-algebra of observables

Until now, the construction of the various C*-algebras has been rather abstract. However, in the discrete case, we can actually identify a function $h \in C^*(R_{punc})$ such that

$$\pi_T(h) = H_T,$$

for all $T \in \Omega_{punc}$, where $\{H_T\}$ is the covariant family of discrete Schrödinger operators affiliated to $C^*(R_{punc})$. Note that this is not possible in the continuous case, because the continuous Hamiltonian is not a bounded operator, in contrast to the discrete one. To prove the above assertion, we first consider an electron moving in a tiling T, hopping from tile to tile. If we change our reference frame to that of the electron, we can choose the electron to stay in the origin, and move the tiling instead. This is exactly what happens in the Hilbert space $\ell^2(R^{-1}(T))$. Recall that the fiber $R^{-1}(T)$ is defined by

$$R^{-1}(T) = \{ (T, T') \in R_{punc} \mid T' = T + x \text{ for some } x \in \mathbb{R}^d \}.$$

So $R^{-1}(T)$ can be identified with the set of all translates of T in Ω_{punc} , i.e.,

$$R^{-1}(T) = \{T - x \mid x \in T^{punc}\}.$$
(8.22)

Now, the family of discrete Hamiltonians H_T acts on $\ell^2(R^{-1}(T))$ by

$$H_T\psi(T') := \sum_{T'' \in R^{-1}(T)} h_T(T', T'')\psi(T''), \qquad (8.23)$$

where $h_T(T', T'')$ is the matrix element indexed by $T', T'' \in R^{-1}(T)$. A more convenient way to define the matrix of H_T can be obtained if one observes that $R^{-1}(T)$ is actually homeomorphic to T^{punc} , which is immediate from (8.22). This homeomorphism between $R^{-1}(T)$ and T^{punc} reflects the equivalence of the different reference frames: in the first case, the electron sits in the origin, and the tilings are translated (that is, the wave function ψ takes different values on different tilings, which are all discrete translates of each other); in the second case, we consider an electron hopping in T^{punc} from punctured tile to punctured tile (note that here everything happens in only one tiling T, so this is the most natural point of view). In the latter case, we can define the Hamiltonian H_T by

$$H_T\psi(x) = \sum_{x'\in T^{punc}} H_T(x, x')\psi(x'),$$
(8.24)

where $\psi \in \ell^2(T^{punc})$ and $H_T(x, x')$ are matrix elements indexed by $x, x' \in T^{punc}$. Note that $H_T(x, x')$ is related to $h_T(T', T'')$ by

$$h_T(T - x, T - x') = H_T(x, x').$$
 (8.25)

If we view (8.25) as the definition of h_T , we see that we can drop the superfluous subscript T. Then the resulting h can actually be seen as a function on R_{punc} .

Now, in the tight binding representation, only local effects contribute to the Hamiltonian, which means that only the punctures x' of the tiles that lie in a finite patch P around x contribute. This means that the sum in (8.24) may be restricted to $x' \in P^{punc}$, the other elements $H_T(x, x')$ being 0. It follows that H_T is a bounded operator on $\ell^2(T^{punc})$, so there is no need to look at the resolvent of H_T anymore. We thus have [8]:

Proposition 8.4.1 Let H_T be given by (8.24). Then there is an element $h \in C^*(R_{punc})$ such that the matrix elements $H_T(x, x')$ of the operator H_T are given by

$$H_T(x, x') = h(T - x, T - x').$$
(8.26)

Moreover, we have $\pi_T(h) = H_T$.

Proof: Define h by (8.25). Note that h is continuous on R_{punc} . Moreover, it has compact support, since $H_T(x, x')$ is only nonzero on a finite patch around x. Finally, we have

$$\pi_T(h)\psi(T') = \sum_{T'' \sim T'} h(T', T'')\psi(T'') = H_T\psi(T'),$$

for all $T' \in R^{-1}(T), \ \psi \in \ell^2(R^{-1}(T)).$

Actually, in $C^*(R_{punc})$ we can even identify the discrete position and the translation operators that generate the C*-algebra of observables, namely by constructing a C*-algebra A_{punc} that is isomorphic to $C^*(R_{punc})$. Recall that the discretization of the Hamiltonian is motivated by the tight binding approximation. In particular, it is assumed that the motion of an electron is subject to local effects only. In other words, we just look at finite patches P in our tiling T. Following [31], we consider triples (P, t_1, t_2) , where P is a finite patch in T, and $t_1, t_2 \in P$ (possibly, $t_1 = t_2$). Two of these triples are called equivalent if one is a translate of the other. We define the **doubly pointed pattern class** $[P, t_1, t_2]$ to be the equivalence class of (P, t_1, t_2) under translation. Next, we define A_{punc} to be the C*-algebra generated by elements $e[P, t_1, t_2]$, subject to the involution

$$e[P, t_1, t_2]^* = e[P, t_2, t_1],$$
(8.27)

and with a product defined as follows: if (P, t_1, t_2) and (P', t'_1, t'_2) are both contained in a larger patch in such a way that $t_2 = t'_1$, then the product is defined by

$$e[P, t_1, t_2]e[P', t_1', t_2'] = e[P \cup P', t_1, t_2'];$$
(8.28)

otherwise, the product is 0. These elements $e[P, t_1, t_2]$ can be identified with the discrete momentum and position operators, cf. below.

Proposition 8.4.2 [31] The C*-algebra A_{punc} , generated by all elements of the form $e[P, t_1, t_2]$, is isomorphic to $C^*(R_{punc})$.

Proof: Recall that the subsets U(P,t) of Ω_{punc} , defined in (8.15), are both open and closed, and that they generate the topology of Ω_{punc} . Consider the map

$$U(P,t_1) \to U(P,t_2); \quad T' \mapsto T' - x(t_2) + x(t_1).$$

Note that this map is well defined, and is in fact a homeomorphism. The graph $G(P, t_1, t_2)$ of this map, defined by

$$G(P, t_1, t_2) := \{ (T', T' - x(t_2) + x(t_1)) \mid T' \in U(P, t_1) \},\$$

is a subset of R_{punc} . Let $f[P, t_1, t_2]$ denote its characteristic function. Using similar arguments as in the proof of Proposition 8.3.3, one can show that $G(P, t_1, t_2)$ is both open and compact, and that these sets generate the topology of R_{punc} . Therefore, $f[P, t_1, t_2] \in C_c(R_{punc})$, and the linear span of the $f[P, t_1, t_2]$'s is dense in $C_c(R_{punc})$. Using the definition of the product and involution on $C_c(R_{punc})$, (8.17) and (8.18), we get

$$f[P,t_1,t_2]f[P',t_1',t_2'](T,T') = \sum_{T''\sim T'} f[P,t_1,t_2](T,T'')f[P',t_1',t_2'](T'',T').$$

Clearly, only if $T'' = T - x(t_2) + x(t_1) = T' - x(t'_2) + x(t'_1)$, the sum is nonzero. Then (8.28) and (8.27) follow. Likewise, $f[P, t_1, t_2]^*(T, T') = f[P, t_1, t_2](T', T) = f[P, t_2, t_1](T, T')$, for all $(T, T') \in G(P, t_1, t_2)$, which coincides with (8.27). \Box

Actually, since U(P, t) is both open and closed, its characteristic function is an element of the C*-algebra $C(\Omega_{punc})$. In this way, we see that there is a unital injective *-homomorphism from $C(\Omega_{punc})$ into A_{punc} , sending the characteristic function of U(P,t) to e[P,t,t]. Therefore, $C(\Omega_{punc})$ can be seen as the subalgebra of A_{punc} generated by the elements e[P,t,t].

Finally, we can identify the elements $e[P, t_1, t_2]$ as discrete translation and position operators: momentum-independent observables will be functions of the elements e[P, t, t], which describe whether an electron is at the tile t in a patch P. Likewise, given two neighbouring tiles t_1 and t_2 , the element $e[\{t_1, t_2\}, t_1, t_2]$ will describe the motion of an electron from a tile t_2 to a tile t_1 . Note however, that $e[\{t_1, t_2\}, t_1, t_2]$ describes the hopping from t_2 to t_1 for all neighbouring tiles t_1 and t_2 in every patch P in a tiling T with a translate of $\{t_1, t_2\}$ lying in P. Recall that in the tight binding approximation, only local effects are taken into account. In particular, we only consider the action of the operator $e[P, t_1, t_2]$ on the patch P, regardless of the position of P in the tiling T. The operators $e[P, t_1, t_2]$ are called "partial translations" in [31]. Observe that

$$e[P, t_1, t_2]e[P, t_1, t_2]^* = e[P, t_1, t_1]$$

$$e[P, t_1, t_2]^*e[P, t_1, t_2] = e[P, t_2, t_2],$$
(8.29)

so hopping from one tile to another and back is the same as not hopping at all. Note that if $\{t_i\}_{i=1}^n$ is the set of prototiles, then

$$\sum_{i=1}^{n} e[\{t_i\}, t_i, t_i]$$

is a unit for the C*-algebra A_{punc} . We have seen that indeed, our discrete C*-algebra of observables $C^*(R_{punc})$ can be identified with the C*-algebra generated by discrete translation and position operators. In the following, we won't distinguish between $C^*(R_{punc})$, $C^*(G_{punc})$ and A_{punc} if this is not necessary. Similarly, we will use the notation A_T for the continuous C*-algebras of observables, $C^*(\Omega \rtimes \mathbb{R}^d)$ and $C^*(R_T)$.

8.5 Comparison with Connes's space of Penrose tilings

The construction of the hull Ω and its noncommutative C*-algebra by Kellendonk resembles the construction of the space of Penrose tilings X = K/R and its noncommutative analogue (Chapter 6), although the resemblance is somewhat blurred by the use of the index sequences in the Penrose case. Recall that in the latter case an index sequence was assigned to a triangle α in some Penrose tiling T. Alternatively, one could assign a similar sequence to the origin of a plane Tcovered by a Penrose tiling, as long as the origin lies in the interior of some triangle. Then isometric tilings define equivalent sequences, i.e., sequences that coincide eventually. So essentially, whereas the hull is the set of all translates of a certain tiling, endowed with a certain topology, the space of Penrose tilings X is the set of all images under isometries (that is, both translations and orthogonal transformations) of a certain Penrose tiling, where equivalent Penrose tilings are identified. We see that in the construction of the space of Penrose tilings every triangle α is reduced to only one point of its interior, and this construction is generalized by Kellendonk, using punctured tiles. Therefore, Ω_{punc} plays the role of K. In particular, observe that these are both Cantor sets.

These Cantor sets are the unit spaces of the equivalence relation groupoids R_{punc} and R, respectively. The difference between the equivalence relations is that for the Penrose case two tilings are equivalent if and only if there is an isometry between them, whereas for the equivalence relation R_T on the hull, two tilings have to be translates of each other to be equivalent. We have seen that R_{punc} is isomorphic to the transformation groupoid G_{punc} , which reduces to $\Omega_{punc} \rtimes_{\alpha} \mathbb{Z}^d$ in many cases. In particular, for Kellendonk's hull, the transformation group is an (abelian) group of translations. We can ask ourselves whether there is a similar transformation groupoid for the space of Penrose tilings. The transformation group is in this case a (non-abelian) subgroup of $SL(2, \mathbb{R})$, because it not only contains translations, but also rotations and reflections. On the level of the Cantor space K of sequences in 0's and 1's, we can define the transformation groupoid G by introducing the group H_{flip} of "finite flips", that transforms finitely many 0's of a sequence in K into 1's and vice versa. Then G can be defined as

$$G := \{ (z, \alpha) \in K \times H_{flip} \mid \alpha(z) \in K \},\$$

and we see that G is isomorphic to R by the map $(z, \alpha) \in G \mapsto (z, \alpha(z)) \in R$,

just as G_{punc} is isomorphic to R_{punc} . On the level of Penrose tilings, we can puncture every tile α in such a way that if α' is an isometric copy of α , i.e. $\alpha' = s \cdot \alpha$ for some $s \in SL(2, \mathbb{R})$, then $x(\alpha') = s \cdot x(\alpha)$, where $x(\alpha)$ denotes the puncture of α , as usual. Then, denoting the space of Penrose tilings with a puncture in the origin by Y (such that $Y \simeq K$, and $X = Y/SL(2, \mathbb{R})$), we get the transformation groupoid

$$Y \rtimes SL(2,\mathbb{R}) := \{ (T,s) \in Y \times SL(2,\mathbb{R}) \mid s \cdot T \in Y \}.$$

Finally, observe that for a Penrose tiling T, Ω_{punc} is certainly not equal to K, and the same holds on the groupoid level and the C*-algebra level [29]. Note that in principle the construction of Connes may be generalized to arbitrary substitution tilings, such as the Fibonacci chain, but since it explicitly uses the index sequence associated to a substitution tiling, it can not be generalized to tilings that do not have the substitution property. In particular, the C*-algebra $C^*(R_{punc})$ will in general not be an AF-algebra, in contrast to $C^*_{red}(R)$. In conclusion, the construction of $C^*(R_{punc})$ by Kellendonk uses the philosophy of the construction of $C^*_{red}(R)$ by Connes, but yields different results.
Chapter 9

Gap labelling

In this chapter we assume that we have an aperiodic tiling T, with hull Ω , and a covariant family of Schrödinger operators $\{H_T\}_{T \in \Omega}$ affiliated to the C*-algebra A_T . We want to know more about the spectrum of H_T . Recall that in the case of a periodic crystal, the spectrum has a band structure, and the integrated density of states is defined as

$$N(E) := \lim_{m \to \infty} \frac{1}{m^d |\mathcal{V}|} N_{\mathcal{V}^{(m)}}(E),$$

where $N_{\mathcal{V}^{(m)}}(E)$ is the number of eigenvalues of $H_{\mathcal{V}^{(m)}}$ up to E, and $\mathcal{V}^{(m)}$ is the subset of \mathbb{R}^d obtained by stacking up m^d unit cells. Essentially, the integrated density of states is the number of one-electron states per unit volume up to a certain energy. We can generalize this to the aperiodic case, provided that the material we are observing is homogeneous, which means that if we compare large regions, they look very much the same. In other words, it turns out to be useful to assume that the tiling T satisfies the finite pattern condition of Theorem 8.1.3, such that the hull is a compact space.

Definition 9.0.1 Let G be a locally compact group. A Følner sequence is a sequence (Λ_n) in G of open subsets Λ_n , each with finite Haar measure $|\Lambda_n|$, such that $\bigcup_{n=1}^{\infty} \Lambda_n = G$, and such that for all $x \in G$,

$$\lim_{n \to \infty} \frac{|\Lambda_n \Delta(x \cdot \Lambda_n)|}{|\Lambda_n|} = 0, \qquad (9.1)$$

where Δ denotes the symmetric difference of sets, $V\Delta W = (V \cup W) \setminus (V \cap W)$.

A Følner sequence (Λ_n) defines an invariant mean M on $C_b(G)$ by

$$M(f) := \lim_{n \to \infty} \frac{1}{|\Lambda_n|} \int_{\Lambda_n} f(x) d\lambda(x),$$

and it can be shown [22] that there is a Følner sequence in G if and only if G is amenable. Specializing to the continuous case, where $G = \mathbb{R}^d$ acts on the hull Ω , it is easy to see that if we define Λ_n to be the hypercube centered at the origin with length n, (Λ_n) is a Følner sequence. Of course, we can apply the same construction to our tiling T, and look at patches P_n , defined as the smallest patch covering the hypercube Λ_n . In this case, Følner's condition (9.1) implies that surface effects are negligible compared to volume effects, i.e.

$$\lim_{n \to \infty} \frac{|\partial P_n|}{|P_n|} = 0,$$

where ∂P_n is the set of tiles that cover the boundary of the hypercube Λ_n , and |P| denotes the Lebesgue measure of the patch P as a subset of \mathbb{R}^d . One can now define

$$N_{T,\Lambda_n}(E) := \sharp \{ E' \in \sigma(H_{T,\Lambda_n}) \mid E' \le E \},\$$

where H_{T,Λ_n} is the Hamiltonian H_T restricted to Λ_n , acting on the Hilbert space $L^2(\Lambda_n)$, subject to certain boundary conditions. The **integrated density of states (IDS)** $N_T : \mathbb{R} \to \mathbb{R}^+$ is then defined by

$$N_T(E) := \lim_{n \to \infty} \frac{1}{|\Lambda_n|} N_{T,\Lambda_n}(E).$$
(9.2)

In the discrete case, when $G = \mathbb{Z}^d$ acts on Ω_{punc} , the density of states can be defined in a similar way. The existence of the limit is in general a delicate matter, but under reasonable conditions [36], it can be shown that the IDS indeed exists, and is independent of the chosen boundary conditions (since surface effects are negligible) [7]. It seems obvious that the integrated density of states $N_T(E)$ is actually independent of $T \in \Omega$, because of the homogeneity of the solid. Actually, we have

$$N_T(E) = N_{T+x}(E),$$

for all $x \in \mathbb{R}^d$, so by minimality of Ω , N_T is constant as a function of T on a dense subset $T + \mathbb{R}^d$ of Ω . This is an immediate consequence of the fact that

$$\sigma(H_T) = \sigma(T(x)H_TT(x)^{-1}) = \sigma(H_{T+x}),$$

where we used the covariance condition and the invariance of the spectrum under unitary transformations. Later, we will couple this to the measure structure on Ω , cf. Section 9.1.

It is clear that the IDS is a nonnegative, nondecreasing function of $E \in \mathbb{R}$ that is constant on gaps in the spectrum, just as in the periodic case. Moreover, one can show that it is absolutely continuous with respect to E if H has no eigenvalues (i.e., if its pure point spectrum is empty) [36]. In this case one can once more define the **density of states** to be the derivative $\frac{dN_T}{dE}$ of the IDS.

9.1 Shubin's formula

Next, we want to link the IDS to our C*-algebra $A_T = C^*(\Omega \rtimes \mathbb{R}^d)$. Define the **operator trace** Tr of a bounded operator A on a separable Hilbert space \mathcal{H} with orthonormal basis e_i by

$$Tr(A) := \sum_{i=1}^{\infty} \langle e_i, Ae_i \rangle.$$

This trace is independent of the choice of a basis in \mathcal{H} if A is **trace-class**, i.e., if $Tr|A| < \infty$, where $|A| := \sqrt{A^*A}$ [32]. Now observe that $N_{T,\Lambda}(E)$ is in fact equal to the operator trace of the eigenprojection $\chi_{(-\infty,E]}(H_{T,\Lambda})$ onto the eigenstates of $H_{T,\Lambda}$ with energy less that or equal to E, where $\chi_{(-\infty,E]}$ is the characteristic function of the interval $(-\infty, E]$. Since there are only finitely many such eigenstates, we get

$$N_T(E) = \lim_{n \to \infty} \frac{1}{|\Lambda_n|} Tr_{\Lambda_n}(\chi_{(-\infty, E]}(H_{T, \Lambda_n})),$$
(9.3)

where Tr_{Λ_n} is the restriction of the operator trace Tr on $L^2(\mathbb{R}^d)$ to $L^2(\Lambda_n)$. Now we can describe the IDS by using the C*-algebra $C^*(\Omega \times \mathbb{R}^d)$ to which H is affiliated. First, we want to show the existence of a translation invariant probability measure on Ω , i.e., a measure μ such that $\mu(\Omega) = 1$ and such that for every $T \in \Omega$ and every $\epsilon > 0$, we have

$$\mu(B(T,\epsilon)) = \mu(B(T+x,\epsilon))$$

for all $x \in \mathbb{R}^d$. Moreover, we assume that μ is **ergodic** under the action of \mathbb{R}^d , i.e., every invariant subset of Ω has measure 0 or 1.

Proposition 9.1.1 There exists a translation invariant, ergodic probability measure μ on Ω .

Proof: [7] Recall from Definition 8.2.3 that since \mathbb{R}^d is amenable, there exists an invariant mean M on the C*-algebra of continuous bounded functions on \mathbb{R}^d . Now let $f \in C(\Omega)$, and define the function $F : \mathbb{R}^d \to \mathbb{C}$ by F(x) := f(T - x)for some fixed $T \in \Omega$. Then F is continuous and bounded on \mathbb{R}^d , and the map $\tilde{\mu}$ defined on $C(\Omega)$ by $\tilde{\mu}(f) := M(F)$ is a positive linear map such that $\tilde{\mu}(\mathbb{I}_{\Omega}) = M(\mathbb{I}_{\mathbb{R}^d}) = 1$. By Riesz' representation theorem, $\tilde{\mu}$ uniquely defines a measure μ (and vice versa) by

$$\tilde{\mu}(f) = \int f d\mu. \tag{9.4}$$

As usual, the functional $\tilde{\mu}$ and the measure μ will be identified with each other, and we will omit the when no confusion arises. From the above, it is clear that μ is a probability measure, which is translation invariant because of the left invariance of the mean M. Moreover, it is easy to see that μ is ergodic: since Ω is minimal, the orbit of every $T \in \Omega$ under the action of \mathbb{R}^d lies densely in Ω , hence every translation invariant subset of Ω must lie densely in Ω , from which ergodicity follows. \Box

Note that μ can actually be seen as the frequency of the occurrence of a patch P in a tiling T: a subset $B(T, \epsilon) \subset \Omega$ consists of tilings with a certain patch P (or a small translate of it) covering the ball $B(0, \frac{1}{\epsilon})$ in \mathbb{R}^d . The larger the value of $\mu(B(T, \epsilon))$, the more often the patch P occurs, because of the translation invariance and the fact that $T + \mathbb{R}^d$ is dense in Ω .

Since μ is ergodic, we can apply the **Birkhoff ergodic theorem**, which can be stated as (see for example [41]):

Theorem 9.1.2 Let Ω be a compact space with a probability measure μ that is ergodic and invariant under the action T of an amenable group G on Ω . Then the left Haar measure λ on G can be normalized in such a way that for all $f \in C(\Omega)$, for μ -almost every $\omega \in \Omega$, we have

$$\int_{\Omega} d\mu(\omega') f(\omega') = \lim_{n \to \infty} \frac{1}{|\Lambda_n|} \int_{\Lambda_n} d\lambda(g) f(T_g \omega),$$

where (Λ_n) is a Følner sequence in G.

Applying this to our situation, we get for all $f \in C(\Omega)$:

$$\int f d\mu = \lim_{n \to \infty} \frac{1}{|\Lambda_n|} \int_{\Lambda_n} d^d x f(T - x),$$

for μ -almost all $T \in \Omega$. Since the same holds for any other ergodic translation invariant probability measure ν on Ω , we see that $\int f d\mu = \int f d\nu$ for all $f \in C(\Omega)$, and therefore, since Ω is a compact metric space, we have:

Proposition 9.1.3 The measure μ defined in (9.4) is the unique ergodic, translation invariant probability measure on Ω .

Next, we define a functional τ_{μ} on $C_c(\Omega \rtimes \mathbb{R}^d)$ by

$$\tau_{\mu}(f) := \int d\mu(T) f(T, 0),$$

which has the properties of a positive trace, i.e., $\tau_{\mu}(f * f^*) \geq 0$ and $\tau_{\mu}(f * g) = \tau_{\mu}(g * f)$, as follows from the translation invariance of μ . Note that τ_{μ} is not bounded, so it cannot be extended to a trace on $C^*(\Omega \rtimes \mathbb{R}^d)$. However, restricting τ_{μ} to the discrete case by noting [8] that the measure μ on Ω induces a (unique) ergodic translation invariant probability measure on Ω_{punc} , also denoted by μ , and recalling that $C^*(G_{punc})$ has a unit \mathbb{I} defined by $\mathbb{I}(T, x) := \delta_{0,x}$, we see that

 $\tau_{\mu}(\mathbb{I}) = 1$. So in the discrete case, the trace is normalized, and therefore, it can be extended to $C^*(G_{punc})$. In the same way, we can define a functional $\tilde{\tau}_{\mu}$ on $C_c(R_T)$ by

$$\tilde{\tau}_{\mu}(g) := \int d\mu(T)g(T,T),$$

and its discrete version extends to a trace on $C^*(R_{punc})$.

Recall that a functional ω on a C*-algebra is **faithful** when every positive $a \in A$ for which $\omega(a) = 0$ is equal to 0. We have the following easy proposition:

Proposition 9.1.4 τ_{μ} is faithful.

Proof: We have to show that if $\tau_{\mu}(f * f^*) = 0$ for some $f \in C_c(\Omega \rtimes \mathbb{R}^d)$, then $f \equiv 0$. Suppose that $\tau_{\mu}(f * f^*) = 0$. Then we get:

$$0 = \int (f * f^*)(T, 0) d\mu(T) = \int f(T, x) f^*(T - x, -x) d^d x d\mu(T)$$

= $\int |f(T, x)|^2 d^d x d\mu(T),$ (9.5)

from which the proposition follows.

Applying Birkhoff's ergodic theorem to $f \in C_c(\Omega \rtimes \mathbb{R}^d)$, we get [7]:

$$\tau_{\mu}(f) = \lim_{n \to \infty} \frac{1}{|\Lambda_n|} \int_{\Lambda_n} d^d x f(T - x, 0),$$

for μ -almost every T. By definition of π_T (8.5) and of the operator trace Tr, we can rewrite this as

$$\tau_{\mu}(f) = \lim_{n \to \infty} \frac{1}{|\Lambda_n|} Tr_{\Lambda_n}(\pi_T(f)), \qquad (9.6)$$

for μ -almost every T, where again Tr_{Λ_n} is the restriction of the operator trace on $L^2(\mathbb{R}^d)$ to $L^2(\Lambda_n)$. Thus, τ_{μ} can be seen as an operator trace per unit volume.

Remark 9.1.5 Note that in Chapter 6 the construction was the other way round: starting from a trace τ that arises in a natural way from the AF-property of the C*-algebra $C^*_{red}(R)$, a unique measure μ on the Cantor set K was constructed.

Note that the trace τ_{μ} defines a noncommutative integration on $C^*(\Omega \rtimes \mathbb{R}^d)$ [15, 8]. However, we will not elaborate on this, since only the noncommutative topological structure is of interest to us.

Next, we return to our case of a covariant family $\{H_T\}$ of Schrödinger operators affiliated to the C*-algebra $A_T = C^*(\Omega \rtimes \mathbb{R}^d)$. Observe that the spectral projection of H_T onto values below E, denoted by $\chi_{(-\infty,E]}(H_T)$, is a function of the operator H_T . **Lemma 9.1.6** $\chi_{(-\infty,E]}$ is continuous and bounded on $\sigma(H_T)$ if and only if $E \notin \sigma(H_T)$, i.e., if $E \in \mathfrak{g}$ for some gap \mathfrak{g} .

Proof: Obviously, $\chi_{(-\infty,E]}$ is bounded, since $0 \leq \chi_{(-\infty,E]}(x) \leq 1$ for all $x \in \mathbb{R}$. To show continuity, observe that $\chi_{(-\infty,E]}^{-1}(\{1\}) = \{x \in \mathbb{R} \mid x \leq E\}$ is always closed in $\sigma(H_T)$. However, if we look at the set

$$\chi_{(-\infty,E]}^{-1}(\{0\}) = \{x \in \mathbb{R} \mid x > E\},\$$

we see that it is closed in $\sigma(H_T)$ if and only if $E \notin \sigma(H_T)$, so $\chi_{(-\infty,E]}$ is continuous on $\sigma(H_T)$ if and only if $E \notin \sigma(H_T)$. \Box

It follows that if E does not lie in the spectrum of H_T , then $\chi_{-\infty,E]}(H_T)$ can be represented as $\pi_T(\chi_{H\leq E})$ for some element $\chi_{H\leq E} \in C^*(\Omega \rtimes \mathbb{R}^d)$, since H_T is affiliated to this C*-algebra (cf. Definition 8.2.9). $\chi_{H\leq E}$ is actually a projection in $C^*(\Omega \rtimes \mathbb{R}^d)$. Now for $f := \chi_{H\leq E}$, note that (9.6) becomes

$$\tau_{\mu}(\chi_{H \le E}) = \lim_{n \to \infty} \frac{1}{|\Lambda_n|} Tr_{\Lambda_n}(\chi_{(-\infty, E]}(H_T)), \qquad (9.7)$$

for μ -almost every T.

Definition 9.1.7 The covariant family $\{H_T\}$ affiliated to A_T) is said to satisfy **Shubin's formula** if for μ -almost all $T \in \Omega$, we have

$$N_T(E) = \tau_\mu \{ \chi_{H \le E} \}.$$
(9.8)

The common value is denoted by N(E). Shubin's formula was established in [8] for continuous Schrödinger operators. We will only prove it for the discrete case [7, 29].

Proposition 9.1.8 A covariant family $\{H_T\}$ of Schrödinger operators affiliated to $C^*(R_{punc})$ satisfies Shubin's formula (9.8).

Proof: Recall that in the discrete case H_T acts on the Hilbert space $\ell^2(T^{punc})$ by

$$H_T\psi(x) = \sum_{x'\in T^{punc}} H_T(x, x')\psi(x'),$$

where $H_T(x, x') \neq 0$ only for the punctures x' in a finite patch around x. Combining (9.3) with (9.7), we see that an operator H satisfies Shubin's formula if we have

$$\lim_{n \to \infty} \frac{1}{|\Lambda_n|} Tr_{\Lambda_n}(\chi_{(-\infty,E]}(H_{T,\Lambda_n}) - \chi_{(-\infty,E]}(H_T)) = 0,$$

for μ -almost all $T \in \Omega_{punc}$. In this case, $|\Lambda_n|$ denotes the number of punctures in the smallest patch $P_n \subset T$ that covers Λ_n . In what follows, we will always denote the smallest patch that covers $\Lambda \subset \mathbb{R}^d$ by P_{Λ} . In particular, P_{Λ}^{punc} will denote the set of punctures in $T^{punc} \cap \Lambda$.

Note that if E lies in a gap, $\chi_{(-\infty,E]}$ is continuous on the spectrum of H_T , so by the Stone-Weierstrass theorem (see for example [41]), it can be uniformly approximated by polynomials. By linearity of the trace, it follows that we have to show that

$$\lim_{n \to \infty} \frac{1}{|\Lambda_n|} Tr(\chi_{\Lambda_n} H_T^k - (\chi_{\Lambda_n} H_T)^k) = 0, \qquad (9.9)$$

for all k and for μ -almost every $T \in \Omega_{punc}$, where χ_{Λ_n} is the characteristic function of Λ_n . Note that we have replaced $Tr_{\Lambda_n}(\cdot)$ by $Tr(\chi_{\Lambda_n} \cdot)$, which is of course the same. Omitting subscripts n and T when they are not necessary, we have

$$\chi_{\Lambda}H^{k} - (\chi_{\Lambda}H)^{k} = \chi_{\Lambda}H(1-\chi_{\Lambda})H^{k-1} + \chi_{\Lambda}H(\chi_{\Lambda}H^{k-1} - (\chi_{Lambda}H)^{k-1}),$$

and applying the same to the second part of the right hand side repeatedly, we finally get

$$\chi_{\Lambda}H^{k} - (\chi_{\Lambda}H)^{k} = \sum_{j=1}^{k-1} (\chi_{\Lambda}H)^{j} (1-\chi_{\Lambda})H^{k-j}.$$

Since we have

$$\frac{1}{|\Lambda|} |Tr((\chi_{\Lambda}H)^{j}(1-\chi_{\Lambda})H^{k-j})| \leq \frac{1}{|\Lambda|} Tr(\chi_{\Lambda}) ||H(\chi_{\Lambda}H)^{k-1}(1-\chi_{\Lambda})H^{k-j}|| \leq ||H||^{k},$$

it follows that the map $H \mapsto \lim_{n\to\infty} \frac{1}{|\Lambda_n|} Tr(\chi_{\Lambda_n} H^k - (\chi_{\Lambda_n} H)^k)$ is continuous, which means that H_T can be approximated by $\pi_T(h)$, with $h \in C_c(R_{punc})$. So we may assume that H_T is the image under π_T of some $h \in C_c(R_{punc})$. Since hhas compact support, the constant C defined by

$$C := \max_{x \in T^{punc}} \sharp \{ x' \in T^{punc} \mid H_T(x, x') \neq 0 \}$$

is finite. Then we get

$$\begin{aligned} Tr\left((\chi_{\Lambda}H_{T})^{j}(1-\chi_{\Lambda})H_{T}^{k-j}\right) &\leq C \Big| \sum_{x \in P_{\Lambda}^{punc}} \sum_{x' \in P_{\mathbb{R}^{d} \setminus \Lambda}^{punc}} H_{T}^{j}(x,x')H_{T}^{k-j}(x',x) \Big| \\ &\leq C^{2} |\partial\Lambda| \max_{x,x' \in T^{punc}} |H_{T}^{j}(x,x')| |H_{T}^{k-j}(x',x)|, \end{aligned}$$

for μ -almost all T, where $|\partial \Lambda|$ denotes the number of tiles that lie on the boundary $\partial \Lambda = \Lambda \cap \mathbb{R}^d / \Lambda$ of Λ . Note that if necessary we could actually get a tighter bound. Finally, we get for μ -almost every T:

$$\left| \lim_{n \to \infty} \frac{1}{|\Lambda_n|} Tr(\chi_{\Lambda_n} H_T^k - (\chi_{\Lambda_n} H_T)^k) \right|$$

$$\leq \lim_{n \to \infty} \frac{|\partial \Lambda_n|}{|\Lambda_n|} C^2 \sum_{j=1}^{k-1} \max_{x, x' \in T^{punc}} |H_T^j(x, x')| |H_T^{k-j}(x', x)|$$

$$= 0,$$

which follows from the fact that $\{\Lambda_n\}$ is a Følner sequence (since this means that $\lim_{n\to\infty} \frac{\partial \Lambda_n}{|\Lambda_n|}$). Thus, we have proven (9.9). \Box

9.2 K-theoretic gap labelling

Shubin's formula implies that

$$\sigma(H_T) = \sigma(H)$$
 for μ - almost all $T \in \Omega$,

since the spectrum of H can be seen as the set of "growing points" of N(E), i.e.,

$$\sigma(H) = \{ E \in \mathbb{R} \mid N(E+\epsilon) - N(E-\epsilon) \neq 0 \ \forall \epsilon > 0 \}.$$

This claim follows from the fact that, by faithfulness of τ_{μ} ,

$$\tau_{\mu} \left(\chi(H \le E + \epsilon) - \chi(H \le E - \epsilon) \right) > 0$$

if and only if the spectral projections $\chi(H \leq E + \epsilon)$ and $\chi(H \leq E - \epsilon)$ are different from each other, which is the case if and only if $E \in \sigma(H)$. Thus we see that the IDS completely determines the spectrum. By unitary invariance of the spectrum, we already had

$$\sigma(H_T) = \sigma(H_{T+x})$$

for every $x \in \mathbb{R}^d$, from which it followed that $\sigma(H_T)$ and N_T are constant on a dense subset $T + \mathbb{R}^d$ of Ω . Using the fact that the metric structure, the topology and the measurable sets are, by construction, all compatible with each other, we have

$$\mu\{T' \in \Omega \mid d(T, T') = 1\} = 0.$$

Figure 9.1: The integrated density of states is constant on gaps in the spectrum

Since the IDS is constant on gaps \mathfrak{g} in the spectrum (see Figure 9.1), the value of the IDS on gaps can serve as a labelling of these gaps. Combining this with Shubin's formula and the fact that $\chi_{H\leq E}$ is a projection in A_{punc} (or in A_T in the continuous case), it follows that the set of gap labels is a subset of $\tau_{\mu}(P_1(A_{punc}))$, where $P_1(A_{punc})$ denotes the set of projections in $A_{punc} = C^*(R_{punc})$. Of course, different values of E in a gap \mathfrak{g} give the same value of the IDS, and this is mathematically unsatisfactory. However, we can associate a projection $P(\mathfrak{g})$ to a gap by putting

$$P(\mathfrak{g}) := \chi_{H \leq E}$$
 for some $E \in \mathfrak{g}$.

j

Now the important thing is that a trace is invariant under unitary transformations, which follows directly from the fact that $\tau_{\mu}(ab) = \tau_{\mu}(ba)$. Thus, τ_{μ} induces a trace $\tau_{\mu*}$ on the set of equivalence classes of projections under unitary transformations. This set is of course just the K_0 -group of $C^*(R_{punc})$, so we have a more canonical form of Shubin's formula on gaps, which can be stated as

$$N(\mathfrak{g}) = \tau_{\mu*}[P(\mathfrak{g})].$$

In particular, using the fact that A_{punc} is separable, and using $\tau_{\mu}(\mathbb{I}) = 1$, where \mathbb{I} is the unit in A_{punc} , and noting that for the gaps at $-\infty$ and $+\infty$ we have $[P(\mathfrak{g}_{-\infty})] = [0]$ and $[P(\mathfrak{g}_{\infty}] = [\mathbb{I}]$, respectively, we can state:

Proposition 9.2.1 The IDS on gaps takes values in $\tau_{\mu*}(K_0(A_{punc})) \cap [0, 1]$, which is a countable subset of \mathbb{R} . \Box

Since $\tau_{\mu*}$ transfers the order of the ordered K_0 -group to the natural order on \mathbb{R} , we see in particular that if $\mathfrak{g}_1 < \mathfrak{g}_2$, then $N(\mathfrak{g}_1) < N(\mathfrak{g}_2)$, just as required.

In the continuous case, things are more complicated, because $C^*(R_T)$ has no unit. However, recall that in a non-unital C*-algebra A, unitary equivalence of projections can be replaced by Murray-von Neumann equivalence, i.e.

$$p \stackrel{MvN}{\sim} q \Leftrightarrow \exists v \in A: \ p = v^*v, \ q = vv^*.$$

The K_0 -group of A is then defined as the kernel of the projection of the K_0 -group of the unitization of A onto $K_0(\mathbb{C})$, i.e.

$$K_0(A) := Ker(K_0(\pi)),$$

where $\pi : \tilde{A} \to \mathbb{C} \cong \tilde{A}/A$ is the obvious projection, and $K_0(\pi)$ is the induced map. For more details, see Section 5.2. Actually, since the K_0 -groups of A_T and A_{punc} are isomorphic by Corollary 8.3.9, we have

Proposition 9.2.2 $\tau_{\mu*}(K_0(A_T)) \simeq \tau_{\mu*}(K_0(A_{punc})).$

So the tight binding approximation does not affect the gap labelling, and in particular, we can compute the gap labels using discrete models, which are often simpler than their continuous counterparts. Summarizing, we have (see e.g. [9]):

Theorem 9.2.3 Let $\{H_T\}$ be a covariant family of Schrödinger operators affiliated to A_T (or A_{punc} , in the tight binding approximation). Then we have the following:

 For μ-almost all T, the value of the IDS on gaps g in the spectrum of H_T is given by

$$N(\mathfrak{g}) = \tau_{\mu*}[P(\mathfrak{g})],$$

where $P(\mathfrak{g})$ is the spectral projection onto energies smaller than E, with $E \in \mathfrak{g}$.

2. $N(\mathfrak{g}) \in \tau_{\mu*}(K_0(A_T)) \cap [0,1]$ gives a labelling of the gaps in the spectrum, which is invariant under norm-continuous perturbations, as long as the gaps do not close.

Proof: The first item is clear from the above. The fact that the gap labelling is invariant under norm perturbations, follows from the fact that if two projections p and q obey ||p - q|| < 1, they belong to the same equivalence class, cf. Proposition 5.2.2. Conversely, if two projections are Murray-von Neumann equivalent, they are homotopic in $P_{\infty}(A_T)$, i.e. there exists a norm-continuous path of projections between them, cf. Corollary 5.2.4.

A few remarks are in order. First of all, if we would purely be interested in labelling the gaps in the spectrum of H, we wouldn't need the trace τ_{μ} , because the elements of $K_0(A_{punc})$ can already serve as gap labels. However, Shubin's formula gives a physical interpretation to the gap labels in $\tau_{\mu*}(K_0(A_{punc}))$ as the value of the integrated density of states on the gaps.

Secondly, it should be noted that computing the K_0 -group of our C*-algebra and its trace does not automatically yield the set of gap labels; if we denote the set of gap labels of H by gap(H), in general, $\tau_{\mu*}(K_0(A_{punc}))$ will be larger than gap(H). This is due to the fact that not all projections in A_{punc} are necessarily spectral projections of H. In particular, we cannot use the additivity rules of the K_0 -group to say that if $N(\mathfrak{g}_1)$ and $N(\mathfrak{g}_2)$ are the values of the IDS on the gaps \mathfrak{g}_1 and \mathfrak{g}_2 respectively, that there is a third gap $\mathfrak{g}_3 \in \text{gap}(H)$ such that

$$N(\mathfrak{g}_3) = N(\mathfrak{g}_1) + N(\mathfrak{g}_2).$$

However, we can use the knowledge about the set of possible gap labels to derive qualitative results on the spectrum of the Hamiltonian, for example whether it is singular continuous or absolutely continuous. In this way, we can derive electronic properties of quasicrystals, for instance whether it is a good or a bad conductor (in general, singular continuous spectrum leads to lower conductivity than absolute continuous (band) spectrum). The fact that in general $\tau_{\mu*}(K_0(A_{punc}))$ may be larger than the set of gap labels, can be rephrased by saying that "not all gaps may be open", so we have

Definition 9.2.4 We say that all gaps are open if

$$\tau_{\mu*}(K_0(A_{punc})) \cap [0,1] = \operatorname{gap}(H).$$

In the next section, we will investigate a one-dimensional example of a quasiperiodic Hamiltonian for which it has been conjectured that indeed all gaps are open. To conclude this section, let us make a few remarks about the actual computation of the K-groups. Useful tools to compute the K-groups are Bott periodicity, the Connes-Thom isomorphism and the Pimsner-Voiculescu exact sequence (see for instance [9, 13]). Another useful tool is the following gap labelling theorem, a proof of which can be found in [10]:

Theorem 9.2.5 Denote the functional associated to the measure μ via Riesz' representation theorem by $\tilde{\mu}$, and let $C(\Omega_{punc}, \mathbb{Z})$ denote the continuous integer-valued functions on Ω_{punc} . Then we have:

$$\tau_{\mu*}(K_0(A_{punc})) = \tilde{\mu}(C(\Omega_{punc}, \mathbb{Z}))$$

We will only indicate why $\tilde{\mu}(C(\Omega_{punc}))$ is a subset of $\tau_{\mu*}(K_0(A_{punc}))$, referring to [10] for the converse inclusion, which is more difficult. Recall that the subalgebra of A_{punc} generated by the position operators e[P, t, t] is isomorphic to $C(\Omega_{punc})$. Now, any $f \in C(\Omega_{punc}, \mathbb{Z})$ can be written as $f = \sum_i n_i \chi_i$, where $n_i \in \mathbb{Z}$ and $\chi_i = e[P, t_i, t_i]$ is the characteristic function of the open and closed subset $U(P_i, t_i)$ of Ω_{punc} . Identifying Ω_{punc} with the diagonal in R_{punc} , we have

$$\tilde{\mu}(f) = \int f d\mu = \sum_{i} n_i \tau_{\mu}(\chi_i) = \sum_{i} n_i \tau_{\mu*}[\chi_i].$$

Thus, the inclusion of $C(\Omega_{punc})$ into A_{punc} yields the inclusion

$$\tilde{\mu}(C(\Omega_{punc},\mathbb{Z})) \subseteq \tau_{\mu*}(K_0(A_{punc})).$$

For the converse inclusion, we refer to [10, 12].

Since μ can be seen as a measure for the frequency of occurrence of patches P in a tiling, the above theorem states that the set of possible gap labels is uniquely determined by these frequencies.

9.3 An example: the Almost Mathieu operator

A well-known example of a quasiperiodic discrete Hamiltonian in one dimension is the **Almost Mathieu operator** (abbreviated AM-operator) $H_{\alpha,\theta,\lambda}$, defined on $\ell^2(\mathbb{Z})$ by

$$H_{\alpha,\theta,\lambda}\psi(n) := \psi(n+1) + \psi(n-1) + 2\lambda\cos(2\pi\alpha n + \theta)\psi(n), \qquad (9.10)$$

where $n \in \mathbb{Z}$, $\psi \in \ell^2(\mathbb{Z})$ and α , θ and λ are real parameters. This model has been extensively studied (see [20, 27, 36, 39, 50] and many others). It is clear that for $\alpha \in \mathbb{Q}$, say $\alpha = \frac{p}{q}$ (with p and q relative prime), the potential

$$V(n) = 2\lambda \cos(2\pi \frac{p}{q}n + \theta),$$

is periodic with period q. Therefore, the spectrum of $H_{\alpha,\theta,\lambda}$ is absolutely continuous for all $\alpha \in \mathbb{Q}$, exhibiting the well-known band structure, with decreasing bandwidth for increasing q. However, for $\alpha \notin \mathbb{Q}$, (9.10) can serve as a model for electronic motion in a one dimensional quasicrystal. For example, if $\alpha = \tau := \frac{1+\sqrt{5}}{2}$, (9.10) describes the motion of an electron on a Fibonacci chain. Although the model looks very simple, it is still not totally clear what the nature of the spectrum of $H_{\alpha,\theta,\lambda}$ is for irrational α . During a talk in 1981, M. Kac offered ten Martini drinks to anybody who could prove or disprove that the AM-operator has Cantor-like spectrum (possibly with positive Lebesgue measure) for all irrational α . Nowadays, this is called the Ten Martini Problem. In fact, B. Simon conjectured a stronger version (the Strong (or Dry) Ten Martini Problem), which stated that "all gaps are open" (see [50, 51, 52] for reviews). This can be reformulated as follows, using the "irrational rotation algebra" A_{α} to which $H_{\alpha,\theta,\lambda}$ is affiliated:

Conjecture 9.3.1 For $\alpha \notin \mathbb{Q}$, we have:

$$gap(H_{\alpha,\theta,\lambda}) = \tau_*(K_0(A_\alpha)).$$

This conjecture has actually been proved for various values of α and λ . In this section, we will review some important results concerning the spectrum of the AM-operator.

Let us first define the C^{*}-algebra $H_{\alpha,\theta,\lambda}$ is affiliated to. For any α , we can define the **rotation algebra** A_{α} (see e.g. [14, 15, 21]) as the C^{*}-algebra generated by a unit I and two elements u, v in the following way: let u and v be subject to the commutation relation

$$uv = e^{2\pi i\alpha}vu.$$

Considering the algebra P_{α} of all Laurent polynomials in u and v, with unique involution * such that $u^* = u^{-1}$ and $v^* = v^{-1}$, we can define representations π as *-homomorphisms from P_{α} to $\mathcal{B}(\mathcal{H})$, and define (as usual) a norm on P_{α} by

$$||p|| := \sup ||\pi(p)||,$$

where $p \in P_{\alpha}$. Then the completion of P_{α} in this norm is a C*-algebra, and this will be our Rotation Algebra A_{α} .

Next, we will make contact to our general formulation in terms of the noncommutative C*-algebra of the hull, showing that this C*-algebra is isomorphic to the above defined rotation algebra A_{α} . Note that in our present case, the hull is S^1 : indeed, for fixed $\lambda \neq 0$ and α , we can view the set of possible θ 's as the hull, and by periodicity of the cosine in (9.10), θ can be limited to the interval $[0, 2\pi)$, with periodic boundary conditions, which is just the circle S^1 or \mathbb{T} . We define an action $\tilde{\alpha}$ of \mathbb{Z} on our hull S^1 by

$$\tilde{\alpha}_m(\theta) := 2\pi\alpha m + \theta.$$

Note that $\tilde{\alpha}$ can be seen as a rotation operator. Then with this action, $S^1 \rtimes_{\alpha} \mathbb{Z}$ is a transformation groupoid, with product and inverse given by

$$(\theta, m)(\tilde{\alpha}_m(\theta), n) = (\theta, m+n); \qquad (\theta, m)^{-1} = (\tilde{\alpha}_m(\theta), -m),$$

and we can form the C*-algebra $C^*(S^1 \rtimes_{\alpha} \mathbb{Z})$ in the usual way. Now if we define $\tilde{u}, \tilde{v} \in C^*(S^1 \rtimes_{\alpha} \mathbb{Z})$ by

$$\tilde{u}(\theta,m) := \delta_{m,1}; \qquad \tilde{v}(\theta,m) := e^{i(\pi\alpha m + \theta)},$$

we see that this is consistent with the involution. Moreover, a simple computation shows that

$$\tilde{u} * \tilde{v} = e^{2\pi i\alpha} \tilde{v} * \tilde{u},$$

where * denotes the convolution product, and one can show [21] that these elements actually generate $C^*(S^1 \rtimes_{\alpha} \mathbb{Z})$, so that we can identify $C^*(S^1 \rtimes_{\alpha} \mathbb{Z})$ with A_{α} . Of course, if we define an equivalence relation R_{α} by

$$R_{\alpha} := \{ (\theta, \theta') \mid \exists n \in \mathbb{Z} : \theta' = \alpha_n(\theta) \},\$$

the resulting C*-algebra $C^*(R_\alpha)$ is isomorphic to A_α as well. It is easy to see that $C^*(S^1 \rtimes_\alpha \mathbb{Z})$ is simple if and only if the action of $\tilde{\alpha}$ is minimal, which is the case if and only if α is irrational. On the other hand, if $\alpha = p/q$ is rational, the C*-algebra $A_{p/q}$ is isomorphic to $C(\mathbb{T}^2) \otimes M_q(\mathbb{C})$ and has center $C(\mathbb{T}^2)$, where \mathbb{T}^2 denotes the 2-torus [21].

Now, define for all $\theta \in S^1$ the operators U and V_{θ} on $\ell^2(\mathbb{Z})$ by

$$U\psi(n) := \psi(n+1); \quad V_{\theta}\psi(n) := e^{i(2\pi\alpha n + \theta)}\psi(n).$$

Then a simple computation, using $\cos x = \frac{1}{2}(e^{ix} + e^{-ix})$, shows that the AM operator can be written as

$$H_{\alpha,\theta,\lambda} = U + U^* + \lambda (V_\theta + V_\theta^*).$$

Now note that A_{α} can be represented on $\ell^2(\mathbb{Z})$ by defining representations π_{θ} , such that $\pi_{\theta}(u) = U$ and $\pi_{\theta}(v) = V_{\theta}$ for all $\theta \in S^1$. We actually have

$$\pi_{\theta}(uv)\psi(n) = UV_{\theta}\psi(n) = V\psi(n+1) = e^{i(2\pi\alpha(n+1)+\theta)}\psi(n+1) = e^{i(2\pi\alpha(n+1)+\theta)}U\psi(n) = e^{2\pi i\alpha}V_{\theta}U\psi(n) = e^{2\pi i\alpha}\pi_{\theta}(vu)\psi(n),$$

so every π_{θ} is well defined, and it can easily be extended to a *-homomorphism from A_{α} to $\mathcal{B}(\ell^2(\mathbb{Z}))$. Note that since the Almost Mathieu operator $H_{\alpha,\theta,\lambda}$ is a linear combination of U, U^*, V_{θ} and V^*_{θ} , it is affiliated to A_{α} .

In the irrational case, all representations π_{θ} are faithful and hence isometric, so that the spectrum of $H_{\alpha,\theta,\lambda}$ is equal to the spectrum of the element $h_{\lambda} \in A_{\alpha}$, defined by

$$h_{\lambda} := u + u^* + \lambda(v + v^*).$$

A straightforward computation shows that the representation π_{θ} of A_{θ} on $\ell^2(\mathbb{Z})$ is precisely the reduced representation of $C^*(S^1 \rtimes_{\alpha} \mathbb{Z})$, where we have identified each fiber $R^{-1}(\theta)$ of the groupoid $S^1 \rtimes_{\alpha} \mathbb{Z}$ with \mathbb{Z} , as usual. For α and λ fixed, we can explicitly check the covariance condition for $H_{\theta} := H_{\alpha,\theta,\lambda}$, yielding

$$T(n)H_{\theta}T(n)^{-1} = H_{2\pi\alpha n+\theta} = H_{\alpha_n(\theta)}$$

as expected, and likewise for the reduced representations π_{θ} .

Since the covariant family $\{H_{\theta}\}_{\theta \in S^1}$ is affiliated to the irrational rotation algebra $A_{\alpha} \simeq C^*(S^1 \rtimes_{\alpha} \mathbb{Z})$, by Proposition 9.2.1 we have

$$gap(H_{\alpha,\theta,\lambda}) \subseteq \tau_*(K_0(A_\alpha)), \tag{9.11}$$

where τ_* comes from the trace τ on A_{α} , uniquely defined by its value on monomials $u^k v^l$ in the following way: note that since we require $\tau(ab) = \tau(ba)$ for all $a, b \in A_{\alpha}$, we must have

$$\tau(u^k v^l) = 0.$$

for all $k, l \in \mathbb{Z}$, if k and l are not equal to 0. With $\tau(\mathbb{I}) = 1$, we get for any element $\sum_{k,l} a_{kl} u^k v^l \in P_{\alpha}$, where $a_{kl} \in \mathbb{C}$ for every $k, l \in \mathbb{Z}$:

$$\tau(\sum_{k,l} a_{kl} u^k v^l) = a_{00}.$$

Actually, the normalized Lebesgue measure plays the role of the unique ergodic translation invariant probability measure on S^1 , and τ can be related to this measure in the same way as usual [21]. Now the main question (Conjecture 9.3.1) is whether the inclusion in (9.11) can be replaced by an equality. But first, let us compute $\tau_*(K_0(A_\alpha))$.

Proposition 9.3.2 For $\alpha \notin \mathbb{Q}$, there is an isomorphism between $\tau_*(K_0(A_\alpha))$ and $(\mathbb{Z} + \alpha \mathbb{Z}) \cap [0, 1]$.

Sketch of the proof: [21] First, observe that we may take $0 < \alpha < 1$. Secondly, observe that for any nonzero $m \in \mathbb{Z}$, the C*-algebra generated by u^m and v is a subalgebra of A_{α} that is isomorphic to $A_{m\alpha}$, due to the commutation relation

$$vu^m = e^{2\pi i m\alpha} u^m v.$$

One can define a **Rieffel projection** $p \in A_{\alpha}$ by [45]

$$p := hv^{-1} + f + gv,$$

where $f, g, h \in C(S^1)$. The condition $p = p^* = p^2$ imposes certain conditions on f, g and h, and one can show that $\tau(p) = \alpha$ [21, 45]. Likewise, one can show that the trace of the Rieffel projection $p_m \in A_{m\alpha}$ is given by $\tau(p_m) = \{m\alpha\}$, where $\{\cdot\}$ denotes the fractional part. Since $A_{m\alpha} \subseteq A_{\alpha}$ for every nonzero $m \in \mathbb{Z}$, and

since $\tau(0) = 0$ and $\tau(\mathbb{I}) = 1$, we see that $(\mathbb{Z} + \alpha \mathbb{Z}) \cap [0, 1]$ is contained in the range of τ on the projections in A_{α} . Hence, we have the inclusion

$$(\mathbb{Z} + \alpha \mathbb{Z}) \cap [0, 1] \subseteq \tau_*(K_0(A_\alpha))$$

To obtain the converse inclusion, we embed A_{α} into an AF-algebra B_{α} in the following way: recall that every irrational number $\alpha > 0$ has a continued fraction expansion

$$\alpha = r_0 + \frac{1}{r_1 + \frac{1}{r_2 + \frac{1}{r_3 + \dots}}},$$

where $r_i \in \mathbb{N}$, or alternatively, $\alpha = \lim_{m \to \infty} \frac{p_m}{q_m}$, where

$$\frac{p_m}{q_m} = r_0 + \frac{1}{r_1 + \frac{1}{\ddots + \frac{1}{r_m}}}$$

Note that if $r_m = 1$ for all m, α is equal to the golden number τ . In general, p_m and q_m can be shown to obey the recurrence relations

$$p_m = r_m p_{m-1} + p_{m-2}; \quad q_m = r_m q_{m-1} + q_{m-2},$$

with initial conditions $p_0 = r_0$, $q_0 = 1$, $p_1 = r_1r_0 + 1$ and $q_1 = r_1$. In this way we obtain an increasing sequence of finite-dimensional C*-algebras $\{(B_m, \varphi_m)\}$ defined by

$$B_m := M_{q_m}(\mathbb{C}) \oplus M_{q_{m-1}}(\mathbb{C}),$$
$$\varphi_m : B_{m-1} \to B_m; \quad a \oplus b \mapsto w_m (a \oplus \dots \oplus a \oplus b) w_m^* \oplus a,$$

where $(a \oplus \cdots \oplus a)$ denotes r_m copies of $a \in M_{q_m}(\mathbb{C})$, and $w_m \in M_{q_m}(\mathbb{C})$ is a suitable unitary matrix. Then B_{α} is defined as the inductive limit of the B_m 's. It can be shown that in each $M_{q_m}(\mathbb{C})$, there are matrices R_m and S_m for which

$$R_m S_m = e^{2\pi i p_m/q_m} S_m R_m$$

Next, define $v_m := R_m \oplus R_{m-1}$ and $u_m := S_m \oplus S_{m-1}$. Then one can show that the unitary matrices w_m can be chosen in such a way that the limits v and u of v_m and u_m respectively, obey

$$vu = \lim_{m \to \infty} e^{2\pi i p_m/q_m} uv = e^{2\pi i \alpha} uv,$$

so that the C*-subalgebra of B_{α} generated by u and v is isomorphic to A_{α} [21]. The construction of the AF-algebra B_{α} is a generalization of the construction of the C*-algebra of Penrose tilings $C^*_{red}(R)$ in Chapter 6, where $\alpha = \tau := \frac{1+\sqrt{5}}{2}$, and $r_m = 1$ for every m. Likewise, the image of the induced trace τ_* on $K_0(B_{\alpha})$ is $(\mathbb{Z} + \alpha \mathbb{Z}) \cap [0, 1]$ (cf. Proposition 6.4.1), which proves the converse inclusion. This concludes the proof. \Box **Corollary 9.3.3** For $\alpha \notin \mathbb{Q}$ and $\lambda \neq 0$, the IDS on gaps in the spectrum of the AM-operator $H_{\theta} := H_{\alpha,\theta,\lambda}$ takes values in

$$(\mathbb{Z} + \alpha \mathbb{Z}) \cap [0, 1],$$

for almost all $\theta \in S^1$.

Note that if $gap(H_{\theta})$ is in fact equal to $(\mathbb{Z} + \alpha \mathbb{Z}) \cap [0, 1]$ (that is, all gaps are open), the spectrum is Cantor-like; in particular, it is nowhere dense and it has no isolated points. Thus, the statement that all gaps are open automatically implies the fact that the spectrum is Cantor-like, and is therefore a stronger statement than the Ten Martini Problem, justifying the name "Strong Ten Martini Problem".

Now let's give some known results about the nature of the spectrum of the AM-operator for various values of λ (see e.g. [20, 27, 51]). Since most proofs use methods different from our K-theoretic approach (for example Lyapunov exponents and Aubry-André duality), we will not discuss these proofs. For Lebesgue-almost every α and θ , we have

- 1. If $|\lambda| < 1$ the spectrum of $H_{\alpha,\theta,\lambda}$ is purely absolutely continuous.
- 2. If $|\lambda| = 1$, the spectrum is purely singular continuous.
- 3. If $|\lambda| > 1$, the spectrum is pure point.

These results were obtained during the last two decades. In most cases, "almost every α " means that α satisfies a so-called **Diophantine equation**, which means there exist constants c, r > 0 such that for all $n \neq 0$,

$$|\sin(2\pi n\alpha)| > \frac{c}{|n|^r}.$$

Note that by increasing the coupling constant λ , one observes a transition from absolutely continuous spectrum ($|\lambda| < 1$ via singular continuous spectrum ($\lambda = 1$) to pure point spectrum ($\lambda > 1$). Now recall that a.c. spectrum corresponds to extended wave functions, whereas p.p. spectrum corresponds to localized wave functions, with s.c. spectrum in between, with critical wave functions (i.e., neither extended nor exponentially localized). Therefore, we see that increasing the potential (via the coupling constant λ) gives a transition where extended electronic wave functions become localized. This transition can be seen as a metal-insulator transition [27].

The latest result on the question whether the spectrum is Cantor-like (possibly with positive Lebesgue measure) has been obtained by Puig [39]. He showed that for Diophantine α , the spectrum is Cantor-like for $|\lambda| \neq 0, 1$. This solves the Ten Martini Problem for almost every α . Moreover, he showed that for α

Diophantine, all spectral gaps are open for small enough and large enough λ , solving the Strong Ten Martini Problem (Conjecture 9.3.1) for these values.

We conclude this section with some remarks. First of all, it should be noted that although the AM-operator describes a simple one-dimensional quasiperiodic model, it is already very difficult to obtain exact results about its spectrum. However, this model shows that singular continuous spectrum may in fact appear in physical situations. Moreover, it gives a hint that Cantor-like spectrum might be generic for quasiperiodic Hamiltonians. This is in agreement with numerical computations on periodic approximants of quasiperiodic tilings, showing a "spiky" density of states (cf. Section 7.3). However, these spikes have so far not been observed in experiments [54], and it may well be possible that the spikiness of the density of states is limited to 1- and 2-dimensional systems. Moreover, the spikiness observed in numerical computations could be an artifact of certain assumptions [58, 57]. To the best knowledge of the author, this is still an open problem.

Secondly, note that in order to determine whether indeed all elements of the countable set $\tau_*(K_0(A_\alpha))$ serve as gap labels, other methods than K-theoretic or operator-algebraic ones are necessary. It appears that it is not possible to determine which elements actually serve as gap labels using only the K-theoretic data. However, Shubin has derived an operator-algebraic condition for all gaps to be open for the AM-operator [50]. It remains an open question whether a similar condition can be formulated for general quasiperiodic Schrödinger operators.

Chapter 10

Conclusion

In this thesis, we have described quasicrystals, which form a new state of longrange order between periodic crystals and amorphous metals. Since Bloch theory does not apply to aperiodic media, a different approach has to be found to handle electronic motion in quasicrystals. Following the work of Bellissard, Connes, Kellendonk and others, we have used K-theory to obtain results about the spectrum of quasiperiodic one-electron Hamiltonians.

To this end, we have generalized ordinary topology to a noncommutative version of it, using C*-algebras as a basic tool. Noncommutative topology turned out to be useful in describing non-Hausdorff spaces, and the groupoid C*-algebra of equivalence relations was introduced for this purpose. We have shown that Ktheory, consisting of abelian groups K_0 and K_1 , is a good topological invariant to characterize non-Hausdorff spaces, and we have indicated why other invariants have been abandoned.

We have reviewed an illuminating example of a non-Hausdorff space constructed by Connes, namely the space of Penrose tilings, and in an analogous way, the noncommutative C*-algebra of the hull, which is basically the space of all translates of a certain tiling, was obtained, following the work of Kellendonk. We have shown that for a (quasi-)crystal that is modeled by this tiling, the C*algebra of the hull can be seen as the C*-algebra of observables, both in the continuous and in the discrete case. Surprisingly, we saw that although this C*-algebra does not depend on the precise shape of the potential, but only on the (quasi-)periodicity of the tiling, it can nevertheless be used to obtain results about the spectrum of the Hamiltonian. For this purpose, the K-theory of the C*-algebra of observables was used to obtain a set of possible labels of the gaps in the spectrum, namely the K_0 -group, and via Shubin's formula, the values of a trace on this K_0 -group were shown to be equal to the values of the integrated density of states on the gaps. An important problem is that the K_0 -group is in general larger than the set of actual gaps, and it remains unclear how one can show which elements actually serve as gap labels. In particular, we cannot use the group laws of the K_0 -group to obtain additivity properties of gap labels. Possibly, more information about the precise form of the potential is needed to derive which elements of the K_0 -group are actual gap labels, but this is still an open problem. Therefore, it remains unclear whether the K-theoretic gap labelling may be used in the future to obtain quantitative results about the spectrum of quasiperiodic Hamiltonians. However, the gap labelling can in fact be used to obtain qualitative results about the nature of the spectrum, for example whether it is absolutely continuous, singular continuous or pure point.

We have studied the one-dimensional example of the Almost Mathieu operator, and we have seen that for almost all values of the parameters, the spectrum is Cantor-like. The coupling constant λ appears to be the decisive parameter for the spectrum to be absolutely continuous, singular continuous or pure point. The appearance of purely singular continuous spectrum is an important example of the fact that s.c. spectrum can in fact be physical, in contrast to what people believed until the eighties.

The Cantor-like nature of the spectrum of the AM-operator has lead people to conjecture that Cantor-like spectrum might be generic for quasiperiodic Hamiltonians. This is also supported by numerical computations for periodic approximants of quasiperiodic tilings, showing a very spiky density of states. However, as far as the author knows, this spikiness has not (yet) been observed in experiments. To solve these matters is still an open question.

In conclusion, the K-theoretic gap labelling may serve as a solid theoretical basis for the description of electronic transport properties of quasicrystals, and noncommutative topology may be used as a building block to generalize Bloch theory from periodic media to aperiodic media. However, it is unclear whether this formulation may be used in the future to obtain any quantitative results.

Chapter 11

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