Hull of Aperiodic Solids and Gap Labelling Theorems

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ABSTRACT. We review the basic constructions liable to replace Bloch theory for aperiodic solids. Point sets describing atomic positions lead to the notion of hull, a topological dynamical system with action of the translation group. We establish that quantities like the hull, the diffraction measure or the electronic density of states are uniquely determined by the Gibbs state describing thermal equilibrium of the solid. We recall the construction of the corresponding non-commutative Brillouin zone for electrons or phonons. We describe its topology through its algebraic K-theory. The gap labelling theory is reviewed and completed by a general conjecture for the case of transversally totally discontinuous hull and by results obtained for two-dimensional media.

Introduction[1]

In 1981, J. Moser [**Mos**], exhibited the first example of a Schrödinger operator with nowhere dense spectrum. Soon after his preprint appeared, several other examples were found (see [**Sim82, Bel82, Bel86, Bel89, Bel93**] for reviews). It was realized at the same time that there was a need for a labelling of the gaps which was robust (namely stable under suitable perturbations of the Hamiltonian) and natural enough from both a mathematical and a physical point of view. Two results were announced in 1981 and published in 1982 in this direction: Johnson & Moser [**JoMo**] showed that for a Schrödinger equation with almost periodic potential, the set of gap labels was the so-called *frequency module*, whereas one of us realized the connection with the K-theory of C^*-algebras [**Bel82**]. In order to show that it was really the K-group that mattered instead of the frequency module, a counter-example was designed [**BS**]. For a long time, all examples of Hamiltonians with nowhere dense spectra were given by ordinary differential equations (ODE) with almost periodic coefficients or discretized version of them. It was not until 1988 that another class of potentials leading to nowhere dense spectra was found, namely potentials generated by *automatic sequences* [**Bel90**] (see also [**Su90**]). In 1989, an example in higher dimension was produced in connection with spectral properties of quasicrystals (QC) [**Sir90**]. However, due to the *Bethe-Sommerfeld conjecture* [**DaTr, Skri, HeMo, Kar**], Schrödinger operators in higher dimension should have no gaps at high energy. For compounds with metallic behaviour, no gaps should occur near the Fermi level, so that the gap labelling theorem should be of limited use in such cases. However, the K-theory still applies in any dimension raising the question of its physical interpretation.

[1] This work will be part of the PhD theses of Daniel Herrmann and Marc Zarrouati.

The main idea behind this construction goes as follows [**Bel93**]. Given a Schrödinger operator H on $\mathbb{R}^d$, or a discretized version of it on $\mathbb{Z}^d$, one constructs a canonical C^*-algebra $\mathcal{A}$ attached to it. In particular all bounded functions of H and of its translates belong to $\mathcal{A}$. If $\mathfrak{g} = (E_-, E_+)$ is a spectral gap, the characteristic function $\chi_{\mathfrak{g}}$ of the interval $(-\infty, E_-]$ is continuous on the spectrum of H so that $P(\mathfrak{g}) = \chi_{\mathfrak{g}}(H)$ is a projection in $\mathcal{A}$. $\mathcal{A}$ is separable in most cases of interest, so that the number of projections in $\mathcal{A}$, modulo "unitary equivalence" is at most countable [**Ped**]. Since the spectrum is an algebraic invariant, one can associate to each gap $\mathfrak{g}$ the equivalence class $n(\mathfrak{g}) = [P(\mathfrak{g})]$ of its gap projection. It turns out that, modulo a slight extension of the notion of equivalence, this set of equivalence classes is endowed with the structure of an Abelian discrete group, with the direct sum of projections, namely $[P] + [Q] = [P \oplus Q]$. This group is called $K_0(\mathcal{A})$. Since the equivalence class of a projection is a homotopy invariant, the gap labels are invariant by norm resolvent perturbations of H, as long as the corresponding gap does not close. This implies, in particular, sum rules and conservation rules as the dynamics is perturbed. Such rules had been observed for a long time without being conceptually understood. The K-theory gives the explanation.

The previous construction is rather abstract so that one can wonder whether there is a more concrete aspect of it that is used by physicists. The link is given by the so-called *Shubin formula* [**Shub, Bel86, Bel93**]. The *trace per unit volume* defines a *trace* $\mathcal{T}$ on $\mathcal{A}$. Since a trace is invariant under unitary transformations, the trace of a projection depends only on the equivalence class of that projection. Moreover a trace is additive on a direct sum. Consequently $\mathcal{T}$ induces a group homomorphism $\mathcal{T}_*$ from $K_0(\mathcal{A})$ into $\mathbb{R}$. On the other hand Shubin showed (see also [**Bel93**] for a generalization of Shubin's formula) that

$$\mathcal{N}(E) = \mathcal{T}\{\chi_{(-\infty,E]}(H)\}$$

where $\mathcal{N}(E)$ is the so-called *integrated density of states* (IDOS), defined as the number of eigenstates of H per unit volume with eigenvalues lower than or equal to E. It turns out that this function is non-decreasing and positive, vanishing below the infimum of the spectrum. Therefore its derivative $d\mathcal{N}$ defines a Stieljes-Lebesgue measure called the *density of states* (DOS). Note that physicists have access to the DOS, especially near the Fermi level, through various experimental techniques. Numerical calculations of band spectra in solids give also a computation of the DOS. In 1D, thanks to the Sturm-Liouville theory for ODE's, the IDOS is also given by the *rotation number* of the wave function (*i.e.* the real solution of the equation $-\psi"(x) + V(x)\psi(x) = E\psi(x)$ vanishing at $-\infty$), obtained by counting the number of sign changes of ψ per unit length. As a consequence of all these remarks

$$E \in \mathfrak{g} \qquad \Rightarrow \qquad \mathcal{N}(E) \;=\; \mathcal{T}_*\left([P(\mathfrak{g})]\right) \;\in \mathcal{T}_*\left(K_0(\mathcal{A})\right)$$

This is a remarkable result implying that the IDOS on gaps must take values in some specific countable subgroup of $\mathbb{R}$ that depends on H only through the C^*-algebra $\mathcal{A}$. Since this set is model independent it can, in principle, be computed without knowing much about the spectrum of H, giving an *a priori* constraint on it.

Since 1981, the set of gap labels has mainly been computed for 1D systems (see [**Bel93**] for a review). In some smooth cases, using the Connes index theorem [**Co82**], one also get the gap labels in higher dimension. However for a long time, the case of QC's was an open problem. It is only since the middle of the nineties that we start to have some results. A deep theorem by Forrest and Hunton [**FoHu**] gives a rational isomorphism (the Chern character) between the K-group and some group homology in some class of systems. It is valid in any dimension and applies to QC's. It has recently been supplemented by explicit calculations [**FHK1, GeKe**] of the group K_0 for QC's with codimension 1 and 2. The computation of its image under the trace is still open to a large extent, even though results for 2D QC's are now available [**vEl, Kel1, BCL, PuAn**]. The 3-dimensional or 3-codimensional cases are still under scrutiny. Recent progress have led to the computation of the cohomology groups [**FoKe**] in this case. However, the gap labelling is not computed yet, mainly because the structure of the K-groups is qualitatively more involved. The aim of this paper is to review the general construction explained above and to give an account of the calculations of gap labels for 2D systems. We will adopt a point of view slightly different from the one given in [**Bel86, Bel93**]. We will take advantage of the recent work of Lagarias and Pleasants on point sets [**LaPle**]. To each point set, liable to represent the set of atomic positions, we associate the point measure supported by this set and give weight n to each point on which n atoms are lying. Such measures will be called *quasi uniformly discrete* and we shall denote the space of such measures by $QD(\mathbb{R}^d)$. Thanks to this representation, the weak-$*$ topology on the space of measures induces a natural topology on the set $QD(\mathbb{R}^d)$ of atomic configurations. It makes quite an easy task to use compactness arguments, leading to the notion of *hull* of an atomic configuration, which is the closure of the orbit of one atomic configuration under the translation group $\mathbb{G}$. This closure is, in most cases of interest, a compact space endowed with an action of $\mathbb{G}$. This dynamical system gives rise to a C^*-algebra in a canonical way which describes electronic observables that are considered for solving the Schrödinger equation. The spectral gaps of the electronic Hamiltonian are then labelled by means of the K-theory of that C^*-algebra.

We also introduce a complementary point of view taking the thermodynamics of the atomic motion into account. By an axiomatic approach, we propose a framework in which the Gibbs state describing the thermal equilibrium of atomic configurations becomes a probability measure on $QD(\mathbb{R}^d)$. Since the translation group acts on $QD(\mathbb{R}^d)$ by homeomorphisms, it acts on such probabilities as well. If the Gibbs state is unique it should be translation invariant and ergodic. Using such properties, we show that the Gibbs state uniquely determines:

(1) The hull of the point set: *the thermodynamic equilibrium defines entirely the relevant family of atomic configurations.*
(2) The diffractive measure associated, which correspond to the diffraction pattern of the point set.
(3) The electronic DOS of the Hamiltonian: the Gibbs state defines in a unique way a *trace per unit volume* on the C^*-algebra of observables. Hence, thermodynamic principles give a natural choice of a trace and this trace is exactly what is needed to obtain the set of gap labels.
(4) The density of phonon modes (this aspect will not be developed here): the matrix defining phonon modes belongs to a similar C^*-algebra.

Examples of solid compounds for which this construction applies will be described in more detail. Three cases will be emphasized due to their importance in modern technology and as paradigm for aperiodic systems: the case of perfect crystals, like most metals, the case of crystals with impurities, like doped semiconductors, and the case of quasicrystals.

The construction of the C^*-algebra of observables will follow together with a description of the construction of the K-group for beginners (the reader is invited to see [**Bla**] for more details). Various standard techniques used to compute the K-group and the set of gap labels will be described. These results will be applied to QC's especially in dimension two. The calculation of the K-groups and gap labels will be given in the known cases. A conjecture for the set of gap labels will be established.

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1. Atomic sites and their hull

A typical equation of motion for conduction electrons in a solid is the Schrödinger equation $H\psi = E\psi$, where H is the following operator acting on $\mathcal{H} = L^2(\mathbb{R}^d)$

$$H = -\frac{\hbar^2}{2m}\Delta + \sum_{j=1}^{c} \sum_{y \in L_j} v_j(\,.\, - y)\ . \tag{1.1}$$

Here d is the physical space dimension, m is the mass of the charge carrier, $\hbar$ is Planck's constant, $j = 1, \dots, c$ labels the chemical atomic species, L_j is the point set of equilibrium positions of atoms of type j and v_j the effective potential for valence electrons near an atom of type j.

1.1. Bloch theory versus aperiodicity. If the solid is a perfect crystal, the point sets L_j are all invariant under a *translation group* $\mathcal{R}$, *i.e.* a discrete subgroup of $\mathbb{R}^d$ generating $\mathbb{R}^d$, namely what mathematicians call a *lattice*. In such a case, $\mathcal{R}$ is represented in $\mathcal{H}$ by unitary operators $U(a)$, $a \in \mathcal{R}$ and

$$U(a)\ H\ U(a)^{-1}\ =\ H \qquad \forall a \in \mathcal{R}\ . \tag{1.2}$$

Therefore one can simultaneously diagonalize H and the $U(a)$'s. Since $\mathcal{R}$ is Abelian, diagonalization of the $U(a)$'s is performed through its character group $\mathcal{R}^*$. Standard results in Pontryagin duality theory imply that $\mathcal{R}^*$ is isomorphic to the quotient $\mathbb{B} = \mathbb{R}^{d\,*}/\mathcal{R}^\perp$ of the dual group of $\mathbb{R}^d$ (isomorphic to $\mathbb{R}^d$) by the orthogonal $\mathcal{R}^\perp$ of $\mathcal{R}$ in this group. It is a well known fact that $\mathcal{R}^\perp$ is a lattice in $\mathbb{R}^d$ (called *the reciprocal lattice* in Solid State Physics [**Jon**]) so that $\mathbb{B} = \mathbb{R}^{d\,*}/\mathcal{R}^\perp$ is a compact group homeomorphic to a d-torus, even if analytically, point symmetries of the crystal may provide it with extra structures. Throughout this paper $\mathbb{B}$ will be called the *Brillouin zone* (strictly speaking this is slightly different from what crystallographers call Brillouin zone).

The concrete calculation of $\mathbb{B}$ goes as follows: any character of $\mathbb{R}^d$ is represented by an element $k \in \mathbb{R}^{d\,*}$. Since $\mathbb{R}^{d\,*}$ and $\mathbb{R}^d$ can be identified canonically, by using the usual Euclidean structure, one can see k as a vector $k = (k_1, \cdots, k_d) \in \mathbb{R}^d$. The corresponding character is given by the map

$$\eta_k : x \in \mathbb{R}^d \mapsto e^{\imath \langle k|x\rangle} \in U(1)$$

In particular η_k restricts to a character of $\mathcal{R}$, with the condition that $\eta_k \restriction_{\mathcal{R}} = \eta_{k'} \restriction_{\mathcal{R}}$ if and only if $k - k' \in \mathcal{R}^{\perp}$, where

$$\mathcal{R}^{\perp} = \{b \in \mathbb{R}^d \,;\, \langle b|a\rangle \in 2\pi\mathbb{Z},\, \forall a \in \mathcal{R}\}.$$

Since $\mathbb{B}$ is a compact group, the diagonalization of the $U(a)$'s requires the use of a direct integral decomposition of $\mathcal{H}$ over $\mathbb{B}$, so that

$$\mathcal{H} = \int_{k\in\mathbb{B}}^{\oplus} d^dk\, \mathcal{H}_k \qquad\qquad H = \int_{k\in\mathbb{B}}^{\oplus} d^dk\, H_k$$

where H_k is an operator acting on the Hilbert space $\mathcal{H}_k$. In the specific case given by Equation (1.1), $\mathcal{H}_k$ is the space of functions ψ on $\mathbb{R}^d$ such that $\psi(x+a) = e^{\imath\langle k|x\rangle}\psi(x)$ for all $a \in \mathcal{R}$ and that $\int_{\mathbb{V}} d^dx |\psi(x)|^2 = \|\psi\|^2_{\mathcal{H}_k} < \infty$, where $\mathbb{V} = \mathbb{R}^d/\mathcal{R}$. H_k is then the partial differential operator formally given by the same expression as H, but with domain $\mathcal{D}_k$ given by the space of elements $\psi \in \mathcal{H}_k$ such that $\partial_i\psi/\partial x_i \in \mathcal{H}_k$, for $1 \leq i \leq d$, and $\Delta_x\psi \in \mathcal{H}_k$. Then H_k is unitarily equivalent to an elliptic operator on the torus $\mathbb{R}^d/\mathcal{R} = \mathbb{V}$. In solid state physics, $\mathbb{V}$ is called the *Wigner-Seitz cell*, whereas it is called the *Voronoi cell* in tiling theory.

As a consequence, it follows that, for each $k \in \mathbb{B}$, the spectrum of H_k is discrete and unbounded. If $E_i(k)$ denotes the eigenvalues, with a convenient labelling i, the maps $k \in \mathbb{B} \mapsto E_i(k) \in \mathbb{R}$ are called the *band functions*. The spectrum of H is recovered as $\mathrm{spec}(H) = \bigcup_{i,k\in\mathbb{B}} E_i(k)$ and is called a *band spectrum*. A discrete spectrum is usually liable to be computable by suitable algorithms, since it restricts to diagonalizing large matrices.

This is a short summary of *Bloch theory*. Strutt first realized the existence of band functions [**Str**], but soon after Bloch wrote his important paper [**Blo**]. In 1930, Peierls gave a perturbative treatment of the band calculations [**Pei**] and Brillouin discussed the $2D$ and $3D$ cases [**Bri**]. The reader is invited to look at [**Jon, AshMe**] to understand why this theory has been so successful in solid state physics. Let us simply mention that the first explicit calculations of bands in $3D$ were performed in 1933 by Wigner & Seitz [**WiSe**] on sodium using the cellular method that holds their names. The symmetry properties of the wave function were explicitly used in an important paper by Bouckaert, Smoluchowski & Wigner [**BSW**] leading to noticeable simplifications of the band calculation.

If the solid is no longer a perfect crystal, Equation (1.2) is violated so that there may not be any space symmetry anymore, even though some point symmetry may survive. How can one deal with such situations in general ? In specific cases, where the breaking of translation symmetry can be considered as a small perturbation one can find ways around. For instance, if there are isolated impurities in the crystal, a good approximation was developed by Slater in 1949 [**Sla**] to compute the change produced in the energy spectrum. But many examples of compounds require another treatment taking into account the aperiodicity: semiconductors at low temperature for impurity bands electrons [**ShEf**], quasicrystals [**HiGra**], amorphous materials, even metallic liquids. To deal with this situation one of us has proposed a long time ago [**Bel86, Bel93**] to replace Bloch theory by the formalism of non-commutative geometry [**Co94**]. It consists in replacing the set of continuous functions over the Brillouin zone $\mathcal{C}(\mathbb{B})$, by a non-commutative algebra over a virtual space, that will be called the *non-commutative Brillouin zone*. This algebra is built from the family $\{U(a)HU(a)^{-1}, a \in \mathbb{R}^d\}$ of the translates of H. The construction leads to $\mathcal{C}(\mathbb{B})$ whenever the crystal is perfect. This is explained in the next sections.

1.2. The hull of a point set. For $x = (x_1, \cdots, x_d) \in \mathbb{R}^d$, we set $|x|_\infty = \max_{1\leq i\leq d}|x_i|$. If $x \in \mathbb{R}^d$ and $r > 0$ we set $B(x,r) = \{y \in \mathbb{R}^d \ ; \ |y-x|_\infty < r\}$: it is the open ball of radius r centered at x for the metric $|\cdot|_\infty$ namely the open hypercube with faces perpendicular to the vectors of the canonical basis, centered at x and with side $2r$.

Atomic sites of type j are located on the discrete point set $L = L_j$ contained in $\mathbb{R}^d$. Following Lagarias and Pleasants [**LaPle**] we define the following hierarchy of properties:

- L is *discrete* if the intersection of any compact set of $\mathbb{R}$ with L is finite.
- L is *uniformly discrete* if there is $r > 0$, such any ball of radius r contains at most one point of L. This means that there is a non-zero minimum distance between points of L.
- L is *relatively dense* if there is $R > 0$ such that any ball of radius R contains at least one point of L.
- L is a *Delone* (or Delaunay) *set* if it is both uniformly discrete and relatively dense.
- A Delone set L is *finitely generated* if the $\mathbb{Z}$-module generated by $L - L$ in $\mathbb{R}^d$ is finitely generated.
- A Delone set L has *finite type* if $L - L$ is discrete and closed.
- L is a *Meyer set*, whenever both L and $L - L$ are Delone sets.

If L is a Delone set, we set $r_0 = \sup\{r > 0; \ |B(x,r) \cap L| \leq 1, \forall x \in \mathbb{R}^d\}$ and $r_1 = \inf\{R > 0; \ |B(x,R) \cap L| \geq 1, \forall x \in \mathbb{R}^d\}$. Then the minimal distance r_L between two distinct points of L is $r_L = 2r_0$. We will say that L is (r,R)-Delone whenever $r \leq r_0$ and $R > r_1$.

EXAMPLE 1.1. A point set in $\mathbb{R}^d$ randomly distributed with respect to a Poisson process, is discrete but not uniformly discrete with probability one.

EXAMPLE 1.2. In practice, due to quantum mechanics, the equilibrium positions of atoms in any solid medium is a uniformly discrete set. Impurities in a semiconductor, distributed randomly, are located on a uniformly discrete set which is not a Delone set in general. This is also the case of zeolithes which may have empty holes of arbitrary size.

EXAMPLE 1.3. Most solids, amorphous, glasses, crystals, quasicrystals, have their atoms on a Delone set. Random tilings built from a quasilattice [**Moss**], have their vertices on finitely generated Delone sets.

EXAMPLE 1.4. Point sets constructed by cut-and-project method [**HiGra**], namely model sets [**Moo**], and more generally point sets obtained by inflation with matching rules or by covering clusters [**JeSt, Gum, Kra99**], are Meyer sets [**Mey**].

Now, we denote by $\mathcal{M}(\mathbb{R}^d)$ the space of measures on $\mathbb{R}^d$. By construction it is the set of linear continuous maps from $\mathcal{C}_c(\mathbb{R}^d)$, the space of continuous functions with compact support on $\mathbb{R}^d$, into $\mathbb{C}$.

Let $QD(\mathbb{R}^d) = \{\nu \in \mathcal{M}(\mathbb{R}^d); \nu$ is pure point and $\nu(\{x\}) \in \mathbb{N}, \forall x \in \mathbb{R}^d\}$. For each $\nu \in QD(\mathbb{R}^d)$, $L^{(\nu)} = \mathrm{supp}(\nu) = \{x; \nu(\{x\}) \geq 1\}$ is a discrete set. Given $x \in L^{(\nu)}$, the integer $N_x = \nu(\{x\})$, that will be called the *multiplicity of* x, can be interpreted as the number of atoms located at x. Conversely, given a discrete set L and for each $x \in L$ an integer $n(x) \in \mathbb{N}_*$, one can define the measure

$$\nu^{(L,\underline{n})}(dx) = \sum_{y \in L} n(y)\delta(x-y)$$

This gives a one-to-one correspondence between discrete sets with multiplicity and measures in $QD(\mathbb{R}^d)$.

One can extend the correspondence between points sets in $\mathbb{R}^d$ and measures by defining $UD_r(\mathbb{R}^d) = \{\nu \in QD(\mathbb{R}^d); \forall x \in \mathbb{R}^d,\ \nu(B(x,r)) \leq 1\}$. This set of measures corresponds to r-uniformly discrete point sets with no degeneracy. We shall set $UD(\mathbb{R}^d) = \bigcup_{r>0} UD_r(\mathbb{R}^d)$, the space of uniformly discrete point sets. In much the same way, (r,R)-Delone sets will be represented by elements $\nu \in UD_r(\mathbb{R}^d)$ such that, for any open ball of radius R, $\nu(B(x,R)) \geq 1$. This subspace will be denoted by $Del_{(r,R)}(\mathbb{R}^d)$. The space of all Delone sets will then be $Del(\mathbb{R}^d) = \bigcup_{0<r<R} Del_{(r,R)}(\mathbb{R}^d)$.

The main properties of these spaces are the following (see Section 2):

THEOREM 1.5. *Let $\mathcal{M}(\mathbb{R}^d)$ be endowed with the weak-$*$ topology with respect to $\mathcal{C}_c(\mathbb{R}^d)$, then:*

(i) *The subspace $QD(\mathbb{R}^d)$ is a closed set. It is therefore a Polish space* (i.e. *a complete metrizable space).*
(ii) *For all $r > 0$ the subspace $UD_r(\mathbb{R}^d)$ of $QD(\mathbb{R}^d)$ is compact.*
(iii) *For all $0 < r \leq R$ the subspace $Del_{(r,R)}(\mathbb{R}^d)$ of $UD_r(\mathbb{R}^d)$ is compact.*
(iv) *The subspaces $UD(\mathbb{R}^d)$ and $Del(\mathbb{R}^d)$ are dense in $QD(\mathbb{R}^d)$.*

Therefore the correspondence between point sets and point measures becomes quite powerful in that it gives immediately a good topological structure. The last claim (iv) in Theorem 1.5 indicates that it is not possible to get away from point sets with multiplicity unless we accept to work on the non-closed F_σ-sets $UD(\mathbb{R}^d)$ or $Del(\mathbb{R}^d)$.

Let us give an intuitive description of what the weak-$*$ topology means (see a precise statement in Section 2.7). Given $\nu \in QD(\mathbb{R}^d)$ one associates $L^{(\nu)}$ its support, but we see each point $x \in L^{(\nu)}$ as a finite set with N_x points in it (its multiplicity). Then a sequence $(\nu_n)_{n\in\mathbb{N}}$ of elements of $QD(\mathbb{R}^d)$ converges to ν if and only if, for any open ball $B(x,r)$, the sets $L^{(\nu_n)}$ counted with their multiplicities, converge to $L^{(\nu)}$ in the sense of the Hausdorff distance [**Barn**]. In other words, convergence of $L^{(\nu_n)}$ towards $L^{(\nu)}$ means convergence of points of $L^{(\nu_n)}$ in any bounded window.

More generally, given the atomic sites with several species, one associates the vector-valued point measure $\vec{\nu} = (\nu_1, \cdots, \nu_c)$ with $\nu_j = \nu^{(L_j)}$. The vector-valued measure $\vec{\nu}$ belongs to $\mathcal{M}(\mathbb{R}^d) \otimes \mathbb{C}^c$ that can be seen as the dual space of $\mathcal{C}_c(\mathbb{R}^d) \otimes \mathbb{C}^c$. The duality between them is given by $\langle \vec{\nu} | \vec{f} \rangle = \int_{\mathbb{R}^d} d\vec{\nu}(x) \vec{f}(x)$.

We endow these spaces with the weak-$*$ topology, namely a sequence $\vec{\nu}_n$ of vector-valued measure converges to $\vec{\nu}$ if and only if $\lim_{n\to\infty} \langle \vec{\nu}_n | \vec{f} \rangle = \langle \vec{\nu} | \vec{f} \rangle$ for every $\vec{f} \in \mathcal{C}_c(\mathbb{R}^d) \otimes \mathbb{C}^c$.

The main result of this subsection is the following theorem, which is a direct consequence of Theorem 1.5.

THEOREM 1.6. *Let* $\vec{\nu} = (\nu_1, \cdots, \nu_c)$, *with* $\nu_j = \nu^{(L_j)}$, *the vector-valued measure attached to the atomic positions. Assume the* L_j*'s are all uniformly discrete. Then the family* $\{\tau^a \vec{\nu}\,; a \in \mathbb{R}^d\}$ *of translates of* $\vec{\nu}$ *by elements of* $\mathbb{R}^d$ *has a compact weak closure in* $\mathcal{M}(\mathbb{R}^d) \otimes \mathbb{C}^c$.

Recall that a *topological dynamical system* is a pair $(X, \mathbb{G})$ where X is a topological space, $\mathbb{G}$ is a locally compact group acting on X by homeomorphisms [**GoHe**]. In all cases considered here, X will be compact metrizable. $(X, \mathbb{G})$ is called *topologically transitive* if X admits one dense $\mathbb{G}$-orbit. It is called *minimal* if all $\mathbb{G}$-orbits are dense. If X is compact, the set $\mathcal{M}_1(X, \mathbb{G})$ of $\mathbb{G}$-invariant probability measures is a non-empty compact convex set if endowed with the weak-$*$ topology. The extremal elements of this set are exactly the $\mathbb{G}$-invariant ergodic probability measures on x. $(X, \mathbb{G})$ is *uniquely ergodic* if $\mathcal{M}_1(X, \mathbb{G})$ reduces to one point only. Two dynamical systems $(X_1, \mathbb{G}_1)$ and $(X_2, \mathbb{G}_2)$ are *semi-conjugated* if it exists a surjective continuous map ϕ from X_1 to X_2 such that $\phi \circ T_1 = T_2 \circ \phi$, where T_i is the action of $\mathbb{G}_i$ on X_i. When ϕ is one-to-one, $(X_1, \mathbb{G}_1)$ and $(X_2, \mathbb{G}_2)$ are *conjugated*. A family $(X_i, \mathbb{G})$ of topological dynamical systems over the group $\mathbb{G}$ is *structurally stable* whenever for any $i \neq j$ there is a homeomorphism $\phi_{i,j} : X_i \mapsto X_j$ that conjugates the actions.

We are now ready to define rigorously the hull:

DEFINITION 1.7. Given a finite family $L = (L_1, \cdots, L_c)$ of uniformly discrete point sets in $\mathbb{R}^d$, the closure $\Omega_{\vec{\nu}}$ of the family of translates of the vector-valued measure $\vec{\nu}^{(L)} = (\nu_1, \cdots, \nu_c)$ (with $\nu_j = \nu^{(L_j)}$), is called the *hull* of L. Endowed with the canonical action T of $\mathbb{R}^d$ by translation, it becomes a topological dynamical system $(\Omega, \mathbb{R}^d, T)$ which is topologically transitive.

The notion of the hull was first introduced by one of us in earlier papers [**Bel86, Bel93**] as the compact strong closure Ω_H, when it exists, of the family $\{U(a)HU(a)^{-1}, a \in \mathbb{R}^d\}$ of the translates of the Schrödinger operator $H = \Delta + V$. These two definitions are not strictly equivalent in general. However we can prove that $(\Omega_\nu, \mathbb{R}^d)$ and $(\Omega_H, \mathbb{R}^d)$ are semi-conjugated (Section 2.7).

EXAMPLE 1.8. The point set of a perfect crystal in $\mathbb{R}^d$ is $\mathcal{R}$-periodic, $\mathcal{R}$ being a lattice in $\mathbb{R}^d$ (cf. Section 1.1). Its hull is then the quotient $\mathbb{R}^d/\mathcal{R}$, namely it is homeomorphic to $\mathbb{T}^d$. Others examples are quoted in Section 3.

In many cases, it is quite convenient to work with a tight-binding representation (see Section 4) instead of using the Schrödinger equation (1.1). This means that Equation (1.1) is replaced by a finite difference equation where the wave functions live in $\ell^2(L)$ instead of belonging to $L^2(\mathbb{R}^d)$ [**Bel86**]. The breaking of translation invariance can be described through the notion of *the canonical transversal* and its *groupoid* (see Section 2.5).

DEFINITION 1.9. Let Ω be a closed $\mathbb{R}^d$-invariant subset of $QD(\mathbb{R}^d)$. Its *canonical transversal* Υ is the closed subset

$$\Upsilon = \{\omega \in \Omega; \omega(\{0\}) \geq 1\}$$

The set of pairs $(\omega, a) \in \Omega \times \mathbb{R}^d$ such that both ω and $\tau^{-a}\omega$ belong to Υ, is a locally compact groupoid G_Υ [**Ren**] called the *groupoid of the transversal.*

1.3. Gibbs measures on the hull. Up to now we have supposed that the atomic positions in a solid are fixed once and for all. As we know however, even solids are subject to phase transitions. The shape of the point set on which atoms are located is usually a consequence of thermodynamics. The description of the Gibbs state in such a situation is still today an open problem to a large extent. Nevertheless let us try to give a (non-rigorous) description of what it should be, so that we can extract which axioms a Gibbs measure is likely to satisfy.

Due to the large mass difference between electrons and atomic nuclei, one usually treats atomic motion in the Born-Oppenheimer approximation. Namely, one diagonalizes the electronic Hamiltonian considering the atomic positions as adiabatic parameters. Then the electronic energy depends upon atomic positions and acts as an extra attractive potential between nuclei. For this reason, it is enough to consider the Hamiltonian for nuclei alone.

In principle, even the atomic motion is quantized. But there are two kinds of simplifications that should be taken into account. First of all, since the system is solid, atoms only vibrate around their equilibrium position. The atomic vibrations built up acoustic waves called *phonons*. With a very good accuracy, one can treat phonons as harmonic waves, at least at low enough energies, namely at low enough temperatures. Nevertheless, one may take into account a small amount of anharmonicity if one wishes to.

The second simplification consists in using the Feynman path integral [**Gin65, Gin71**] to represent the Gibbs state describing atomic equilibrium. This gives the atomic partition function only in terms of the atomic potential energy, the contribution of the kinetic energy being represented by random fluctuations around the equilibrium position.

For all these reasons, the Gibbs state can be described with a rather good accuracy through the potential energy alone. The construction of such state can be found in [**Rue, Lan, Sin**]. The main properties of the potential energy are the following.

U1: In any finite ball Λ, the potential energy is a function $U_\Lambda(x_1, \cdots, x_N)$ of the positions $x_1, \cdots, x_N$ of atoms located in Λ. Hence one can see it as a function over the space $QD(\mathbb{R}^d)$.

U2: The potential energy is *translation-invariant* that is to say

$$U_{\Lambda+a}(x_1 + a, \cdots, x_N + a) = U_\Lambda(x_1, \cdots, x_N)$$

for all $a \in \mathbb{R}^d$.

U3: The potential energy is *repulsive at short distances*, namely it diverges as two atoms become too close to each other. In other words, the potential energy is finite if and only if the atomic sites are located on a uniformly discrete point set, namely an element of $UD(\mathbb{R}^d)$.

U4: The potential energy is a continuous function of the atomic positions away from coincident points. That means the U_Λ's are continuous on $UD(\mathbb{R}^d)$.

U5: The potential energy is *asymptotically extensive*, namely:

$$U_{\Lambda_1 \cup \Lambda_2 + a}(x_1, \cdots, x_M, y_1 + a, \cdots, y_N + a)$$
$$-U_{\Lambda_1}(x_1, \cdots, x_M) - U_{\Lambda_2+a}(y_1 + a, \cdots, y_N + a) \to 0$$

as $a \to \infty$ and $x_i \in \Lambda_1$ and $y_j \in \Lambda_2$.

U6: The potential energy is *attractive at large distances.* The exact description of this property is technical. Let us simply say that one decreases the potential energy in a large box by restricting it to the space $Del(\mathbb{R}^d)$ of Delone sets.

In the limit for which quantum effects on the atomic motion become negligible, the Gibbs state $\mathbb{P}$ is then described as a limit point, whenever it exists, of the following family of probability measures on $QD(\mathbb{R}^d)$

$$\mathbb{P}_\Lambda(F) = \frac{1}{\Xi_\Lambda(\beta,\mu)} \sum_{N=0}^{\infty} \frac{e^{\beta\mu N}}{N!} \int_{\Lambda^{\times N}} d^d x_1 \cdots d^d x_N \, e^{-\beta U_\Lambda(x_1,\cdots,x_N)} F(x_1,\cdots,x_N)$$

where $\beta = 1/kT$, μ is the chemical potential, $\Xi_\Lambda(\beta,\mu)$ (the normalization factor) is the *grand partition function* and F is a uniformly continuous bounded function on $QD(\mathbb{R}^d)$. Using **U1-U6**, one expects that $\mathbb{P}$ will be supported by the space $Del(\mathbb{R}^d)$. As usual, *pure phases* in the sense given to that word by physicists, are described by extreme points of the set of Gibbs states and are usually ergodic with respect to the translation group. Moreover we may expect $\mathbb{P}$ to be translation invariant. Such a property is a consequence of the unicity of the Gibbs state. However, this last requirement is not always satisfied even in practice, since inhomogeneous boundary conditions may lead to mixed phases with phase boundaries.

Whatever the hypothesis made to built the Gibbs measure $\mathbb{P}$, we expect that it should satisfy the following axioms:

G1: $\mathbb{P}$ is *uniformly discrete* namely, it gives probability one to $UD(\mathbb{R}^d)$.
G1': $\mathbb{P}$ is *Delone*, namely it gives probability one to $Del(\mathbb{R}^d)$.
G2: $\mathbb{P}$ is translation invariant.
G3: $\mathbb{P}$ is ergodic with respect to the translation group.

Remarkably enough, the mathematical framework developed previously gives several useful informations about the nature of typical atomic configurations. The first ones are summarized in the following (see Section 3.1):

THEOREM 1.10. (i) *Let $\mathbb{P}$ be a probability measure on $QD(\mathbb{R}^d)$ such that* **G1**, **G2** *and* **G3** *holds. Then there is $r_0 > 0$ such that for $\mathbb{P}$-almost all ν, its support $L^{(\nu)}$ is r_0-uniformly discrete and not r-uniformly discrete for $r > r_0$.*

(ii) *If in addition $\mathbb{P}$ satisfies $G1'$, there is $R_0 > 0$ such that for $\mathbb{P}$-almost all ν, its support $L^{(\nu)}$ is R_0-relatively dense and not R-relatively dense for $R < R_0$.*

The next result concerns the hull of a typical atomic configuration. If $\mathbb{P}$ satisfies **G1'**, then it is supported by the compact space $Del_{(r_0,R_0)}(\mathbb{R}^d)$. The *topological support* of $\mathbb{P}$ is the smallest closed subset of $Del_{(r_0,R_0)}(\mathbb{R}^d)$ of probability one. Then (see Section 3.1):

THEOREM 1.11. *Let $\mathbb{P}$ be a probability measure on $QD(\mathbb{R}^d)$ obeying* **G1'**, **G2**, **G3**. *Then, for $\mathbb{P}$-almost all $\nu \in QD(\mathbb{R}^d)$, its hull Ω_ν coincides with the topological support Ω of $\mathbb{P}$.*

This last theorem shows that the hull is entirely defined by the thermodynamic properties of the solid. We may also wonder whether the hull is structurally stable as the Gibbs state $\mathbb{P}$ varies in a region of uniqueness of the phase diagram. If this is correct, it means that the hull cannot bifurcate unless a phase boundary is crossed. This conjecture would give an explanation of why the lattice symmetry of a perfect crystal is fixed within a region of uniqueness.

Now, if we identify an element $\nu \in QD(\mathbb{R}^d)$ with a point set in $\mathbb{R}^d$ representing the position of atoms in a solid, the diffraction pattern seen on a screen, in an X-ray diffraction experiment or in a transmission electronic microscope (T.E.M.), can be computed from the Fourier transform of ν restricted to the domain Λ occupied by the sample in $\mathbb{R}^d$. Namely the intensity seen on the screen is proportional to

$$I_\Lambda(k) = \frac{1}{|\Lambda|} \left| \sum_{x\in\Lambda} \nu(\{x\}) e^{\imath\langle k|x\rangle} \right|^2 \tag{1.3}$$

where $k \in \mathbb{R}^d$ represents the wave vector of the diffraction beam, the direction of which gives the position on the screen. In practice however, the intensity seen is $f(k)I_\Lambda(k)$ instead, where f is a *form factor* which takes into account that the incident beam sees atoms as composite objects rather than as points. The main problem is whether such quantity converges as $\Lambda \uparrow \mathbb{R}^d$. Before answering that question, let us remark that the Fourier transform of $I_\Lambda(k)$ is given by the following expression: if $f \in \mathcal{C}_c(\mathbb{R}^d)$, its Fourier transform is denoted by $\tilde{f}$ and

$$\int_{k\in\mathbb{R}^d} dk \tilde{f}(k) I_\Lambda(k) = \frac{1}{|\Lambda|} \sum_{x,y\in\Lambda} \nu(\{x\})\nu(\{y\}) f(x-y) = \rho_\nu^{(\Lambda)}(f) \tag{1.4}$$

where $\rho_\nu^{(\Lambda)}$ will be called the *finite volume diffraction measure.* ¿From Equation (1.4), it follows that $\rho_\nu^{(\Lambda)} \in \mathcal{M}(\mathbb{R}^d)$ is a positive measure with a Fourier transform being also a positive measure.

The next theorem gives conditions under which convergence hold as $\Lambda \uparrow \mathbb{R}^d$ (see Section 3.2).

THEOREM 1.12. *Let $\mathbb{P}$ be a uniformly discrete translation-invariant probability measure on $QD(\mathbb{R}^d)$ supported by $UD_r(\mathbb{R}^d)$ for some $r > 0$. Then:*

(i) *The averaged diffraction measure $\rho_\mathbb{P}^{(\Lambda)} = \int_{\nu\in QD(\mathbb{R}^d)} d\mathbb{P}(\nu)\rho_\nu^{(\Lambda)}$ converges as $\Lambda \uparrow \mathbb{R}^d$ (Λ varying within the set of hypercubes in $\mathbb{R}^d$), to a positive measure $\rho_\mathbb{P} \in \mathcal{M}(\mathbb{R}^d)$.*

(ii) *The distributional Fourier transform of $\rho_\mathbb{P}$ is also a positive measure on $\mathbb{R}^d$.*

(iii) *If in addition $\mathbb{P}$ is ergodic, then for $\mathbb{P}$-almost every $\nu \in QD(\mathbb{R}^d)$ the family $\rho_\nu^{(\Lambda)}$ of measures on $\mathbb{R}^d$ converges to $\rho_\mathbb{P}$.*

In other words, each invariant ergodic uniformly discrete probability measure on $QD(\mathbb{R}^d)$ determines in a unique way the diffraction pattern. In particular, if we look into the phase diagram in a region of uniqueness of the Gibbs state, the diffraction pattern is entirely defined.

1.4. C^*-algebra of observables. The previous subsections have shown that the set of atomic sites gives rise to a canonical dynamical system $(\Omega, \mathbb{R}^d)$, its hull, over the translation group $\mathbb{R}^d$. There is always a C^*-algebra associated to such dynamical system, namely the crossed product $\mathcal{C}(\Omega) \rtimes \mathbb{R}^d$ [**Ped**]. We will show that this C^*-algebra, suitably modified if a uniform magnetic field is applied to the system, is nothing but the smallest C^*-algebra $\mathcal{A}$ generated by bounded continuous functions of the Schrödinger operator and its translates by $\mathbb{R}^d$, at least for an atomic potential satisfying sufficient regularity conditions (see Section 2.7). Moreover, when applied to a perfect crystal, we will see that $\mathcal{A}$ is isomorphic to $\mathcal{C}(\mathbb{B}) \otimes \mathcal{K}$, namely the space of matrix-valued continuous functions on the Brillouin zone. If the solid is no longer a perfect crystal, $\mathcal{A}$ is no longer of type I, namely it becomes non-commutative in a non-trivial way. It then replaces the C^*-algebra of continuous functions on the Brillouin zone. That is why we will associate to it a *non-commutative manifold* that we will call the *non-commutative Brillouin zone* (NCBZ) [**Bel86, Bel93**].

Given a uniform magnetic field $B = (B_{\nu\mu})$, namely a real-valued antisymmetric $d \times d$-matrix, we associate the C^*-algebra $C^*(\Omega \times \mathbb{R}^d, B)$ defined as follows. We first consider the topological vector space $\mathcal{C}_c(\Omega \times \mathbb{R}^d)$ of continuous functions with compact support in $\Omega \times \mathbb{R}^d$. It is endowed with the following structure of *-algebra

$$fg(\omega, x) = \int_{\mathbb{R}^d} dy\, f(\omega, y) g(T^{-y}\omega, x-y) e^{i\pi(e/h)\, B.x\wedge y}\,, \tag{1.5}$$

$$f^*(\omega, x) = \overline{f(T^{-x}\omega, -x)}\,, \tag{1.6}$$

where $f, g \in C_c(\Omega \times \mathbb{R}^d)$, $B.x \wedge y = \sum B_{\nu\mu} x_\nu y_\mu$ and $\omega \in \Omega$, $x \in \mathbb{R}^d$. Here e is the electric charge of the particle and $h = 2\pi\hbar$. This *-algebra is represented on $L^2(\mathbb{R}^d)$ by the family of representations $\{\Pi_\omega;\ \omega \in \Omega\}$ given by

$$\Pi_\omega(f)\psi(x) = \int_{\mathbb{R}^d} dy f(T^{-x}\omega, y-x) e^{i\pi(e/h)\, B.x\wedge y}\psi(y), \qquad \psi \in L^2(\mathbb{R}^d) \tag{1.7}$$

where Π_ω is linear, $\Pi_\omega(fg) = \Pi_\omega(f)\Pi_\omega(g)$ and $\Pi_\omega(f)^* = \Pi_\omega(f^*)$. In addition $\Pi_\omega(f)$ is a bounded operator and the representations $(\Pi_\omega)_{\omega\in\Omega}$ are related by the covariance condition:

$$U(a)\,\Pi_\omega(f)\,U(a)^{-1} = \Pi_{T^a\omega}(f)\,. \tag{1.8}$$

Here the U's are the so-called *magnetic translations* [**Zak**] defined by:

$$U(a)\psi(x) = \exp\Big\{(ie/\hbar)\int_{[x-a,x]} dy^\mu A_\mu(y)\Big\}\psi(x-a), \tag{1.9}$$

where $\vec{A} = (A_1, ..., A_d)$ is the vector potential defined by $B_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$, $a \in \mathbb{R}^d$, $\psi \in L^2(\mathbb{R}^d)$ and $[x-a, x]$ is the line segment joining $x-a$ to a in $\mathbb{R}^d$. Now, we set

$$\|f\| = \sup_{\omega\in\Omega} \|\Pi_\omega(f)\|\,, \tag{1.10}$$

which defines a C^*-norm.

DEFINITION 1.13. The non-commutative Brillouin zone is the topological manifold associated to the C^*-algebra $\mathcal{A} = C^*(\Omega \rtimes \mathbb{R}^d, B)$ obtained by completion of $\mathcal{C}_c(\Omega \times \mathbb{R}^d)$ under the norm $\|\cdot\|$ defined in Equation (1.10).

For $B = 0$ we recover the construction of the C^*-crossed product $\mathcal{C}(\Omega) \rtimes \mathbb{R}^d$ [**Ped, Bla**]. In the case of a perfect crystal (see Section 1.1), with lattice translation group $\mathcal{R}$, the hull $\Omega = \mathbb{R}^d/\mathcal{R}$ is homeomorphic to $\mathbb{T}^d$ (see Example 1.8). We get:

THEOREM 1.14. [**Bel93**] *The C^*-algebra $C^*(\mathbb{R}^d/\mathcal{R} \rtimes \mathbb{R}^d, B = 0)$ associated to a perfect crystal with lattice translation group $\mathcal{R}$, is isomorphic to $\mathcal{C}(\mathbb{B}) \otimes \mathcal{K}$, where $\mathcal{C}(\mathbb{B})$ is the space of continuous functions over the Brillouin zone and $\mathcal{K}$ the algebra of compact operators.*

Even though the algebra $\mathcal{C}(\mathbb{B}) \otimes \mathcal{K}$ is already non-commutative, its non-commutative parts come from $\mathcal{K}$, the smallest C^*-algebra generated by finite rank matrices. It describes the possible vector bundles over $\mathbb{B}$. Theorem 1.14 is the reason to claim that $\mathcal{A}$ generalize the Brillouin zone for aperiodic systems.

At last, a very similar construction can be performed within the tight-binding representation. One starts from the space $\mathcal{C}_c(G_\Upsilon)$ of continuous functions with compact support on the groupoid of the transversal (see Definition 1.9 and Section 2.5). We proceed as before replacing the Hilbert space $L^2(\mathbb{R}^d)$ by $\ell^2(G_\Upsilon^\omega)$ where G_Υ^ω is the fiber of range ω in G_Υ. In this way we construct $C^*(G_\Upsilon, B=0)$ (see Section 4).

Given any translation-invariant probability measure $\mathbb{P}$ on Ω, one can define a *trace* on $\mathcal{A} = C^*(\Omega \rtimes \mathbb{R}^d, B)$ as follows. If $f \in \mathcal{C}_c(\Omega \times \mathbb{R}^d)$ we set [**Bel86, Bel93**]:

$$\mathcal{T}_{\mathbb{P}}(f) \;=\; \int_\Omega d\mathbb{P}(\omega) f(\omega, x=0) \tag{1.11}$$

This is a densely-defined linear form on $\mathcal{A}$ such that $\mathcal{T}_{\mathbb{P}}(f^* \cdot f) = \mathcal{T}_{\mathbb{P}}(f \cdot f^*) \geq 0$, namely it is an unbounded trace on $\mathcal{A}$. It has been shown [**Bel93**] that, whenever $\mathbb{P}$ is $\mathbb{R}^d$-ergodic, this trace satisfies

$$\mathcal{T}_{\mathbb{P}}(f) \;=\; \lim_{\Lambda \uparrow \mathbb{R}^d} \frac{1}{|\Lambda|} \mathrm{Tr}_\Lambda\left(\Pi_\omega(\mathrm{f})\right) \qquad \text{for } \mathbb{P}\text{-almost all } \omega\text{'s}, \tag{1.12}$$

if $f \in \mathcal{C}_c(\Omega \times \mathbb{R}^d)$ and Λ varies in the family of open balls centered at one point in $\mathbb{R}^d$. It is therefore the *trace per unit volum*. For a perfect crystal, it is easy to show that this trace equals the integral over the Brillouin zone. Using a Gibbs state to built the equilibrium atomic configurations, we see that it not only defines uniquely the hull, but also endows the C^*-algebra of the hull with a physically natural trace.

1.5. K-theory: main results. We recalled in the Introduction the main ideas leading to the definition and the construction of the K_0-group of a C^*-algebra. Let us give more details and summarize the main results here.

Together with $K_0(\mathcal{A})$ there is another K-group, denoted by $K_1(\mathcal{A})$, necessary in dealing with exact sequences and spectral sequences in K-theory. $K_1(\mathcal{A})$ classifies the homotopy classes of invertible elements of $\mathcal{A} \otimes \mathcal{K}$ (or $(\mathcal{A} \otimes \mathcal{K})^+$, the algebra obtained by adding a unit).

By construction of the K-groups, $\mathcal{A}$ and $\mathcal{A} \otimes \mathcal{K}$ have always the same K-theory (Morita equivalence). As a matter of facts, this leads to group isomorphisms between $K_i(C^*(\Omega \rtimes \mathbb{R}^d, B)$ and $K_i(C^*(G_\Upsilon, B))$.

For $B=0$ the situation becomes a bit simpler. Through the Thom-Connes theorem [**Co81**], one gets an isomorphism between $K_i(\mathcal{C}(\Omega) \rtimes \mathbb{R}^d)$ and $K_{i+d}(\mathcal{C}(\Omega))$, where $i+d$ is defined modulo 2. On $\mathcal{C}(\Omega)$ the K-theory is isomorphic to the topological K-group $K^*(\Omega)$ over Ω, that is the classification modulo stable isomorphisms of vector bundles over Ω. Whenever Ω is a smooth manifold, the Chern character gives a rational isomorphism between $K^*(\Omega)$ and the cohomology of Ω with integer coefficients $H^*(\Omega, \mathbb{Z})$. Unfortunately, in most cases of interest in solid state physic, the topological space Ω is totally disconnected transversally to the $\mathbb{R}^d$-action. This means that its canonical transversal is totally disconnected. Therefore, we need to develop other techniques to compute the K-theory. This is exactly the purpose of this work.

As indicated in the Introduction, the trace per unit volume $\mathcal{T}_{\mathbb{P}}$ attached to any invariant probability measure $\mathbb{P}$ on the hull, gives rise to a group homomorphism $\mathcal{T}_{\mathbb{P}*} : K_0(C^*(\Omega \rtimes \mathbb{R}^d, B)) \mapsto \mathbb{R}$. The *gap labels* are the elements of the image of this map. Our main conjecture is given as follows

PROBLEM 1.15. *Prove or disprove that, if the hull Ω of a point set has a totally disconnected canonical transversal, the set of gap labels is given by*

$$\mathcal{T}_{\mathbb{P}*}\left(K_0(C^*(\Omega \rtimes \mathbb{R}^d, B=0))\right) \;=\; \int_\Omega d\mathbb{P}\, \mathcal{C}(\Omega, \mathbb{Z}),$$

where $\mathcal{C}(\Omega,\mathbb{Z})$ is the space of continuous functions on Ω with values in $\mathbb{Z}$.

Evidences for this conjecture are provided by the following results:

THEOREM 1.16. *Let Ξ be a totally disconnected compact space with a $\mathbb{Z}^d$-action. For any $\mathbb{Z}^d$-invariant ergodic probability measure $\mathbb{P}$ on Ξ one has*

$$\mathcal{T}_{\mathbb{P}*}\left(K_0(\mathcal{C}(\Xi) \rtimes \mathbb{Z}^d)\right) \;=\; \int_\Xi d\mathbb{P}\, \mathcal{C}(\Xi, \mathbb{Z}) \qquad \text{for} \quad d = 1, 2\,.$$

This theorem was proved in [**Bel93**] for $d = 1$. Note that it solves Problem 1.15 in this case. For indeed every $\mathbb{R}$-action on a compact space reduces to a $\mathbb{Z}$-action on any transversal (the Poincaré first return map). Moreover, integrating integer-valued continuous functions on Ω is equivalent to integrating integer-valued continuous functions on a transversal.

For $d \geq 2$ an $\mathbb{R}^d$-action on a compact space does not reduce, in general, to a $\mathbb{Z}^d$-action on a transversal, so that Problem 1.15 remains open in general. However, in many cases, including quasicrystals, the K-theory can be computed through a $\mathbb{Z}^d$-action. The proof of 1.15 for $d = 2$ for some class of $\mathbb{Z}^2$-actions was given by A. van Elst [**vEl**] (see Section 6.3). Unfortunately van Elst's proof for $d = 3$ is not correct. The explicit computations provided by physicists for $3D$ quasicrystals (see for instance [**KaGr**]), give strong indications that Problem 1.15 should have a positive answer in any dimensions. In the last chapter a list of explicit useful cases will be given together with the explicit values of the set of gap labels.

2. Construction and properties of the hull

2.1. Points sets with multiplicity. Let $QD(\mathbb{R}^d) = \{\nu \in \mathcal{M}(\mathbb{R}^d); \forall x \in \mathbb{R}^d,\ \nu$ is pure point and $\nu(\{x\}) \in \mathbb{N}\}$ (cf. Section 1.2). It is straightforward to check that for each $\nu \in QD(\mathbb{R}^d)$, $L^{(\nu)} = \mathrm{supp}(\nu) = \{x; \nu(x) \geq 1\}$ is a discrete set. Let us call N_x the *multiplicity* of x, and define $N_\nu = (N_x)_{x \in L^{(\nu)}}$.

LEMMA 2.1. *$QD(\mathbb{R}^d)$ is closed in $\mathcal{M}(\mathbb{R}^d)$.*

PROOF: Let $\nu \in \mathcal{M}(\mathbb{R}^d)$ be such that $\nu = \lim_{n\to\infty} \nu_n$ where $(\nu_n)_{n\in\mathbb{N}} \in QD(\mathbb{R}^d)$. Let $x \in \mathbb{R}^d$ and $N \in \mathbb{N}$ be such that $N \leq \nu(\{x\}) < N+1$. Continuity properties of ν imply the existence of a real r such that $N \leq \nu(B(x,s)) \leq \nu(\overline{B(x,s)}) < N+1$ for $0 \leq s \leq r$. A sequence $(\nu_n)_{n\in\mathbb{N}}$ of positive Radon measures in $\mathcal{M}(\mathbb{R}^d)$ converges weakly to ν if and only if for every compact set K and for every relatively compact open set U,

$$\limsup_{n\to\infty} \nu_n(K) \leq \nu(K), \quad \text{and} \quad \liminf_{n\to\infty} \nu_n(U) \geq \nu(U). \tag{2.1}$$

Using these inequalities, for $0 < s < s' < r$ we get

$$\begin{aligned} N \;&\leq\; \limsup_{n\to\infty} \nu_n(B(x,s)) \;\leq\; \nu(\overline{B(x,s)}) \;\leq\; \cdots \\ \cdots \;&\leq\; \nu(B(x,s')) \;\leq\; \liminf_{n\to\infty} \nu_n(B(x,s')) \;<\; N+1 \end{aligned} \tag{2.2}$$

Since $\nu_n \in QD(\mathbb{R}^d)$, it follows that $\{\nu_n(B(x,s));\, n \in \mathbb{N}\} \subset \mathbb{N}$ so that the liminf and the limsup must be integers. Thus $\nu(B(x,s)) = N$ for all $0 < s < r$ implying that for all $x \in \mathbb{R}^d$, $\nu(\{x\}) \in \mathbb{N}$ and that the support $L^{(\nu)}$ of ν is a discrete set. □

Now, we are interested in defining natural compact subsets of $QD(\mathbb{R}^d)$. By "natural" we mean compact subsets which we expect to be the actual support of some Gibbs measure of the system (cf. Section 3.1). Let us first mention a general result on compactness we will extensively use afterwards.

THEOREM 2.2 ([**Bau**]). *Let E be a locally compact space and $\mathcal{M}(E)$ be the set of all Radon measures endowed with the weak-$*$ topology. A set $\mathcal{F} \subset \mathcal{M}(E)$ has a weakly compact closure if and only if*

$$\sup_{\nu\in\mathcal{F}} |\nu(f)| \;<\; \infty$$

holds for all $f \in \mathcal{C}_c(E)$.

Following Section 1.2, let us introduce

$$UD_r(\mathbb{R}^d) = \{\nu \in QD(\mathbb{R}^d); \forall x \in \mathbb{R}^d,\ \nu(B(x,r) \leq 1\}.$$

As previously noticed, for such measures N_ν is trivial and $L^{(\nu)}$ is r-discrete. Elements of $UD_r(\mathbb{R}^d)$ can then be seen as point sets in $\mathbb{R}^d$. The choice of these spaces comes from the fundamental theorem

LEMMA 2.3. *$UD_r(\mathbb{R}^d)$ is a compact subset of $QD(\mathbb{R}^d)$ which is invariant under the action of $\mathbb{R}^d$.*

PROOF: Let $f \in \mathcal{C}_c(\mathbb{R}^d)$. Let us define $\delta(f) = \inf\{R > 0; \exists x \in \mathbb{R}^d,\ \mathrm{supp}(f) \subset B(x,R)\}$. If $\nu \in UD_r(\mathbb{R}^d)$, we have $\nu(f) = \sum_{x\in L^{(\nu)}} f(x)$, then $|\nu(f)| \leq \|f\|\,|L^{(\nu)} \cap B(0,R)|$. Uniform discreteness gives

$$|L^{(\nu)} \cap B(0,R)| r^d \leq |\bigsqcup_{x\in L_\nu\cap B(0,R)} B(x,r/2)| < |B(0,R+r)|$$

where $\bigsqcup$ is a disjoint union, due to r-discreteness of ν. It implies the following bound, uniformly in ν: $|\nu(f)| \leq \|f\|.(\delta(f)/r+1)^d$. Thanks to Theorem 2.2, $UD_r(\mathbb{R}^d)$ is relatively compact. As in the proof of Lemma 2.1, a similar argument shows that $UD_r(\mathbb{R}^d)$ is closed, then compact. The translation invariance and metrizability of $UD_r(\mathbb{R}^d)$ are left to the reader. □

Let $UD(\mathbb{R}^d) := \bigcup_{r>0} UD_r(\mathbb{R}^d)$. It is the set of all uniformly discrete subsets of $\mathbb{R}^d$.

LEMMA 2.4. $\overline{UD(\mathbb{R}^d)} = QD(\mathbb{R}^d)$.

PROOF: Since $QD(\mathbb{R}^d)$ is closed, we only have to prove $QD(\mathbb{R}^d) \subset \overline{UD(\mathbb{R}^d)}$. Let ν belong to $QD(\mathbb{R}^d)$. For $n \in \mathbb{N}$ we set $L_n = L^{(\nu)} \cap B(0,n)$. For each $x \in \mathbb{R}^d$, let $e_x \in \mathbb{R}^d$ be chosen such that $|e_x|_\infty = 1$ and let $r_n > 0$ be the minimal distance between points of L_n. For $x \in L_n$ we set $y_i(x) = x + ([(i-1)r_n]/2nN_x)e_x$ for $1 \leq i \leq N_x$ and $L^{(n)} = \{y_i(x)\ ;\ x \in L_n, 1 \leq i \leq N_x\} + 2(n+r_n)\mathbb{Z}$. Remark that $(e_x)_{x\in L_n}$ is chosen such that $\{y_i(x), x \in L_n\} \subset B(0,n)$. Clearly, $L^{(n)}$ is uniformly discrete. We set $\nu_n = \nu^{(L^{(n)})} \in UD(\mathbb{R}^d)$. Now, let $f \in \mathcal{C}_c(\mathbb{R}^d)$ and $n_f \in \mathbb{N}$ be such that $\mathrm{supp}(f) \subset B(0,n_f)$. For $n \geq n_f$ we get

$$|\nu(f) - \nu_n(f)| \;\leq\; \sum_{x\in L_n}\sum_{i=1}^{N_x} |f(x + \frac{r_n(i-1)}{2nN_x}\, e_x) - f(x)| \;\leq\; \eta_f(\frac{r_n}{2n})\, \nu(B(0,n_f))$$

where η_f is the modulus of continuity of f. Thus $\nu = \lim_{n\to\infty} \nu_n$. □

2.2. Delone measures. Following the Lagarias classification of point sets, we introduce $Del_{(r,R)}(\mathbb{R}^d) = \{\nu \in UD_r(\mathbb{R}^d);\ \nu(\overline{B(x,R)}) \geq 1, \forall x \in \mathbb{R}^d\}$.

PROPOSITION 2.1. *ν belongs to $Del_{(r,R)}(\mathbb{R}^d)$ if and only if $L^{(\nu)}$ is a Delone set.*

PROOF: Obvious. □

LEMMA 2.5. *$Del_{(r,R)}(\mathbb{R}^d)$ is a compact and metrizable set, invariant under the action of $\mathbb{R}^d$.*

PROOF: Since it is included in the compact set $UD_r(\mathbb{R}^d)$, it is enough to show that $Del_{(r,R)}(\mathbb{R}^d)$ is a closed set. The same argument as in Lemma 2.1 gives this result. □

We set $Del_r(\mathbb{R}^d) = \bigcup_{R>0} Del_{(r,R)}(\mathbb{R}^d)$.

LEMMA 2.6. $\overline{Del_r(\mathbb{R}^d)} = UD_r(\mathbb{R}^d)$

PROOF: Let $\nu \in UD_r(\mathbb{R}^d)$ and for $n \in \mathbb{N}, L_n = L^{(\nu)} \cap B(0,n), L^{(n)} = L_n + 2(n+r)\mathbb{Z}$. $2R_n = \max\{2n, \sup\{d(x,y), (x,y) \in L_n \times L_n\}\}$. Then, if $L_n \neq \emptyset$, $\nu_n = \nu^{(L^{(n)})} \in Del_{(r,R_n)}(\mathbb{R}^d)$. Now, let $f \in \mathcal{C}_c(\mathbb{R}^d)$ and let $n_f \in \mathbb{N}$ be such that $\operatorname{supp}(f) \subset B(0,n_f)$. $\nu(f)$ coincides with $\nu_n(f)$ for each n greater than n_f. So, $\nu = \lim_{n\to\infty} \nu_n$. □

REMARK 2.7. $Del_r(\mathbb{R}^d)$ is not closed. However it is an F_σ, namely a countable union of closed sets.

Proof of Theorem 1.5: It follows from Lemmas 2.1, 2.3, 2.4, 2.5 and 2.6. □

2.3. General properties of the hull. Let ν be a measure in $UD_r(\mathbb{R}^d)$. Since $UD_r(\mathbb{R}^d)$ is compact, the closure Ω_ν of the $\mathbb{R}^d$-orbit of any $\nu \in UD_r(\mathbb{R}^d)$ is compact, too. Ω_ν has been called the hull of ν (see Definition 1.7).

In what follows, we will consider the hull as an abstract compact metrizable set Ω and we will denote the vector-valued measures corresponding to $\omega \in \Omega$ by $\vec{\nu}_\omega$. The first important result about the hull is the following consequence of Theorem 1.5:

THEOREM 2.8. (i) *Let $L = (L_1, \cdots, L_c)$ be a finite family of uniformly discrete point sets in $\mathbb{R}^d$ and let Ω be its hull. Then for every $\omega \in \Omega$, there is a finite family $L_\omega = (L_{\omega,1}, \cdots, L_{\omega,c})$ of uniformly discrete sets such that the vector-valued measure corresponding to ω is $\vec{\nu}_\omega = (\nu_{\omega,1}, \cdots, \nu_{\omega,c})$, with $\nu_{\omega,j} = \nu^{(L_{\omega,j})}$.*

(ii) *If, in addition, L_j is a (r,R)-Delone set, so is $L_{\omega,j}$ for any $\omega \in \Omega$.*

REMARK 2.9. Let L be a Delone set with hull Ω, and let r_0, r_1 be defined as in Section 1.2. For $\omega \in \Omega$, L_ω may have $r_0(L_\omega) > r_0$ and $r_1(L_\omega) < r_1$. An example of such a set is given as follows: let L_0 be the lattice $\mathbb{Z}^d$ in $\mathbb{R}^d$. Then L is obtained by removing 0 from L_0 and by adding $x_0 = (3/2, 1/2, \cdots, 1/2)$. Then $r_0 = 1/4$, $r_1 = 2$, whereas L_0 is clearly an element of the hull with $r_0 = r_1 = 1$. □

REMARK 2.10. If L is a finitely-generated Delone set with hull Ω, for $\omega \in \Omega$, L_ω need not be finitely generated anymore. This can be seen on the following counterexample: let $\mathcal{Z}$ be a finitely-generated dense subgroup of $\mathbb{R}^d$. Let $0 < \delta < 1/4$ and let $D = B(0,\delta)$. Let now $\underline{u} = (u_m)_{m\in\mathbb{Z}^d}$ be a sequence such that $u_m \in \mathcal{Z} \cap D$, $\forall m \in \mathbb{Z}^d$. Our example is given by $L_{\underline{u}} = \{m + u_m\ ;\ m \in \mathbb{Z}^d\}$.

By construction $L_{\underline{u}}$ is a Delone set and it is finitely generated since the differences $m + u_m - m' - u_{m'}$ all belong to $\mathcal{Z}$. Now choose $\underline{u}$ as follows: let $\underline{v} = (v_m)_{m\in\mathbb{Z}^d}$ be a sequence chosen randomly where the v_m's are considered as independent random variables, uniformly distributed on D. Then we choose $u_m \in \mathcal{Z} \cap D$ so that $|u_m - v_m|_\infty \leq 2^{-|m|_\infty}\delta$. Using the same argument as the one proved in Section 3.3, it is possible to show that the hull is homeomorphic to the *mapping torus* of $D^{\mathbb{Z}^d}$ and that, if $\underline{v} \in D^{\mathbb{Z}^d}$, the corresponding point set is $L_{\underline{v}}$. Then it is clear that $\underline{v}$ can be chosen such that $L_{\underline{v}}$ is not finitely generated. □

2.4. Dynamical properties of the hull. One can wonder whether global properties of the dynamical system defined by the hull Ω of a uniformly discrete point set L can be read off from its local properties. Among these properties, let us examine the structure of orbits. By construction the orbit of L is dense. Which conditions are necessary and sufficient for the hull to define a minimal system ? The following result give a necessary condition.

THEOREM 2.11. *Let L be uniformly discrete but not Delone. Then the hull admits one fixed point corresponding to the empty set.*

PROOF: If L is not Delone, there is a sequence $(x_n)_{n\in\mathbb{N}}$ in $\mathbb{R}^d$ such that $B(x_n, n) \cap L = \emptyset$. Therefore given any $f \in \mathcal{C}_c(\mathbb{R}^d)$ one gets $\lim_{n\to\infty} T^{-x_n}\nu^{(L)}(f) = 0$. Hence the measure $\nu_\infty = 0$ belongs to the hull and the corresponding point set is empty. It is clearly a fixed point of the translation group. □

This results shows that if L is not Delone, the hull cannot be minimal unless $L = \emptyset$. The following definition will characterize minimal hulls.

DEFINITION 2.12. Let L be a Delone set in $\mathbb{R}^d$. It is called *uniformly distributed* if and only if for every $f \in C_c(\mathbb{R}^d)$, $f \geq 0$ and every $s \in \mathbb{R}_+$ the set $L^{f,s} = \{x \in L;\ T^{-x}\nu^{(L)}(f) > s\}$ is either empty or a Delone set.

THEOREM 2.13. *Let L be a Delone set in $\mathbb{R}^d$. Then the hull Ω of L is minimal if and only if L is uniformly distributed.*

PROOF: (I) Let L be a uniformly distributed Delone set.

(i) Let ω be a point in the hull of L. Then there is a sequence $(a_l)_{l\in\mathbb{N}}$ in $\mathbb{R}^d$ such that $\nu_\omega = \nu^{(L_\omega)} = \lim_{l\to\infty} T^{a_l}\nu^{(L)}$. If $f \in \mathcal{C}_c(\mathbb{R}^d), f \geq 0$, let $t \geq 0$ so that $L^{f,t} \neq \emptyset$. Then one can find $s > t$ such that $L^{f,s} \neq \emptyset$ so that it is a Delone set. Moreover, by definition, $L^{f,s} + a = (L + a)^{f,s}$ for any $a \in \mathbb{R}^d$, so that this is also a Delone set.

(ii) We claim that $L_\omega^{f,t}$ is a Delone set for all $\omega \in \Omega$. Let us consider $L_l = L^{f,s} + a_l$, which is a Delone set, and denote by $\nu_l = \nu^{(L_l)}$ the corresponding measure. Using the Corollary 1.6 and the Theorem 2.8, it follows that ν_l has a limit point ν in $\mathcal{M}(\mathbb{R}^d)$ corresponding to a Delone set denoted by L_ν. Using the properties of the weak limit, if $x \in L_\nu$, one can find $x_l \in L_l$ such that $x = \lim_{l\to\infty} x_l$. Since $x_l \in L_l \subset L + a_l$ it follows that $x \in L_\omega$ so that $L_\nu \subset L_\omega$. By definition of the x_l's, $T^{a_l - x_l}\nu^{(L)}(f) > s$ for all $l \in \mathbb{N}$ leading to:

$$T^{a_l - x_l}\nu^{(L)}(f) \ = \ \nu^{(L+a_l)}(f \circ T^{-x_l}).$$

Since f is continuous with compact support, it is uniformly continuous so that, since x_l converges to x, there is $R_1 > 0$ with $\mathrm{supp}(f \circ T^{x_l}) \subset B(0, R_1)$ for all l. In addition, for every $\varepsilon > 0$ there is $l_0 \in \mathbb{N}$ with $\|f \circ T^{-x} - f \circ T^{-x_l}\| \leq (R_1/r_0 + 1)^{-d}\varepsilon/2$

for $l \geq l_0$. In particular, using the inequality (2.1)

$$|\nu^{(L+a_l)}(f \circ T^{-x}) - \nu^{(L+a_l)}(f \circ T^{-x_l})| \leq \varepsilon/2.$$

Moreover, since ν_ω is the limit of the $\nu^{(L+a_l)}$'s there is $l_1 \geq l_0$ so that if $l \geq l_1$, $|\nu_\omega(f \circ T^{-x}) - \nu^{(L+a_l)}(f \circ T^{-x})| \leq \varepsilon/2$. It follows that $\nu_\omega(f \circ T^{-x}) = T^{-x}\nu_\omega(f) \geq s > t$, thus $x \in L_\omega^{f,t}$. As a consequence

$$L_\nu \subset L_\omega^{f,t} \subset L_\omega.$$

Since L_ν is relatively dense, so is $L_\omega^{f,t}$ and since L_ω is uniformly discrete so is $L_\omega^{f,t}$. Hence $L_\omega^{f,t}$ is a Delone set.

(iii) To prove that the hull is minimal, it is enough to show that the orbit of L_ω is dense for all $\omega \in \Omega$. Since the orbit of L is dense by definition of the hull, it is sufficient to show that there is a sequence $(x_l)_{l\in\mathbb{N}}$ in $\mathbb{R}^d$ such that L is the limit of $L_\omega + x_l$. Without loss of generality we can assume $0 \in L$, otherwise we choose $x \in L$ and we replace L by $L - x$.

We built a sequence g_l of continuous functions with compact support as follows. Let r_0 be such that any open ball of radius r_0 contains at most one point of L. For $l \geq 1$ let $f_l(x) = \phi(l|x|_\infty/r_0)$ with

$$\phi(\xi) = \begin{cases} 1-\xi & \text{if } 0 \leq \xi \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

and

$$g_l(x) = \sum_{y \in L \cap B(0,lr_0)} f_l(y-x).$$

The properties of g_l are the following:

(a) Its support is $\text{supp}(g_l) = \bigcup_{y\in L\cap B(0,lr_0)} \overline{B(y, r_0/l)}$. For $l \geq 2$, these balls are disjoint.
(b) $0 \leq g_l(x) \leq 1$ for all $x \in \mathbb{R}^d$, and $g_l(x) = 1$ if and only if $x \in L \cap B(0, lr_0)$.
(c) Let $n_l = |L \cap B(0, lr_0)|$ and let L' be a point set in $\mathbb{R}^d$. Let us define

$$\hat{g}_l(L; L') = \sum_{x\in L'} g_l(x).$$

Then $0 \leq \hat{g}_l(L; L') \leq n_l$ and if $\text{dist}(L, L') \geq \rho$ then $\hat{g}_l(L; L') \leq n_l - l\rho/r_0$.

Thanks to (c) above, we get $\nu^{(L)}(g_l) = n_l > s_l = n_l - 1/l$, namely, since $0 \in L$, $0 \in L^{g_l,s_l}$. Since it is not empty, it must be a Delone set, because L is uniformly distributed. From part (ii) it follows that $L_\omega^{g_l,s_l}$ is a Delone set. Let then $x_l \in L_\omega^{g_l,s_l}$. This means

$$n_l - \frac{1}{l} < T^{-x_l}\nu_\omega(g_l) = \sum_{y\in L_\omega - x_l} g_l(y) = \hat{g}_l(L; L_\omega - x_l)$$

which, by the property (c) above, implies that the distance between points of L and of $L_\omega - x_l$ contained in $B(0, lr_0)$ is smaller than or equal to r_0/l^2. Hence $L_\omega - x_l$ converges (in the sense of the weak topology for measures), to L. Consequently, the hull is indeed minimal.

(II) Let L be a non-empty Delone set with minimal hull. If L is not uniformly distributed, using (I.i), there is $\omega \in \Omega$, $f \in \mathcal{C}_c(\mathbb{R}^d)$, $f \geq 0$ and $s > 0$ such that $L_\omega^{f,s} \neq \emptyset$ and $L_\omega^{f,s}$ is not a Delone set. Since $L_\omega^{f,s} \subset L_\omega$, it is uniformly discrete. Let $r > 0$ be such that every ball of radius r meets L_ω at one point at most. One can find a sequence $(x_l)_{l\in\mathbb{N}}$ in $\mathbb{R}^d$ such that the open balls $B(x_l, lr)$ never meet $L_\omega^{f,s}$.

Extracting a subsequence if necessary, there is $\sigma \in \Omega$ such that $\lim_{l\to\infty} T^{-x_l}\nu_\omega = \nu_\sigma$.

Let $x \in L_\omega^{f,s}$, then $T^{-x}\nu_\omega(f) > s$. Moreover, for $a \in \mathbb{R}^d$, $T^{-a-x_l}\nu_\omega(f)$ converges to $T^{-a}\nu_\sigma(f)$. But we remark that

$$T^{-a-x_l}\nu_\omega(f) \;=\; \sum_{y\in L_\omega - x_l} f(y-a).$$

If this sum were not vanishing, there would be $y \in L_\omega - x_l$ such that $y-a \in \operatorname{supp}(f)$, namely $|a-y|_\infty \le R$ for some $R>0$. Since the ball $B(0, lr_0)$ does not intersect $L_\omega - x_l$, it would follow that $|a|_\infty \ge lr_0 - R$. This condition cannot be satisfied for all l's, so that the sum vanishes eventually, leading to $T^{-a}\nu_\sigma(f) = 0$ for all $a \in \mathbb{R}^d$. Thus

$$\inf_{a\in\mathbb{R}^d} |T^{-x}\nu_\omega(f) - T^a\nu_\sigma(f)| \;\ge\; s \;>\; 0$$

showing that the orbit of σ is not dense, a contradiction, since we assumed the hull to be minimal. □

2.5. The canonical transversal. For usual dynamical systems where the group $\mathbb{G} = \mathbb{R}$ represents the time evolution, a transversal, also called a *Poincaré section*, is used to replace the continuous time evolution by a discrete time, through the so-called *first return map*. For other groups, this construction can be generalized by using the notion of *groupoid* [**Co79, Co94, Ren**].

A *groupoid* G is the data of two sets $G^{(0)}$, the set of *objects* or the *basis* of G, and $G^{(1)}$, the set of *arrows*, together with the following structure:

- **G1:** There are two maps $r, s : G^{(1)} \mapsto G^{(0)}$, called the *range* and the *source*, respectively. If $\gamma \in G^{(1)}$ is such that $x = s(\gamma), y = r(\gamma)$ we set $\gamma : x \mapsto y$.
- **G2:** The subset $G^{(2)}$ of $G^{(1)} \times G^{(1)}$ of pairs (γ_1, γ_2) of arrows such that $s(\gamma_1) = r(\gamma_2)$ is the set of *composable arrows*.
- **G3:** There is a *composition* $(\gamma_1, \gamma_2) \in G^{(2)} \mapsto \gamma_1 \circ \gamma_2 \in G^{(1)}$, which is associative and satisfies: $r(\gamma_1 \circ \gamma_2) = r(\gamma_1)$, $s(\gamma_1 \circ \gamma_2) = s(\gamma_2)$.
- **G4:** To each object $x \in G^{(0)}$ there is an arrow e_x, *the unit at* x, such that $r(e_x) = s(e_x) = x$ and $\forall \gamma : x \mapsto y$, $\gamma = e_y\gamma = \gamma e_x$.
- **G5:** There is a map called the *inverse* $\gamma \in G^{(1)} \mapsto \gamma^{-1} \in G^{(1)}$ such that $r(\gamma^{-1}) = s(\gamma)$, $s(\gamma^{-1}) = r(\gamma)$, with $\gamma \circ \gamma^{-1} = e_{r(\gamma)}$, $\gamma^{-1} \circ \gamma = e_{s(\gamma)}$ and also $(\gamma_1 \circ \gamma_2)^{-1} = \gamma_2^{-1} \circ \gamma_1^{-1}$.

Thanks to **G4**, $G^{(0)}$ can be identified with the set of units and becomes a subset of $G^{(1)}$. Thus G can be identified with the set $G = G^{(1)}$. The groupoid G is *topological* if both $G^{(0)}$ and $G^{(1)}$ are topological space and if all maps defined in **G1**, ... , **G5** are continuous. If $x \in G^{(0)}$ we denote by G^x the *fiber of range* x, namely the set of arrows with range x. If $X \subset G^{(0)}$, the groupoid G_X *induced by* X is defined by $G_X^{(0)} = X$ and $G_X^{(1)} = \{\gamma \in G^{(1)}\;;\; r(\gamma), s(\gamma) \in X\}$.

Given a topological dynamical system $(X, \mathbb{G})$, there is a canonical groupoid attached to it, denoted by $G = X \rtimes \mathbb{G}$ and called the *crossed product of* X *by the action of* $\mathbb{G}$. Its set of objects is X and an arrow is a pair $\gamma = (x, g) \in X \times \mathbb{G}$ with $r(x, g) = x$, $s(x, g) = g^{-1}x$ and $(x, g) \circ (g^{-1}x, g') = (x, gg')$.

A *transversal* of this (topological) dynamical system $(X, \mathbb{G})$ is a closed subset Y of X which meets every $\mathbb{G}$-orbit and such that $\{g \in \mathbb{G}; g^{-1}x \in Y\}$ is non-empty, discrete for all $x \in X$ and continuous with respect to x (let us remark that this definition is compatible with Definition 1.9).

Let $L \subset \mathbb{R}^d$ be a uniformly discrete point set with hull Ω and let $\Omega \rtimes \mathbb{R}^d$ be the corresponding groupoid. Then we get

PROPOSITION 2.2. *Let $L \subset \mathbb{R}^d$ be a uniformly discrete point set with hull Ω. The set $\Upsilon = \{\omega \in \Omega \ ; \ L_\omega \ni 0\}$ is a compact transversal such that for all $\omega \in \Omega$, $\{a \in \mathbb{R}^d \ ; \ T^a\omega \in \Upsilon\} = L_\omega$.*

PROOF: The proof is straightforward and left to the reader. □

DEFINITION 2.14. The transversal Υ defined in Proposition 2.2 is the canonical transversal attached to L. The corresponding groupoid will be denoted by G_Υ.

REMARK 2.15. Υ is compact in Ω, thus the transversal can be endowed with the topology induced by $\Omega \subset QD(\mathbb{R}^d)$.

REMARK 2.16. This groupoid plays an important rôle in our approach since it is at the origin of the so-called *tight-binding representation* (see Section 4) in which the electronic wave function is restricted to atomic sites and the Schrödinger operator is discretized to become a matrix indexed by atomic sites.

There are special cases for which the groupoid of the transversal is itself a dynamical system. An example is given as follows: let $\mathcal{R}$ be a lattice in $\mathbb{R}^d$, namely a discrete subgroup generating $\mathbb{R}^d$ as a vector space. The point set L is built as the image of a map $a \in \mathcal{R} \mapsto x_a \in \mathbb{R}^d$ such that $\sup_{a\in\mathcal{R}} |x_a - a|_\infty \leq r_2$ for some $r_2 > 0$. If $D = B(0, r_2)$ one has $u_a = x_a - a \in D$. Let then Σ be the closure in $D^{\mathcal{R}}$ of the family $\{T^a\underline{u}; a \in \mathcal{R}\}$ where $T^a\underline{u} = (u_{b-a})_{b\in\mathcal{R}}$. This is a compact space on which $\mathcal{R}$ acts through the family of homeomorphisms $(T^a)_{a\in\mathcal{R}}$. It is a simple fact that the canonical transversal of L is homeomorphic to Σ and that the corresponding groupoid is isomorphic to $\Sigma \rtimes \mathcal{R}$. One can then reconstruct the hull of L by means of the *mapping torus*, also called *suspension*. Namely, on the space $\Sigma \times \mathbb{R}^d$ there are two types of actions: (i) $\mathbb{R}^d$ itself acts through $\phi_s : (\underline{u}, x) \mapsto (\underline{u}, x + s)$; (ii) $\mathcal{R}$ acts through $\eta_a : (\underline{u}, x) \mapsto (T^a\underline{u}, x - a)$. These actions commute with each other. The quotient space $M\Sigma = \Sigma \times \mathbb{R}^d/\mathcal{R}$ inherits an action of $\mathbb{R}^d$ through the quotient map associated to ϕ. It then follows that the hull of L is homeomorphic to $M\Sigma$ and the corresponding actions of $\mathbb{R}^d$ are conjugate through this homeomorphism.

2.6. Hulls with totally disconnected transversal. If $\nu \in UD(\mathbb{R}^d)$, let $(\Omega_\nu, \mathbb{R}^d)$ be its hull. Very often, the hull is totally disconnected transversally. Which conditions on ν are sufficient to provide such a property?

Let us endow Υ with the metric δ_H defined as

$$\delta_H(\omega_1, \omega_2) = \inf\{\frac{1}{R+1}; \delta_{R,H}(\omega_1, \omega_2) \leq \frac{1}{R}, R \in \mathbb{R}_+\} \tag{2.3}$$

where $\delta_{R,H}(\omega_1, \omega_2) = d_H((L_{\omega_1} \cap B(0, R)) \cup \partial B(0, R), (L_{\omega_2} \cap B(0, R)) \cup \partial B(0, R))$ and d_H is the Hausdorff distance on point set spaces ([**RadWo, FHK2**]). It is elementary to show that the topology induced by δ_H is the weak-$*$ topology on $UD(\mathbb{R}^d)$. This confirms the intuitive view of the weak-$*$ topology outlined in Section 1.2, and precise actually the link with the hulls introduced in [**KelPu**]. As a direct consequence, δ_H endows Υ with the weak-$*$ topology (Remark 2.15).

LEMMA 2.17. *If a metric d on Υ takes values in a discrete set away from zero, Υ is totally disconnected for the topology induced by d.*

PROOF: If $B(\omega_0, r)$ is an open ball it is closed. For indeed, let $\omega \neq \omega_0$ belongs to the closed ball $\overline{B(\omega_0, r)}$. ω is a limit of points $(\omega_n)_n$ of $B(\omega_0, r)$ so that $d(\omega_0, \omega) = \lim_n d(\omega_0, \omega_n) \leq \sup_n d(\omega_0, \omega_n)$. Discretness of values taken by d away from zero implies that $\sup\{d(\omega_0, \omega_n), n \in \mathbb{N}\} \subset \{d(\omega_0, \omega_n), n \in \mathbb{N}\}$. Thus ω belongs to $B(\omega_0, r)$, too, and the ball is closed. □

PROPOSITION 2.3. *Let* $\Omega_R(\nu) = \overline{\bigcup_{x \in \mathrm{supp}(\nu)} \mathrm{supp}(T^{-x}\nu) \cap B(0, R)}$. *If for every* $R > 0$, $\Omega_R(\nu)$ *has no accumulation point, then the transversal* Υ *of* Ω_ν *is totally disconnected for the topology induced by the metric* δ_H.

PROOF: Let $\rho(R)$ be the number of points in $\Omega_R(\nu)$. Since $\Omega_R(\nu)$ is finite for all $R > 0$, ρ is finite on $\mathbb{R}_+$, integer-valued, and non-decreasing. Thus the set $D(\nu) = \{R; |\Omega_{R+\epsilon}(\nu)| > |\Omega_{R-\epsilon}(\nu)|, \epsilon \in \mathbb{R}_*^+, R \in \mathbb{R}_+\}$ is discrete. Let $d_{u.m}$ be the distance defined by $d_{u.m}(\omega_1, \omega_2) = \inf\{1/(R+1); d_H(L_{\omega_1} \cap B(0, R), L_{\omega_2} \cap B(0, R)) = 0, R \in \mathbb{R}_+\}$. The set of values of $d_{u.m}$ on Υ is included in $\{1/(R+1); R \in D(\nu), R \in \mathbb{R}_+\}$ and is discrete away from zero. By Lemma 2.17, the topology induced by $d_{u.m}$ on Υ is totally disconnected. It is elementary to check that this topology coincides with weak-$*$ topology on Υ. □

REMARK 2.18. Kellendonk proves a similar result in [**Kel1**] (ref. (a) p. 122).

COROLLARY 2.1. *Let* $\nu \in UD(\mathbb{R}^d)$ *with* L_ν *a Delone set of finite type. Then the transversal* Υ *of* Ω_ν *is totally disconnected.*

PROOF: For every $R > 0$ and every Delone set of finite type L the set $L - L \cap B(0, R)$ is finite. Therefore $\Omega_R(\nu)$ in Proposition 2.3 has no accumulation point. □

2.7. Hull of a Schrödinger operator. Let us consider a Schrödinger operator on $L^2(\mathbb{R}^d)$

$$H = (\vec{P} - e\vec{A})^2/2m + V = H_0 + V\ , \tag{2.4}$$

where V is the effective potential seen by an electron and $\vec{A}$ is the vector potential corresponding to a uniform magnetic field. In general H is not translation invariant. However, the physical properties of a homogeneous medium do not depend upon the choice of an origin. In particular, H can be replaced by any of its translated $H_x = U(x)HU(x)^{-1},\ x \in \mathbb{R}^d$, and the physics will be the same. This choice being arbitrary, the smallest possible algebra of observables should contain all bounded functions of the $\{H_x,\ x \in \mathbb{R}^d\}$'s. Following [**Bel93**], the homogeneity of the Hamiltonian H will be defined by:

DEFINITION 2.19. Let $\mathcal{H}$ be a Hilbert space with a countable basis. Let $\mathbb{G}$ be a locally compact group (for instance $\mathbb{R}^d$ or $\mathbb{Z}^d$). Let U be a unitary projective representation of $\mathbb{G}$, namely for each $a \in \mathbb{G}$ there is a unitary operator $U(a)$ acting on $\mathcal{H}$ such that the family $U = \{U(a);\ a \in \mathbb{G}\}$ satisfies the following properties:

(i) $U(a)U(b) = U(a+b)e^{i\phi(a,b)}$, where $\phi(a,b)$ is some phase factor.
(ii) For each $\psi \in \mathcal{H}$, the map $a \in \mathbb{G} \to U(a)\psi \in \mathcal{H}$ is continuous.

Then a self-adjoint operator H on $\mathcal{H}$ is *homogeneous* with respect to $\mathbb{G}$ if the family $S = \{R_a(z) = U(a)(z\,\mathbf{1} - H)^{-1}U(a)^{-1};\ a \in \mathbb{G}\}$ admits a compact closure in the strong operator topology (for some $z \in \mathbb{C}$).

Let us now define the "hull" of a homogeneous operator H . For z in the resolvent set $\rho(H)$ of H, let $\Omega_H(z)$ be the strong closure of the family $\{R_a(z) = U(a)(z\mathbf{1} - H)^{-1}U(a)^{-1};\ a \in \mathbb{G}\}$. By definition of homogeneity, it is a metrizable compact space. Moreover, $\Omega_H(z)$ is endowed with a $\mathbb{G}$-action by means of the representation U of $\mathbb{G}$. Actually, $\Omega_H(z)$ does not depend on the choice of z [**Bel93**]. Identifying $\Omega_H(z)$ and $\Omega_H(z')$ for $z, z' \in \mathbb{C}$ gives rise to an abstract compact space Ω_H endowed with an action of $\mathbb{G}$. If $\omega \in \Omega_H$ and $a \in \mathbb{G}$ we will denote by $T^a\omega$ the result of the action of a on ω, and $R(z,\omega)$ the representative of ω in $\Omega_H(z)$. Then one gets

$$\begin{aligned} U(a)R(z,\omega)U(a)^{-1} &= R(z,T^a\omega)\ , \\ R(z',\omega) - R(z,\omega) &= (z-z')R(z,\omega)R(z',\omega) = (z-z')R(z',\omega)R(z,\omega) \end{aligned}$$

In addition, $z \to R_\omega(z)$ is norm-holomorphic in $\rho(H)$ for every $\omega \in \Omega_H$, and $\omega \to R_\omega(z)$ is strongly continuous.

DEFINITION 2.20. Let H be a homogeneous operator on the Hilbert space $\mathcal{H}$ with respect to the representation U of the locally compact group $\mathbb{G}$. Then the *hull* of H is the dynamical system $(\Omega_H, \mathbb{G}, T)$, where Ω_H is the (abstract) compact space given by the strong closure of the family $\{R_a(z) = U(a)(z\mathbf{1}-H)^{-1}U(a)^{-1};\ a \in \mathbb{G}\}$ for some $z \in \rho(H)$, and the $\mathbb{G}$-action T on Ω_H is induced by U.

In the case of a Schrödinger operator (2.4) the situation has been clarified in [**Bel93**]. The vector potential $\vec{A}$ satisfies

$$\partial_\mu A_\nu - \partial_\nu A_\mu = B_{\mu\nu} = \text{const.} \tag{2.5}$$

and therefore the kinetic part H_0 is actually translation invariant provided one uses the magnetic translations (1.9).

THEOREM 2.21. [**Bel93, NaBel**] *Let $H = H_0 + V$ be given by (2.4) with $V \in L^\infty_{\mathbb{R}}(\mathbb{R}^d)$, i.e. a real, measurable, essentially bounded function over $\mathbb{R}^d$. Then H is homogeneous with respect to the representation of $\mathbb{R}^d$ given by* (1.9)*. Moreover, the hull of H is homeomorphic to the weak closure Ω_V of the family $\{U(a)VU(a)^{-1}; a \in \mathbb{R}^d\}$ in the space $L^\infty_{\mathbb{R}}(\mathbb{R}^d)$ endowed with the weak topology w.r.t. $L^1(\mathbb{R}^d)$. Furthermore, there exists a Borelian function v on Ω_V such that $V_\omega(x) = v(T^{-x}\omega)$ for almost every $x \in \mathbb{R}^d$ and every $\omega \in \Omega_V$. If in addition V is uniformly continuous, then v is continuous.*

The Schrödinger operator (1.1) acting on $\mathcal{H} = L^2(\mathbb{R}^d)$ was given by

$$H = -\frac{\hbar^2}{2m}\Delta + \sum_{j=1}^{c}\sum_{y\in L_j} v_j(\ .\ - y) = -\frac{\hbar^2}{2m}\Delta + \sum_{j=1}^{c} \nu_j * v_j\ . \tag{2.6}$$

where $v_j(\ .\ - y)$ is the effective potential for valence electrons due to an atom of species j at position y. Here $\nu_j * v_j$ denotes the convolution of the measure $\nu_j = \nu^{(L_j)}$ and of the potential v_j. For simplicity, we assume in the following that we have only one species of atoms and that the point set of atomic positions is r-discrete. The second sum in (2.6) being infinite, the following lemma provides a sufficient condition for its convergence. Let

$$L^1_{K,r}(\mathbb{R}^d) = \{f \in L^1(\mathbb{R}^d); |f(x)| \le \frac{K}{r^d}\int_{|x-y|<r/2} d^dy|f(y)|, \quad \text{for a.e. x}\}$$

be the set of integrable K-subharmonic functions on $\mathbb{R}^d$. It is elementary to check that $L^1_{K,r}(\mathbb{R}^d)$ is closed in $L^1(\mathbb{R}^d)$ and contained in $L^\infty(\mathbb{R}^d)$.

LEMMA 2.22. *Let $v \in L^1_{K,r}(\mathbb{R}^d)$. Then $\nu * v \in L^\infty_{\mathbb{R}}(\mathbb{R}^d)$ and the map $v \mapsto \nu * v$ is continuous.*

PROOF: For almost all $x \in \mathbb{R}^d$,

$$\begin{aligned} |\nu * v(x)| = |\sum_{y\in L^{(\nu)}} v(x-y)| &\le \sum_{y\in L^{(\nu)}} |v(x-y)| \\ &\le \sum_{y\in L^{(\nu)}} \left\{ \frac{K}{r^d} \int_{|y'-(x-y)|<r/2} d^d y' |v(y')| \right\}. \end{aligned}$$

Since $\nu \in UD_r(\mathbb{R}^d)$, $L^{(\nu)}$ is r-discrete and we get

$$\begin{aligned} \sum_{y\in L^{(\nu)}} \left\{ \frac{K}{r^d} \int_{|y'-(x-y)|<r/2} d^d y' |v(y')| \right\} &\le \frac{K}{r^d} \int_{\mathbb{R}^d} d^d y' |v(y')| \\ &\le \frac{K}{r^d} \|v\|_1. \end{aligned}$$

□

According to Theorem 2.21 and Lemma 2.22, the Hamiltonian (2.6) is homogeneous if $\nu \in UD_r(\mathbb{R}^d)$ and its hull is well defined. As outlined in Section 1.2, the definition of the hull of an operator came earlier than the definition of the hull of a point set. The following gives a link between these two notions:

THEOREM 2.23. *Let $v \in L^1_{K,r}(\mathbb{R}^d)$ be a real-valued atomic potential. For $\nu \in UD_r(\mathbb{R}^d)$ the map $\varphi_v : T^a_1(\nu) \in \Omega_\nu \to U(a)R_z(H_\nu)U(a)^{-1}$ can be continued in a unique way as a surjective, strongly continuous function from Ω_ν onto $\Omega_H(z)$ fulfilling*

$$\varphi_v \circ T^x_1(\omega) = U(x)R_z(H_\omega)U(x)^{-1} \,. \tag{2.7}$$

In particular, φ_v semi-conjugate the hull of ν, $(\Omega_\nu, \mathbb{R}^d, T_1)$, and the hull $(\Omega_H, \mathbb{R}^d, T_2)$ of the Schrödinger operator H.

PROOF: By Lemma 2.22, we have $\nu_\omega * v \in L^\infty_{\mathbb{R}}(\mathbb{R}^d)$. We will prove that $\omega \in \Omega_\nu \to \nu_\omega * v \in L^\infty_{\mathbb{R}}(\mathbb{R}^d)$ is continuous in the sense of Theorem 2.21 implying the continuity of φ_v.

For $f \in L^1(\mathbb{R}^d)$, let $f_n \in C_c(\mathbb{R}^d)$, $n \in \mathbb{N}$ be such that $\lim_{n\to\infty} \|f_n - f\|_1 = 0$ and let $v_k \in C_c(\mathbb{R}^d) \cap L^1_{K,r}(\mathbb{R}^d), k \in \mathbb{N}$, be such that $\lim_{k\to\infty} \|v_k - v\|_1 = 0$. Let $\omega, \omega_l \in \Omega_\nu$, $l \in \mathbb{N}$ be such that $\lim_{l\to\infty} \omega_l = \omega$ and let us define $L_l = \mathrm{supp}(\nu_{\omega_l}), L = \mathrm{supp}(\nu_\omega)$. Then

$$\begin{aligned} |\langle f|(\nu_{\omega_l} * v - \nu_\omega * v)\rangle| \le\ & |\langle f - f_n|(\nu_{\omega_l} * v - \nu_\omega * v)\rangle| \\ & + |\langle f_n|(\nu_{\omega_l} * v - \nu_{\omega_l} * v_k) - (\nu_\omega * v - \nu_\omega * v_k)\rangle| \\ & + |\langle f_n|\nu_{\omega_l} * v_k - \nu_\omega * v_k)\rangle| \end{aligned}$$

The first term is bounded by:

$$\left\|(\nu_{\omega_l} * v - \nu_\omega * v)\right\|_\infty \int |f(y) - f_n(y)|\, dy \;\le\; 2\, \frac{K}{r^d} \|v\|_1 \left\|f - f_n\right\|_1 ,$$

the second term by:

$$\left\|(\nu_{\omega_l}-\nu_\omega)*(v-v_k)\right\|_\infty \left\|f_n\right\|_1 \;\leq 2\,\frac{K}{r^d}\left\|f_n\right\|_1 \left\|v-v_k\right\|_1$$

(we use Lemma 2.22), and the third by:

$$|\langle f_n*\check{v}_k|\nu_\omega-\nu_{\omega_l}\rangle|$$

where $\check{v}(x)=v(-x)$. Since $f_n*\check{v}_k\in\mathcal{C}_c(\mathbb{R}^d)$, this third term tend to zero for $l\to\infty$ by definition of the weak-$*$ topology on the space of measures. The continuity follows from a 3ε argument. The covariance property (2.7) is obvious and is left to the reader. The surjectivity follows from the continuity of φ_v: the image of Ω_ν is compact and the orbit of $R_z(H_\nu)$ is dense in it. Therefore this image coincides with the operator hull. Hence, φ_v semi-conjugate the two dynamical systems. □

COROLLARY 2.2. *Let $\nu\in UD_r(\mathbb{R}^d)$ and $v\in L^1_{K,r}(\mathbb{R}^d)$ be a real-valued atomic potential with* supp $(v)\subset B(0,r_v)$ *for some $r_v\leq r$. Then the map φ_v of Theorem 2.23 is one-to-one.*

PROOF: According to Theorem 2.23 it is enough to prove that the map φ_v is injective. Let $\nu_1,\nu_2\in\Omega_\nu$ and let x be such that $\nu_1*v(x)=\nu_2*v(x)\neq 0$. Then, there exists $(y_1,y_2)\in L^{(\nu_1)}\times L^{(\nu_2)}$ such that $x\in\Delta=B(y_1,r_v)\cap B(y_2,r_v)$. If $y_1\neq y_2$ then $B(y_2,r_v)\setminus\Delta\neq\emptyset$. Since $r_v\leq r$, $I=B(y_1,r)\cap[B(y_2,r_v)\setminus\Delta]\neq\emptyset$. Let $x'\in I$, then $\forall y\in L^{(\nu_1)}$ $v(x'-y)=0$, but $v(x'-y_2)\neq 0$, a contradiction. Thus $\nu_1=\nu_2$. □

Let us conclude this section by the following result.

THEOREM 2.24. [**Bel93**] *Let H be the Schrödinger operator $H=\Delta+V$ with $V\in L^\infty(\mathbb{R}^d)$ and let $(\Omega_H,\mathbb{R}^d,T)$ be the hull of H. Then for each z in the resolvent set of H and for every $x\in\mathbb{R}^d$ there is an element $r(z;x)\in C^*(\Omega_H\times\mathbb{R}^d,B)$, such that for each $\omega\in\Omega_H$, we have $\Pi_\omega(r(z;x))=(z-H_{T^{-x}\omega})^{-1}$.*

COROLLARY 2.3. *Let $\nu\in UD_r(\mathbb{R}^d)$ and let $(\Omega_\nu,\mathbb{R}^d)$ be the hull of ν. Let H be the Schrödinger operator (2.6). Then for each z in the resolvent set of H, and for every $x\in\mathbb{R}^d$, there is an element $r(z,x)\in C^*(\Omega_\nu\times\mathbb{R}^d,B)$, such that for each $\omega\in\Omega_\nu$, we have $\Pi_\omega(r(z,x))=(z-H_{T^{-x}\omega})^{-1}$.*

PROOF: By Theorem 2.23 the two hulls are semi-conjugate. Hence $C^*(\Omega_H\times\mathbb{R}^d,B)$ is *-isomorphic to a subalgebra of $C^*(\Omega_\nu\times\mathbb{R}^d,B)$. □

Though Theorem 2.24 shows that the C^*-algebra generated by H and its translates lies in $C^*(\Omega_H\times\mathbb{R}^d)$, we do not know under which conditions $C^*(\Omega_H\times\mathbb{R}^d)$ is strictly larger.

3. Hulls and thermodynamics

In this section, we will explicitly compute the hull of the few examples of realistic solids we quote in Section 1.2. We develop here a new point of view in comparison with [**Bel86, Bel93**], by emphasizing upon the Gibbs measure describing the thermal equilibrium of the solid under consideration, as a natural choice of an invariant ergodic measure for taking space averages. This point of view is developed in Section 3.1 below. We follow an approach already suggested by Radin [**Rad**] on the basis of works done in rigorous statistical mechanics [**Rue, Sin**]. Then in Section 3.3, we built the hull for a random distribution of impurities in a crystal. In

Section 3.4 we consider the case of a quasicrystal for which the hull is explicitly constructed supplementing various results obtained previously [**BCL, Kel1, PuAn**].

3.1. Thermal equilibrium for atoms. It follows from the definition of $QD(\mathbb{R}^d)$ (see Section 2) that it is a *Polish space* [**Par**], namely a metrizable space with a metric making it complete. In $QD(\mathbb{R}^d)$ there are two special families of compact spaces given by the $UD_r(\mathbb{R}^d)$'s and the $Del_{(r,R)}(\mathbb{R}^d)$'s with $r>0, R>0$ and $\overline{UD(\mathbb{R}^d)} = \overline{Del(\mathbb{R}^d)} = QD(\mathbb{R}^d)$ (see Theorem 1.5). This structure motivates the following definitions (for a discussion see Section 1.3). Let $\mathbb{P}$ be a probability measure on $QD(\mathbb{R}^d)$:

G1: $\mathbb{P}$ is *uniformly discrete* namely, it gives probability one to $UD(\mathbb{R}^d)$.
G1': $\mathbb{P}$ is *Delone*, namely it gives probability one to $Del(\mathbb{R}^d)$.
G2: $\mathbb{P}$ is translation invariant.
G3: $\mathbb{P}$ is ergodic with respect to the translation group.

Proof of Theorem 1.10: Let $\mathbb{P}$ satisfy **G1**. One remembers that

$$r_1 > r_2 \Rightarrow UD_{r_2}(\mathbb{R}^d) \subset UD_{r_1}(\mathbb{R}^d), \forall r_1, r_2 > 0.$$

Let then $(r_n)_{n\in\mathbb{N}}$ be a decreasing sequence of positive numbers, converging to zero. We get $\lim_n \mathbb{P}(UD_{r_n}(\mathbb{R}^d)) = \mathbb{P}(\lim_n UD_{r_n}(\mathbb{R}^d)) = \mathbb{P}(UD(\mathbb{R}^d)) = 1$. Thus, $\forall\epsilon > 0$ there exists $r_0 > 0$ such that $\forall r \le r_0, \mathbb{P}(UD_r(\mathbb{R}^d)) \ge 1-\epsilon$. Since $\mathbb{P}$ is $\mathbb{R}^d$-invariant and ergodic, and since $UD_r(\mathbb{R}^d)$ is an $\mathbb{R}^d$-invariant compact set, for all $r>0$, $\mathbb{P}(UD_r(\mathbb{R}^d)) = 0$ or 1. Let $r_0 = \sup\{r > 0; \mathbb{P}(UD_r(\mathbb{R}^d)) = 1\}$. Since $\bigcap_{r<r_0} UD_r(\mathbb{R}^d) = UD_{r_0}(\mathbb{R}^d)$, by σ-additivity, we get $\mathbb{P}(UD_{r_0}(\mathbb{R}^d)) = 1$. Moreover, by definition of r_0 we also get $\mathbb{P}(UD_r(\mathbb{R}^d)) = 0$ for $r > r_0$. Hence $\mathbb{P}$ is concentrated on $UD_{r_0}(\mathbb{R}^d) \setminus \bigcup_{r>r_0} UD_r(\mathbb{R}^d)$. If $\mathbb{P}$ satisfies condition **G1'** instead of **G1**, a similar argument proves that $\mathbb{P}$ is concentrated on $Del_{(r_0,R_0)}(\mathbb{R}^d)\setminus\bigcup_{r>r_0,R<R_0} Del_{(r,R)}(\mathbb{R}^d)$ in $QD(\mathbb{R}^d)$. □

Proof of Theorem 1.11: The proof of Theorem 1.11 is a simple corollary of the following lemma, that is a general property of topological dynamical systems. If $\mathbb{P}$ satisfy condition **G1'** instead of **G1**, a similar argument prove the concentration of $\mathbb{P}$ on a $Del_{(r_0,R_0)}(\mathbb{R}^d) \subset QD(\mathbb{R}^d)$. □

LEMMA 3.1. *Let X be a compact metrizable set, $\mathbb{G}$ a group acting on X, and $\mathbb{P}$ an ergodic and $\mathbb{G}$-invariant probability measure on X. Then* $\mathrm{supp}(\mathbb{P}) = \overline{Orb(x)}$ *for $\mathbb{P}$-almost every $x \in X$.*

PROOF: In the following the support of $\mathbb{P}$ will be denoted by Ω and the closure of the orbit of $x \in X$ by Ω_x.

(I) Let f be a continuous function on Ω. By Birkhoff's theorem there is a $\mathbb{P}$-measurable set $\Sigma_f \subset \Omega$ such that $\mathbb{P}(\Sigma_f) = 1$ and $\forall y \in \Sigma_f$:

$$\lim_{\Lambda\to\mathbb{R}^d} \frac{1}{|\Lambda|}\int_{a\in\Lambda} f(T^a y) = \int_\Omega d\mathbb{P}(y) f(y)$$

Since X is metrizable, so does Ω, so that there is a countable dense subset $(f_n)_{n\in\mathbb{N}}$ in $\mathcal{C}(\Omega)$. If $\Sigma_\infty = \cap_n \Sigma_{f_n}$, the σ-additivity of $\mathbb{P}$ gives $\mathbb{P}(\Sigma_\infty) = 1$.

(II) Now, for $f \in \mathcal{C}(\Omega)$ and $y \in \Sigma_\infty$ we set:

$$I_{(\Lambda,y)}(f) = \int_\Omega d\mathbb{P}(y')f(y') \; - \frac{1}{|\Lambda|}\int_{a\in\Lambda} f(T^a y)$$

If $\epsilon > 0$, let $N \in \mathbb{N}$ be such that $\|f - f_n\| < \epsilon/2, \forall n \geq N$. Using $|I_{(\Lambda,y)}| \leq 2\|f\|$, we get $|I_{(\Lambda,y)}(f) - I_{(\Lambda,y)}(f_n)| = |I_{(\Lambda,y)}(f - f_n)| \leq \epsilon$. This result holds for every $\epsilon > 0$. Since $\lim_\Lambda |I_{(\Lambda,y)}(f_n)| = 0$, one has $\limsup_\Lambda |I_{(\Lambda,y)}(f)| = 0$ for all $y \in \Sigma_\infty$.

(III) Ω being the support of $\mathbb{P}$, it is the smallest closed subset of X such that any open subset O of X with $O \cap \Omega \neq \emptyset$ satisfies $\mathbb{P}(O) > 0$. Let $x \in \Omega$ be such that $\Omega_x \subset \Omega$ and $\Omega_x \neq \Omega$. Let then $y \in \Omega \setminus \Omega_x$. Since Ω_x is closed, there is an open set $O \ni y$ such that $O \cap \Omega_x = \emptyset$. Since X is metrizable, there is an open set $O' \subset O$, such that $\overline{O'} \subset O$ and $\mathbb{P}(O') = \epsilon > 0$. By Urysohn's lemma [**ReSi**], there is a continuous function f, vanishing on $\overline{O'}$, taking the value one on Ω_x and such that $0 \leq f \leq 1$. In particular $0 \leq \int_\Omega d\mathbb{P} f \leq 1 - \epsilon$. Then $\forall x' \in \Omega_x$,

$$1 \;=\; \lim_{\Lambda \to \mathbb{R}^d} \frac{1}{|\Lambda|} \int_{a \in \Lambda} f(T^a x') \;>\; \int_\Omega d\mathbb{P}(y)\, f(y). \tag{3.1}$$

It follows from (I) and (II) that $x \notin \Sigma_\infty$, so that the set of x's for which $\Omega_x \neq \Omega$ has $\mathbb{P}$-measure zero. □

3.2. Diffraction measure. *Proof of Theorem 1.12:* The existence of the limit will be proved by using subadditivity and the Birkhoff ergodic theorem.

(i) Since $\mathbb{P}$ is translation invariant, one has $\rho_{\mathbb{P}}^{(\Lambda)} = \rho_{\mathbb{P}}^{(\Lambda+x)}$ for all $x \in \mathbb{R}^d$. Therefore one can always choose Λ of the form $\Lambda_R = (0, R)^{\times d}$. We also remark that if $R' > R$ then

$$\frac{|\Lambda_{R'} \setminus \Lambda_R|}{|\Lambda_R|} \leq d \left(\frac{R'}{R}\right)^{d-1} \frac{R' - R}{R}$$

Let now f be a continuous function with compact support contained in the ball $B(0, r(f))$. For $\nu \in QD(\mathbb{R}^d)$, we set $f_\nu(x) = \sum_{y \in \mathbb{R}^d} f(x - y)\nu(\{y\})$. Since $\mathbb{P}$ is supported by $UD_r(\mathbb{R}^d)$, for $\mathbb{P}$-almost every ν we get (if $L^{(\nu)}$ is the support of ν)

$$\|f_\nu\| \;=\; \sup_x |\sum_{y \in L^{(\nu)}} f(x - y)| \;\leq\; \|f\| \left(\frac{r(f)}{r} + 1\right)^d \;=\; C_0(f)$$

where $\|f\| = \sup_{x \in \mathbb{R}^d} |f(x)|$. Hence $|\rho_\nu^{(\Lambda)}(f)| \leq C_0(f)$ uniformly with respect to $R > 0$ and to $\nu \in UD_r(\mathbb{R}^d)$. This shows in particular that the family $\rho_\nu^{(\Lambda)}$ is compact in $\mathcal{M}(\mathbb{R}^d)$, so that limit points do exist. We also conclude that if

$$S_\nu^{\Lambda,\Lambda'}(f) \;=\; \sum_{x \in \Lambda \cap L^{(\nu)}} \left(\sum_{y \in \Lambda' \cap L^{(\nu)}} f(x - y)\right)$$

then, if both Λ and Λ' are hypercubes

$$|S_\nu^{\Lambda,\Lambda'}(f)| \;\leq\; C(f)\; \min\left(|\Lambda|, |\Lambda'|\right) \tag{3.2}$$

with $C(f) = C_0(f) \max\left((2/r)^d, 1\right)$. Let R_1, R be real numbers such that $2r(f) < R_1 < R$. Let $a \in \mathbb{N}$ be the integer such that $aR_1 < R \leq (a+1)R_1$. Let $\Lambda, \Lambda_a, \delta\Lambda, \Lambda_1$ denote respectively $\Lambda_R, (0, aR_1]^d, \Lambda_R \setminus \Lambda_a$ and $(0, R_1]^d$. Then

$$S_\nu^{\Lambda,\Lambda}(f) \;=\; S_\nu^{\Lambda_a,\Lambda_a}(f) + S_\nu^{\Lambda_a,\delta\Lambda}(f) + S_\nu^{\delta\Lambda,\Lambda_a}(f) + S_\nu^{\delta\Lambda,\delta\Lambda}(f)$$

Using the previous bound (3.2), we get

$$|\rho_\nu^{(\Lambda)}(f) - \rho_\nu^{(\Lambda_a)}(f) \;\leq\; \frac{2^{d+1} d C(f)}{a}$$

One now decomposes Λ_a into the (disjoint) union of the smaller hypercubes $\Lambda(k) = \Lambda_1 + kR_1$ where $k \in I_a = \{0, \cdots, a-1\}^d$

$$S_\nu^{\Lambda_a,\Lambda_a}(f) = \sum_{k,k' \in I_a} S_\nu^{\Lambda(k),\Lambda(k')}(f)$$

Since $f(x-y) = 0$ whenever $|x-y|_\infty \geq r(f)$, we conclude that $\sum_{k' \in I_a} S_\nu^{\Lambda(k),\Lambda(k')}(f)$ coincides with $S_\nu^{\Lambda(k),\Lambda(k)'}(f)$ if $\Lambda(k)'$ is the set of points in $\mathbb{R}^d$ within a distance at most $r(f)$ from $\Lambda(k)$. Thus if $\delta\Lambda(k) = \Lambda(k)' \setminus \Lambda(k)$, we do get

$$S_\nu^{\Lambda_a,\Lambda_a}(f) = \sum_{k \in I_a} \left(S_\nu^{\Lambda(k),\Lambda(k)}(f) + S_\nu^{\Lambda(k),\delta\Lambda(k)}(f) \right)$$

This implies, using again the same estimates,

$$|\rho_\nu^{(\Lambda_a)}(f) - \frac{1}{a^d} \sum_{k \in I_a} \rho_{T^{-kR_1}\nu}^{(\Lambda_1)}(f)| \leq \frac{2^{d-1} d r(f) C(f)}{R_1} \tag{3.3}$$

In particular, integrating over ν with respect to $\mathbb{P}$ gives

$$|\rho_{\mathbb{P}}^{(\Lambda_a)}(f) - \rho_{\mathbb{P}}^{(\Lambda_1)}(f)| \leq \frac{2^{d-1} d r(f) C(f)}{R_1}$$

There is no loss of generality in assuming that $f \geq 0$. Then, gluing the previous estimates together leads to

$$\limsup_{R \uparrow \infty} \rho_{\mathbb{P}}^{(\Lambda_R)}(f) \leq \inf_{R_1} \rho_{\mathbb{P}}^{(\Lambda_1)}(f)$$

showing that both sides converge to some measure $\rho_{\mathbb{P}}(f)$.

(ii) Since the Fourier transform of $\rho_{\mathbb{P}}^{(\Lambda)}$ is a positive measure for any Λ, one has equivalently

$$\int_{\mathbb{R}^d} d\xi \overline{f(\xi)} \int_{\mathbb{R}^d} d\rho_{\mathbb{P}}^{(\Lambda)}(\eta) f(\xi - \eta) \geq 0$$

for all Λ . Therefore this is also true in the limit, showing that the Fourier transform of $\rho_{\mathbb{P}}$ is a positive measure (Bochner theorem).

(iii) If $\mathbb{P}$ is ergodic, using Birkhoff's ergodic theorem, we obtain that the sum $a^{-d} \sum_{k \in I_a} \rho_{T^{-kR_1}\nu}^{(\Lambda_1)}(f)$ converges $\mathbb{P}$-almost surely to $\rho_{\mathbb{P}}^{(\Lambda_1)}(f)$. It follows from (3.3) that $\mathbb{P}$-almost surely

$$\lim_{R \uparrow \infty} \rho_\nu^{(\Lambda_R)}(f) = \rho_{\mathbb{P}}(f).$$

□

3.3. Impurities in a crystal. Our first example of point sets is given by impurities in a crystal. A typical example in solid state physics is given by doped semiconductor. Let $\mathcal{R}$ be a lattice of $\mathbb{R}^d$. We denote by $\mathfrak{C}$ a discrete $\mathcal{R}$-invariant subset of $\mathbb{R}^d$. Any crystal is represented by such point set. To each type of atomic species that can be found in the crystal, one associates a *letter* $\mathfrak{a}, \mathfrak{b}, \ldots$. The set $\mathfrak{A}$ of such letters will be called an *alphabet* and will be assumed to be finite. An *atomic configuration* is a sequence $\omega = (\omega_x)_{x \in \mathfrak{C}}$ with $\omega_x \in \mathfrak{A}, \forall x \in \mathfrak{C}$. We will set $\Omega_\infty = \mathfrak{A}^{\mathfrak{C}}$ for the space of atomic configurations. It is compact if endowed with the product topology. If $a \in \mathcal{R}$ we set $T^a\omega = (\omega_{x-a})_{x \in \mathfrak{C}}$. The maps T^a $(a \in \mathcal{R})$ define an action of $\mathcal{R}$ by homeomorphisms. To each $\omega \in \Omega_\infty$ we associate the following subsets of $\mathfrak{C}$

$$\mathfrak{a} \in \mathfrak{A} \quad \Rightarrow \quad L_\omega(\mathfrak{a}) = \{x \in \mathfrak{C}\,;\, \omega_x = \mathfrak{a}\}$$

By construction, $L_\omega(\mathfrak{a})$ is uniformly discrete and $L_\omega(\mathfrak{a})+a = L_{T^a\omega}(\mathfrak{a})$. Conversely, any partition of $\mathfrak{C}$ by subsets $L_\mathfrak{a},\ \mathfrak{a}\in\mathfrak{A}$ defines a unique atomic configuration by setting $\omega^L = (\omega_x)_{x\in\mathfrak{C}}$ with $\omega_x = \mathfrak{a}$ if and only if $x \in L(\mathfrak{a})$. Therefore the *hull* of the family $\{L(\mathfrak{a})\ ;\ \mathfrak{a}\in\mathfrak{A}\}$ under translations by $\mathcal{R}$ can be identified with the closure of the family of translates of ω^L. Then we set $\forall\omega\in\Omega_\infty,\ \Omega_\omega\ =\ \overline{\{T^a\omega; a\in\mathcal{R}\}}$. Ω_ω is called the $\mathcal{R}$-hull of ω.

Let now $\mathbb{P}$ be a $\mathcal{R}$-invariant ergodic probability measure on Ω_∞. We say that $\mathbb{P}$ is *doping* whenever for any finite subset Λ of $\mathfrak{C}$ and any configuration $\sigma_\Lambda\in\mathfrak{A}^\Lambda$,

$$\mathbb{P}(\{\omega\in\Omega_\infty\ ;\ \omega\restriction_\Lambda = \sigma_\Lambda\}) > 0\,.$$

Good examples of such probability measures are provided by *Gibbs states* describing *pure phases* at non-zero temperature for the thermal distribution of impurities [**Rue**]. More precisely, Gibbs measures have always exponential factors which forbid finite volume configurations of zero probability (doping property).

THEOREM 3.2. *Let $\mathbb{P}$ be a $\mathcal{R}$-invariant ergodic and doping probability measure on Ω_∞. Then, for $\mathbb{P}$-almost every $\omega\in\Omega_\infty$ the $\mathcal{R}$-hull Ω_ω coincides with $\Omega_\infty = \mathfrak{A}^\mathfrak{C}$.*

PROOF: Doping property implies that each cylinder of $\mathfrak{A}^\mathfrak{C}$ is contained in $\mathrm{supp}(\mathbb{P})$. Since the set of cylinders is a basis of open sets for the topology of $\mathfrak{A}^\mathfrak{C}$, $\mathrm{supp}(\mathbb{P}) = \Omega_\infty$. Lemma 3.1 then gives the result. □

3.4. Hull of quasicrystals. In 1984, Shechtman, Blech, Gratias and Cahn [**SBGC**] identify, in a quench of the melt of AlMn alloys, an apparently new object in condensated matter, different from crystals or amorphous in terms of order and symmetry, for which neutron diffraction pattern was point like but five-fold symmetric.

The direct evidence by high resolution electron microscopy imaging [**Boi**] of the existence of Bragg peaks is the signature of a long-range order of the atomic structure. However, this corresponds to a non-crystalline order for the Bragg peaks are not periodically distributed in the reciprocal space, or equivalently because the diffraction pattern exhibits rotation axis of order forbidden by translational symmetry (only rotation axis of order 2,3,4 or 6 are consistent with 3-dimensional periodicity). In the case of AlMn, Shechtman et al. showed that the alloy admits an icosahedral point group of symmetry, with six 5-fold axis, ten 3-fold axis, fifteen 2-fold axis and the inversion operation. Then, they gave the name of icosahedral to this AlMn phase (i-AlMn). Other types of quasicrystalline symmetries where soon reported: octagonal, decagonal and dodecagonal phases, with 8-fold, 10-fold and 12-fold order respectively, with periodicity parallel to the corresponding axis. Very small at the beginning, single quasicrystal grains reach now a size of the order of the centimeter, with a very good quality in i-AlPdMn system (see [**Tsa**] for a review), allowing for precise measurements of physical properties.

The simplest example of non-periodic tiling was provided by R. Penrose [**Pen**]. It is built from two types of tiles in the 2D plane, through inflation rules, and exhibits a five-fold symmetry. It was extensively studied by de Bruijn [**dBr**]. But it was recognized only later on by physicists that it is quasiperiodic. However, de Bruijn and also Kramer & Neri [**KraNe**] built examples of quasiperiodic tilings. Most models describing the quasiperiodic order in quasicrystals, are based upon the so-called *cut-and-project method*, independently proposed by Duneau & Katz [**DuKa85, DuKa86**], Kalugin, Kitaev & Levitov [**KKL**], Elser [**Els**] and Levine

& Steinhardt [**LeSt**]. It was not until 1995 that this method was recognized as equivalent to the notion of *model sets* provided by Meyer [**Moo**] in his thesis work [**Mey**].

The cut-and-project method is defined with spaces and maps as follows

$$\begin{array}{ccccc} \mathbb{R}^d & \xleftarrow{\pi_1} & \mathbb{R}^d \times \mathbb{R}^n & \xrightarrow{\pi_2} & \mathbb{R}^n \\ & & \cup & & \\ \Lambda(M) & \xleftarrow{\pi_1} & \mathcal{R} & \xrightarrow{\pi_2} & M \end{array} \tag{3.4}$$

where $\mathcal{R} \subset \mathbb{R}^d \times \mathbb{R}^n$ is a lattice and π_1 and π_2 are the projections onto $\mathbb{R}^d$ and $\mathbb{R}^n$, respectively. Furthermore π_1 restricted on $\mathcal{R}$ is *injective* and $\pi_2(\mathcal{R})$ is *dense* in $\mathbb{R}^n$. We call $\mathbb{R}^d$ the *physical space* and $\mathbb{R}^n$ the *internal space*. We assume that π_1 and π_2 are the restriction maps on the corresponding coordinate of $\mathbb{R}^d \times \mathbb{R}^n$. Therefore the setting of a cut-and-project scheme is given by the triple $(\pi_1, \pi_2, \mathcal{R})$. For a subset M in the internal space $\mathbb{R}^n$ we define the corresponding point set in the physical space $\mathbb{R}^d$ as

$$\Lambda(M) = \{\pi_1(a) | a \in \mathcal{R}, \pi_2(a) \in M\}. \tag{3.5}$$

M is called the *acceptance domain* of the point set $\Lambda(M)$. For a lattice vector $a \in \mathcal{R}$ we have

$$\Lambda(M + \pi_2(a)) = \Lambda(M) + \pi_1(a). \tag{3.6}$$

DEFINITION 3.3. A point set L in $\mathbb{R}^d$ is called *a model set* if there exists a bounded set M with non-empty interior such that $L = \Lambda(M)$.

PROPOSITION 3.1. *A model set is a Meyer set.*

PROOF: (I) If M is bounded, $\Lambda(M)$ and $\Lambda(M) - \Lambda(M)$ are uniformly discrete. For indeed, let $\Sigma_M = \pi_2^{-1}(M)$ and let $r_1, r_2 > 0$ be such that $M \subset B(0, r_2)$. We set $B = \overline{B(0, r_1)} \times \overline{B(0, 2r_2)}$. If x belongs to $\Lambda(M)$ there is $\xi \in \mathcal{R} \cap \Sigma_M$ such that $\pi_1(\xi) = x$. Then $\overline{B(x, r_1)} \times \overline{B(0, r_2)} \subset \overline{B(\pi_1(\xi), r_1)} \times \overline{B(\pi_2(\xi), 2r_2)} = \xi + B$. If now $y \in \Lambda(M), y \neq x$, either $|y - x|_\infty > r_1$ or there is $b \in \mathcal{R} \cap B$ such that $y - x = \pi_1(b)$. Thus, $|y - x|_\infty \geq \min\{|\pi_1(b)|_\infty ; b \in \mathcal{R} \cap B, \pi_1(b) \neq 0\} = r_0 > 0$, because $\mathcal{R} \cap B$ is finite. The same argument applies for $\Lambda(M) - \Lambda(M)$ using the fact that $\mathcal{R} - \mathcal{R} = \mathcal{R}$.

(II) If M has a non-empty interior $\Lambda(M)$ and $\Lambda(M) - \Lambda(M)$ are relatively dense in $\mathbb{R}^d$. For indeed, one remarks that a point set L in $\mathbb{R}^N$ is relatively dense if and only if there is a closed ball B such that $L + B$ covers $\mathbb{R}^N$. Since $\mathcal{R}$ is a lattice, it is relatively dense and there is such a ball B in $\mathbb{R}^d \times \mathbb{R}^n$. If B_1, B_2 denote its projections, they are compact subsets of $\mathbb{R}^d$ and $\mathbb{R}^n$ respectively, and $B \subset B_1 \times B_2$. By hypothesis, $\pi_2(\mathcal{R})$ is dense in $\mathbb{R}^n$ and since M has a non-empty interior, the subsets $\pi_2(a) - M$ cover $\mathbb{R}^n$, whenever a varies in $\mathcal{R}$. By compactness, there is a finite subset J of $\mathcal{R}$ such that $\pi_2(J) - M$ covers B_2. Let B_3 be the smallest closed ball containing $B_1 - \pi_1(J)$. We claim that $\Lambda(M) + B_3$ covers $\mathbb{R}^d$. For if $x \in \mathbb{R}^d$, there is $a \in \mathcal{R}$ such that $(x, 0) - a \in B$. Thus $\pi_2((x, 0) - a) = -\pi_2(a) \in B_2$, so that there is $j \in J$ such that $\pi_2(a + j) \in M$, hence $\pi_1(a + j) \in \Lambda(M)$. On the other hand $x - \pi_1(a) \in B_1$ implying that $x - \pi_1(a + j) \in B_3$ and therefore that $x \in \Lambda(M) + B_3$. Since $M - M$ has also a non-empty interior, the same argument shows that $\Lambda(M) - \Lambda(M)$ is relatively dense in $\mathbb{R}^d$. □

REMARK 3.4. The cut-and-project construction used by physicists for describing the atomic positions in a quasicrystal is obtained by chosing M as the π_2-projection of a suitable unit cell of $\mathcal{R}$ [**KaGr**] (see Figure 1).

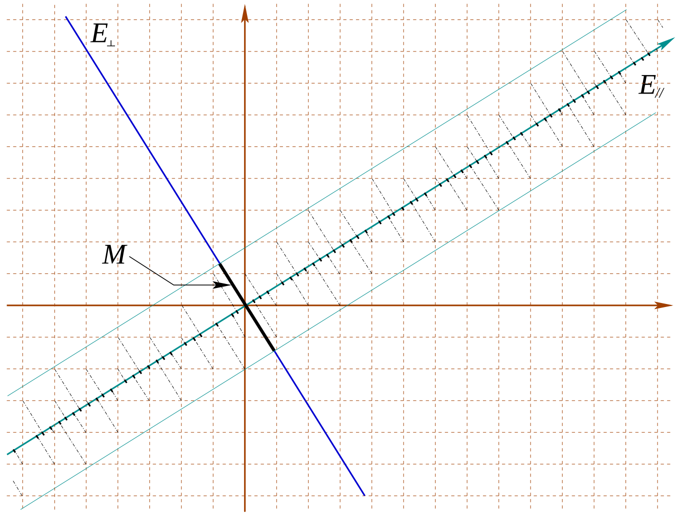

FIGURE 1. The Cut-and-Project Construction

DEFINITION 3.5. Let M be a bounded subset of $\mathbb{R}^n$ with non-empty interior. M is called *admissible* if for every ball $B(x,\epsilon)$ with $\epsilon > 0$ and x in $\pi_2(\mathcal{R}) \cap M$, there exists a finite family $\{a_1, \dots, a_p\}$ in $\pi_2(\mathcal{R})$ such that $M \cap (M + a_1) \cap \dots \cap (M + a_p)$ is a subset of $B(x,\epsilon)$ with non-empty interior. A model set L is called *admissible* if there exists an admissible set M such that $L = \Lambda(M)$.

EXAMPLE 3.6. A convex polytope is an admissible set.

Let us now consider an admissible model set $L = \Lambda(M)$ and let us denote by $\mathcal{A}_M$ the C^*-algebra generated by the set of functions $\{f \otimes (\chi_M \circ T_n^{\pi_2(a)}); a \in \mathcal{R}, f \in \mathcal{C}_c(\mathbb{R}^d)\}$, where $T_n^{\pi_2(a)}$ denotes the translation in $\mathbb{R}^n$ by $\pi_2(a)$. Here χ_M denotes the characteristic function of M. Let $\mathbb{R}_M^{n+d}$ be the set of characters of $\mathcal{A}_M$ so that, by Gelfand's theorem, $\mathcal{A}_M$ is isomorphic to $\mathcal{C}_0(\mathbb{R}_M^{n+d})$. Since M is admissible $\mathcal{C}_0(\mathbb{R}^{n+d})$ is a closed subalgebra of $\mathcal{A}_M$. By duality there is a surjective continuous map $\pi_M : \mathbb{R}_M^{n+d} \to \mathbb{R}^{n+d}$. Therefore $\mathbb{R}_M^{n+d}$ can be seen as the completion of $\mathbb{R}^{n+d}$ for a finer topology than the usual one, that will be called the M-topology, in which the sets $\mathbb{R}^d \times M + a$, for $a \in \mathcal{R}$, are open and closed. By construction, for $a \in \mathcal{R}$, the map $x \in \mathbb{R}^d \times \mathbb{R}^n \to x + a \in \mathbb{R}^d \times \mathbb{R}^n$ extends to $\mathbb{R}_M^{n+d}$ by continuity. One sets $\mathbb{T}_M^{n+d} = \mathbb{R}_M^{n+d}/\mathcal{R}$. By construction, for $y \in \mathbb{R}^d \times \{0\}$, the map $x \in \mathbb{R}^d \times \mathbb{R}^n \to x + y \in \mathbb{R}^d \times \mathbb{R}^n$ extends also by continuity to $\mathbb{R}_M^{n+d}$ and commutes with the action of $\mathcal{R}$. Thus it defines a $\mathbb{R}^d$-action $\hat{T}$ on $\mathbb{T}_M^{n+d}$. Similarly one can define $\mathbb{R}_M^n$ as the set of characters of the C^*-algebra generated by the set $\{\chi_M \circ T_n^{\pi_2(a)}; a \in \mathcal{R}\}$. Since it is a set of idempotents, $\mathbb{R}_M^n$ is totally disconnected and $\mathbb{T}_M^{n+d}$ is transversally totally disconnected.

DEFINITION 3.7. The dynamical system $\left(\mathbb{T}_M^{n+d}, \mathbb{R}^d\right)$ is called the *pseudo-torus* associated to the window M.

THEOREM 3.8. *Let $L = \Lambda(M)$ be an admissible model set in $\mathbb{R}^d$, and $\nu = \nu^{(L)}$. Then $(\Omega_\nu, \mathbb{R}^d, T)$ is topologically conjugated to $(\mathbb{T}_M^{n+d}, \mathbb{R}^d, \hat{T})$. This dynamical system is minimal. It is uniquely ergodic, providing M is a Borel set in $\mathbb{R}^n$.*

PROOF: By definition,

$$\nu = \nu^{(\mathcal{R},M)} = \sum_{a\in\mathcal{R}} \chi_M(\pi_2(a))\delta(x - \pi_1(a)).$$

Let $\omega \in \Omega_\nu$. Then there is a sequence $(x_n)_{n\in\mathbb{N}}$ in $\mathbb{R}^d$ such that $\omega = \lim_{n\to\infty} T^{-x_n}\nu$. Then $\forall f \in \mathcal{C}_c(\mathbb{R}^d)$,

$$\begin{aligned}\omega(f) &= \lim_{n\to\infty} \nu(f \circ T^{x_n}) \\ &= \lim_{n\to\infty} \sum_{a\in\mathcal{R}} (f \otimes \chi_M) \circ \hat{T}^a((x_n, 0))\end{aligned}$$

Let $f_M := f \otimes \chi_M$ and let $\hat{f}_M := \sum_{a\in\mathcal{R}} f_M \circ \hat{T}^a$. Since f_M has compact support, the sum defining $\hat{f}_M$ converges uniformly. Clearly, $f_M \in \mathcal{A}_M = \mathcal{C}_0(\mathbb{R}_M^{n+d})$ and since $\hat{f}_M$ is invariant under the action of $\mathcal{R}$, $\hat{f}_M \in \mathcal{C}(\mathbb{T}_M^{n+d})$. Consequently $\hat{f}_M(x_n, 0)$ converges to $\omega(f)$. Since f is arbitrary in $\mathcal{C}_c(\mathbb{R}^d)$ $\hat{T}^{(x_n,0)}(0)$ converges in $\mathbb{T}_M^{n+d}$. Let Φ_ω denote this limit point. Hence $\omega(f) = \hat{f}_M(\Phi_\omega)$ for all $f \in \mathcal{C}_c(\mathbb{R}^d)$.
From this formula it follows immediately that the map Φ is well defined because the family $\{\hat{f}_M, f \in \mathcal{C}_c(\mathbb{R}^d)\}$ separate the points of $\mathbb{T}_M^{n+d}$. Morever it also shows that Φ is continuous. Since $\overline{Orb(0)} = \mathbb{T}_M^{n+d}$ since $\pi_2(\mathcal{R})$ is dense in $\mathbb{R}^n$ the map is also surjective. At last the same formula shows that Φ conjugates the two actions of $\mathbb{R}^d$.
Since $\pi_2(\mathcal{R})$ is dense in $\mathbb{R}^n$, it follows that the dynamical systems defined by the hull is minimal [**KaHa**]). Moreover, since any function of the form $\hat{f}_M$ with $f \in \mathcal{C}_c(\mathbb{R}^d)$ is a Borel function over $\mathbb{T}^{n+d}$, any probability on Ω_ν is uniquely defined by a probability on $\mathbb{T}^{n+d}$. Since $\mathbb{T}^{n+d}$ is a compact group, its Haar measure is the unique ergodic and $\mathbb{R}^d$-invariant measure, showing that the hull is uniquely ergodic. □

PROPOSITION 3.2. *Let $\mathcal{O}$ be a bounded subset of $\mathbb{R}^n$. Then $\pi_M^{-1}(\mathcal{O})$ is a relatively compact subset of $\mathbb{R}_M^n$.*

The proof requires the following two lemmas.

LEMMA 3.9. *Let X be a locally compact space and let $\chi \in \mathcal{C}_0(X)$ satisfy $\chi^2 = \chi$. Then the support of χ is open and compact.*

PROOF: Since $\chi^2 = \chi$, for any $x \in X$, $\chi(x) \in \{0, 1\}$. Hence, its support is both open and closed. Moreover, since χ vanishes at infinity, there is a compact subset $K \subset X$ such that whenever $x \notin K$ then $\chi(x) = 0$. □

LEMMA 3.10. *Let $x \in \mathbb{R}^n$ and $\epsilon > 0$. Then there is a bounded set $\mathcal{U}_x$ of the form $\mathcal{U}_x = \bigcap_{i=1}^p (M + a_i)$, containing x in its interior and contained in the ball $B(x, \epsilon)$.*

PROOF: M being admissible, there are $b_1, \cdots, b_p$ in $\pi_2(\mathcal{R})$ such that $\mathcal{V}_x = \bigcap_{i=1}^p (M + b_i)$ has a non-empty interior and is contained in the ball $B(x, \epsilon/2)$. Therefore there is $y \in B(x, \epsilon/2)$ and $\epsilon_1 < \epsilon/2$ with $B(y, \epsilon_1) \subset \mathcal{V}_x$. Since $\pi_2(\mathcal{R})$ is dense in $\mathbb{R}^n$, there is $a \in \pi_2(\mathcal{R})$ such that $x - a \in B(y, \epsilon_1)$. Thus $|a|_\infty < \epsilon$ so that $\mathcal{U}_x = \mathcal{V}_x + a$ gives the required set. □

Proof of the Proposition 3.2: Since $\mathcal{O}$ is bounded, its closure is compact. The family $(\mathcal{U}_x)_{x\in\overline{\mathcal{O}}}$ is such that the interiors of its elements cover $\overline{\mathcal{O}}$. There is therefore a finite family $x_1, \cdots, x_l$ in $\overline{\mathcal{O}}$ such that $\overline{\mathcal{O}} \subset \bigcup_{i=1}^{l} \mathcal{U}_{x_i}$. In particular

$$\chi_{\overline{\mathcal{O}}} \leq \sum_{i=1}^{l} \chi_{\mathcal{U}_{x_i}} = F \in \mathcal{A}_M$$

Clearly, F takes values in $\mathbb{N}$. So that if g is the continuous bounded function on $\mathbb{R}$ defined by $g(s) = 0$ for $s \leq 0$, $g(s) = s$ for $0 \leq s \leq 1$ and $g(s) = 1$ for $s \geq 1$, the function $g \circ F = \chi$ belongs to $\mathcal{A}_M$ and satisfies $\chi^2 = \chi$. Thanks to lemma 3.9 the support K of χ is open and compact. Since $\overline{\mathcal{O}}$ is closed, it is closed for the M-topology too, its characteristic function $\chi_{\overline{\mathcal{O}}}$ is Borelian in this topology so that it extends as the characteristic function of $\pi_M^{-1}(\overline{\mathcal{O}})$ showing that $\pi_M^{-1}(\mathcal{O}) \subset K$. □

Since $\pi_2(\mathcal{R})$ is dense in $\mathbb{R}^n$, the π_2-image of the generators of $\mathcal{R}$ on $\mathbb{R}^n$ give a generating set $\{e_1, \ldots, e_{n+d}\}$ of vectors. After relabelling if necessary, they can be chosen such that $\{e_1, \ldots, e_n\}$ be linearly independent on $\mathbb{R}^n$ leading to a splitting of the $\mathcal{R}$-action on $\mathbb{R}^n$ into $(\mathbb{Z}^n \times \mathbb{Z}^d)$-action. By construction, one gets such a splitting of the $\mathcal{R}$-action on $\mathbb{R}^n_M$, too. One sets $\mathbb{T}^n = \mathbb{R}^n/\mathbb{Z}^n$ and $\mathbb{T}^n_M = \mathbb{R}^n_M/\mathbb{Z}^n$. Since $\{e_1, \ldots, e_n\}$ are linearly-independent vectors $\mathbb{T}^n$ is a compact set. Since the $\mathbb{Z}^n$-action and the $\mathbb{Z}^d$-action commute on $\mathbb{R}^n_M$, $\mathbb{T}^n_M$ is canonically endowed with a $\mathbb{Z}^d$-action.

Proposition 3.3. *$\mathbb{T}^n_M$ is a compact, totally disconnected, metrizable space, endowed with a $\mathbb{Z}^d$-action. Moreover $\mathcal{C}(\mathbb{T}^n_M) \rtimes \mathbb{Z}^d$ and $\mathcal{C}_0(\mathbb{R}^n_M) \rtimes \mathbb{Z}^{n+d}$ are Morita equivalent.*

Proof: Let $\mathbb{D}^n$ be the open fundamental domain for the $\mathbb{Z}^n$-action defined by $\mathbb{D}^n = \{\sum_{i=1}^n s_i e_i; 0 < s_i < 1\}$. Then the closure $\mathbb{D}^n_M$ of $\pi_M^{-1}(\mathbb{D}^n)$ in $\mathbb{R}^n_M$ is a fundamental domain for the $\mathbb{Z}^n$-action. Since $\mathbb{D}^n$ is relatively compact in $\mathbb{R}^n$, by Proposition 3.2 $\mathbb{D}^n_M$ is a compact set in $\mathbb{R}^n_M$. Let $f_0 \in \mathcal{C}_c(\mathbb{R}^n_M)$ be such that $f_0(x) = 1, \forall x \in \mathbb{D}^n_M$ and $0 \leq f_0 \leq 1$ elsewhere. Let $\hat{f}_0 := \sum_{a\in\mathbb{Z}^n} f_0 \circ T^a_n$. $f_0 \in \mathcal{C}(\mathbb{T}^n_M)$. One gets $\hat{f}_0(x) \neq 0, \forall x \in \mathbb{T}^n_M$. Thus f_0 is invertible in $\mathcal{C}(\mathbb{T}^n_M)$ and $\mathbb{T}^n_M$ is a compact set.
Since the vectors $\{e_1, \ldots, e_n\}$ are linearly independent, the $\mathbb{Z}^n$-action on $\mathbb{R}^n$ is free and wandering, namely there is no orbit reduced to a single point and for each compact set K in $\mathbb{R}^n$ the set $\{g \in \mathbb{Z}^n, g.K \cap K \neq \emptyset\}$ is finite. Since π_M is a continuous surjection, the $\mathbb{Z}^n$-action on $\mathbb{R}^n_M$ is free and wandering, too. Then $\mathcal{C}(\mathbb{T}^n_M)$ and $\mathcal{C}_0(\mathbb{R}^n_M) \rtimes \mathbb{Z}^n$ are Morita equivalent [**Rie82b**] and such an equivalence can be extended to the $\mathbb{Z}^d$-crossed products. □

Up to now, M has only been assumed to be admissible. The following property actually holds in quasicrystals:

Definition 3.11. A polytope in $\mathbb{R}^n$ is said *$\mathcal{R}$-compatible* if its vertices belong to $\pi_2(\mathcal{R})$.

If the acceptance domain M is an $\mathcal{R}$-compatible polytope, let $F_1, \cdots, F_p$ be the hyperplanes of $\mathbb{R}^{n+d}$ parallel to the maximal faces of $\mathbb{R}^n \times M$. For each $j \in \{1, \cdots, p\}$, let $u_j \in \mathbb{R}^{n+d}$ be a unit vector perpendicular to F_j so as to define $F_j^+ =$

$\{x \in \mathbb{R}^{n+d}; \langle u_j|x\rangle \geq 0\}$ and $F_j^- = \mathbb{R}^{n+d} \setminus F_j^+$. Let then $\mathcal{F}$ be the family of affine hyperplanes $F_j + a$ with $j \in \{1, \cdots, p\}$ and $a \in \pi_2(\mathcal{R})$. $\mathbb{R}^d \times \mathbb{R}^n$ is then endowed with the coarsest topology for which, given any $F \in \mathcal{F}$, the closed half-space F^+ is both closed and open. It will be called the $\mathcal{F}$-topology. The same construction can be performed in $\mathbb{R}^n$. Let $\mathbb{R}^{n+d}_{\mathcal{F}}$ and $\mathbb{R}^n_{\mathcal{F}}$ be the completions of $\mathbb{R}^d \times \mathbb{R}^n$ and $\mathbb{R}^n$ with this topology, respectively. In much the same way, $\mathbb{T}^{n+d}_{\mathcal{F}} = \mathbb{R}^{n+d}_{\mathcal{F}}/\mathcal{R}$ is well defined and can be endowed with an $\mathbb{R}^d$-action. The following proposition is easy to prove:

PROPOSITION 3.4. *If M is $\mathcal{R}$-*compatible*, the M-topology and the $\mathcal{F}$-topology are equivalent on $\mathbb{R}^{n+d}$. In particular $\mathbb{T}^{n+d}_{\mathcal{F}} = \mathbb{T}^{n+d}_{M}$.*

REMARK 3.12. An alternative description of this pseudo-torus is proposed in [**Le, FHK1**] under very general hypothesis on M.

REMARK 3.13. In a Meyer set obtained through the cut-and-project method any bounded pattern repeats itself infinitely often. More generally, each Meyer set is a Delone set of finite type. Thanks to Corollary 2.1, this implies that the canonical transversal is totally disconnected. This can also be seen from the particular topology described just before.

4. Tight-binding representation

The Schrödinger operator H describing the electronic motion (see Section 2.7), is an unbounded selfadjoint operator on $L^2(\mathbb{R}^d)$. The unboundedness introduces useless technical difficulties in most cases. For indeed, only those electrons with energy close to the Fermi level really matter for the description of electronic property of the material in which they evolve. Restricting H to such an energy window leads to the so-called *tight-binding representation*, at least if the atomic orbitals contributing to such energy range are sufficiently well localized on the atom. In the physics literature, such a construction leads to the *tight-binding approximation* [**AshMe**], obtained by truncating the effective Hamiltonian to a finite set of hopping terms, such as the nearest neighbours.

Let H be defined by Equation (2.6), and $v \in L^1(\mathbb{R}^d)$ be the atomic potential describing the electron-ion interactions. Then v is attractive at large distance in order to bind the electrons, and it vanishes at infinity. Consequently the atomic Hamiltonian $H_{at} = \Delta + v$ has bound states. Let E be the energy of such a bound state and let ψ the corresponding wave function. ΔE will denote the energy gap between E and the energy level closest to E. Since the atomic potential vanishes at infinity, the wave function ψ decreases exponentially fast with a rate of decreasing given by $|E|$ [**Agm**]. Therefore, if $\nu \in UD_r(\mathbb{R}^d)$ with r sufficiently large, the functions $(\psi_y(x)) = (\psi(x-y)_{y \in L^{(\nu)}})$ are approximate eigenfunctions of H, and E is the corresponding approximate eigenvalue. More precisely let M^ν be the matrix indexed by $L^{(\nu)}$ and defined by:

$$M^\nu_{y,y'} = \langle \psi_y|\psi_{y'}\rangle = \delta_{yy'} + O(e^{-E|y-y'|_\infty}) \quad \text{as } r \to \infty \tag{4.1}$$

This matrix, seen as an operator acting on $\ell^2(L^{(\nu)})$, is non-negative and there is an r_0 such that if $r > r_0$ then $\|M^\nu - 1\| < 1$. Thus, $(M^\nu)^{-1/2}$ is well defined leading to the following lemma, the proof of which being left to the reader:

LEMMA 4.1. *Let $\mathcal{H}$ be the the subspace of $L^2(\mathbb{R}^d)$ spanned by the ψ_y's. Let $(\phi_y)_{y\in L^{(\nu)}}$ be the family of functions in $\mathcal{H}$ defined by:*

$$\phi_y = \sum_{y'\in L^{(\nu)}} ((M^\nu)^{-1/2})_{y',y}\psi_{y'} \tag{4.2}$$

Then, $(\phi_y)_{y\in L^{(\nu)}}$ is an orthogonal basis of $\mathcal{H}$. In addition, $\|\phi_y - \psi_y\| = O(e^{-|E|r})$ as $r \to \infty$.

Let now P be the orthogonal projection onto $\mathcal{H}$ and $Q = 1 - P$. For r large enough the spectrum of PHP is contained in the open interval $I_E = (E-\Delta E/2, E+\Delta E/2)$ which does not meet the spectrum of $(1-P)H(1-P)$. The part of the spectrum of H contained in I_E can be investigated through the projection method, known as the Schur complement formula or Feshback method [**Fesh58, Fesh62, Bel88**] which consists in defining the following energy dependent operator:

$$H_{eff}(z) = PHP + PHQ\frac{1}{z - QHQ}QHP, \tag{4.3}$$

$H_{eff}(z)$ is the effective Hamiltonian associated to H. The following theorem describes the relation between H and $H_{eff}(z)$ corresponding to the energy window I_E.

THEOREM 4.2. [**Bel86**] *Let $z \in \mathbb{C} \setminus \mathrm{spec}(QHQ)$. Then z belongs to the spectrum of $H_{eff}(z)$ if and only if z belongs to the spectrum of H. λ is an eigenvalue of H with eigenvector φ, if and only if λ is an eigenvalue of $H_{eff}(\lambda)$ with eigenvector $P\varphi$. φ can be recovered from the formulae:*

$$Q\varphi = \frac{1}{\lambda - QHQ}QHP\varphi \tag{4.4}$$

Since the two parts of the spectrum of H are separated by a gap, $H_{eff}(z)$ is norm-analytic in z. It follows from (4.3) that if P is close enough from an eigenprojection of H, the second term is a second-order perturbative term. If λ_0 is the first order approximation for an eigenvalue, (4.3) can be systematically expanded in powers of $z - \lambda_0$, providing a method for calculating the eigenvalues and eigenfunctions.

The exponential decay of ψ leads to the boundedness of QHP and $PHQ(z - QHQ)^{-1}QHP$ is bounded by $O(e^{-2|E|r})$ as $r \to \infty$, uniformly for z in any compact subset of I_E. Consequently:

LEMMA 4.3. [**Bel86**] *The matrix of $H_{eff}(z)$ in the basis of the $(\phi_y)_{y\in L^{(\nu)}}$ is diagonally dominant, namely:*

$$\langle\phi_y|H_{eff}(z)\phi_{y'}\rangle = O(e^{-2|E||y-y'|}) \qquad \textit{as } r \to \infty \tag{4.5}$$

REMARK 4.4. $(M^\nu)_{y',y}$ is a function of $y - y'$ only; thus there is a function $\phi \in L^2(\mathbb{R}^d)$ such that $\forall y \in L^{(\nu)}, \phi_y = U(y)\phi$ (where $U(y)$ is the operator of translation by y), so that $\langle\phi_y|H_\omega(z)\phi_{y'}\rangle = \langle\phi|H_{T^{-y}\omega}(z)U(y-y')\phi\rangle$.

The unbounded operator H, acting on $L^2(\mathbb{R}^d)$, has been replaced by a bounded operator acting on $\ell^2(L^{(\nu)})$, the Hilbert space attached to the atomic sites. The tight-binding approximation is obtained by replacing all matrix elements between sites farther than a given distance ℓ by zero. Choosing ℓ large enough, this gives a good approximation since the error is of order $O(e^{-|E|\ell})$. The discrete hull for

$H_{eff}(z)$ can be directly defined only whenever $L^{(\nu)}$ is invariant by some lattice $\mathcal{R}$ of translations. In the general case of a tight-binding Hamiltonian on a point set the hull can be defined through using the notion of groupoid G_Υ of the transversal Υ (see Proposition 2.2 and Theorem 2.23).

4.1. C^*-algebra of a groupoid. The construction of the C^*-algebra of a groupoid can be found in [**Ren**]. In the special case given here, it goes as follows. Thanks to Proposition 2.2, the groupoid of the transversal can be defined as $G_\Upsilon = \{(\omega, a) \in \Upsilon \times \mathbb{R}^d,\ a \in L^{(\omega)}\}$. Since $L^{(\omega)}$ is uniform discrete and depends continuously on ω, G_Υ is a closed subspace of $\Omega \times \mathbb{R}^d$ (Remark 2.15). Let $\mathcal{C}_c(G_\Upsilon)$ be the vector space of continuous functions on G_Υ with compact support. It is endowed with a structure of *-algebra in the following way:

$$fg(\omega, a) = \sum_{t \in L^{(\omega)}} f(\omega, t) g(T^{-t}\omega, a - t), \tag{4.6}$$

$$f^*(\omega, a) = \overline{f(T^{-a}\omega, -a)} \tag{4.7}$$

For $\omega \in \Upsilon$ we denote by Π_ω the *-representation of $\mathcal{C}_c(G_\Upsilon)$ on $\ell^2(L^{(\omega)})$ given by [**Co79, Co82**]:

$$\Pi_\omega(f)\psi(a) = \sum_{t \in L^{(\omega)}} f(T^{-a}\omega, t - a)\psi(t), \qquad a \in L^{(\omega)}. \tag{4.8}$$

These representations satisfy also a covariance condition. Namely, for $\gamma = (\omega, t) \in G_\Upsilon$, let $U_\omega(t)$ be the unitary operator from $\ell^2(L^{(T^{-t}\omega)})$ into $\ell^2(L^{(\omega)})$ given by

$$U_\omega(t)\psi\,(y) = \psi(y - t).$$

It satisfies:

$$U_\omega(t)\Pi_{T^{-t}\omega}(f) = \Pi_\omega(f)U_\omega(t) \tag{4.9}$$

Then a C^*-norm is given by

$$\|f\| = \sup_{\omega \in \Upsilon} \|\Pi_\omega(f)\| \tag{4.10}$$

$C^*(G_\Upsilon)$ will denote the completion of $\mathcal{C}_c(G_\Upsilon)$ under this norm. For $\omega \in \Upsilon$ let H_ω be given by

$$H_\omega = H_0 + \sum_{y \in L^{(\omega)}} v(. - y) = H_0 + \nu_\omega * v\ , \tag{4.11}$$

(where v is an atomic potential, see the precise definition in Section 2.7). Then, according to Lemma 4.3 and Remark 4.4, the effective Hamiltonian for H_ω acts on $\mathcal{H}_\omega = \overline{\text{Span}\,\{U(y)\phi|\ y \in L^{(\omega)}\}} \cong \ell^2(L^{(\omega)})$. Thanks to its covariance and continuity properties, it satisfies:

PROPOSITION 4.1. [**Bel86**] *Let $h(z)$ be the function on G_Υ defined by:*

$$h(z)(\omega, y) = \langle \phi | H_\omega(z) U(y) \phi \rangle,$$

where ϕ is defined in Remark 4.4. Then $h(z)$ belongs to $C^*(G_\Upsilon)$ for any $z \in I_E$. Furthermore, the matrices of $H_\omega(z)$ and of $\Pi_\omega(h(z))$, with respect to the basis $(\phi_y)_{y \in L^{(\omega)}}$, coincide.

Therefore, $C^*(G_\Upsilon)$ can be used to described the spectrum of H locally. The following connection between the discretized and the continuum algebras should be noted:

THEOREM 4.5. [**Rie82a**] *The C^*-algebras $\mathcal{B} = C^*(\Omega \times \mathbb{R}^d)$ and $\mathcal{C} = C^*(G_\Upsilon)$ are Morita equivalent, namely $\mathcal{B} \otimes \mathcal{K}$ and $\mathcal{C} \otimes \mathcal{K}$ are isomorphic (not in a canonical way).*

The proof consists in constructing a Hilbert $\mathcal{B}$-$\mathcal{C}$-bimodule implying an isomorphism of the stabilized algebras of $\mathcal{B}$ and $\mathcal{C}$. Another strong consequence of the existence of this bimodule will be seen in Theorem 6.1.

4.2. Physical models on quasilattices. This section is devoted to the description of the tight-binding representations for quasicrystals. As described in Section 3.4, the set of atomic positions is an admissible model set L that will be called a *quasilattice*. Let $\mathcal{R}$ be a lattice in $\mathbb{R}^{n+d}$, let $M \in \mathbb{R}^n$ be an *admissible* acceptance domain for a cut-and-project scheme $(\pi_1, \pi_2, \mathcal{R})$ and $L = \Lambda(M)$ be the corresponding model set.

Then π_1 induces an isomorphism between the physical Hilbert space $\mathcal{H} = \ell^2(L)$ and $\ell^2(\mathcal{S}_M)$, where $\mathcal{S}_M$ is the strip $\mathcal{S}_M = \{a \in \mathcal{R} | \pi_2(a) \in M\}$. By definition π_1 is injective on $\mathcal{R}$. Therefore $\mathcal{H}$ can be seen as a subspace of the large Hilbert space $\mathcal{E} = \ell^2(\mathcal{R})$. If χ_M denotes the characteristic function of $\mathcal{S}_M$ in $\mathcal{R}$, the orthogonal projection onto $\mathcal{H}$ in $\mathcal{E}$ can be identified with the multiplication operator by χ_M also denoted by χ_M. In general for $K \subset \mathbb{R}^n$ and $b \in \mathcal{R}$, χ_{K+b} will denote the projection onto $\ell^2(\{a \in \mathcal{R},\ \pi_2(a-b) \in K\})$.

The C^*-algebra generated by the translation operators T_a $(a \in \mathcal{R})$ contains all $\mathcal{R}$-invariant observables. It is isomorphic to the algebra $\mathcal{C}(\mathbb{T}^{d+n})$ of continuous functions on the $(n+d)$-dimensional torus. Physical models on L will be rather obtained by restricting the action of $\mathcal{R}$ to $\mathcal{H}$. More precisely, the quasitranslation operators are defined by $S_a = \chi_M T_a \chi_M$ for $a \in \mathcal{R}$ and the C^*-algebra they generate will be denoted by $\mathcal{Q}(n, d, M)$. The operators S_a are partial isometries which do not commute. Thus, since $\mathcal{Q}(n, d, M)$ is unital, it can be seen as the set of continuous functions on a non-commutative compact space. The commutation rules for the partial isometries are given as follows:

$$S_{a_1} S_{a_2} ... S_{a_k} = \chi_{M(\underline{a})} T_{a_1 + \ldots + a_n} \chi_{M(\overline{a})} \tag{4.12}$$

where $\underline{a} = (a_1, ..., a_n)$, $M(\underline{a}) = M \cap (M + a_1) \cap ... \cap (M + a_1 + \ldots + a_n)$, and $M(\overline{a}) = M \cap (M - a_n) \cap ... \cap (M - a_1 - \ldots - a_n)$.
In particular $S_a = \chi_{M \cap (M+a)} T_a \chi_{M \cap (M-a)}$ and

$$S_a S_a^* = \chi_{M \cap (M+a)}, \qquad S_a^* S_a = \chi_{M \cap (M-a)}. \tag{4.13}$$

An integral and differential calculus can be defined on $\mathcal{Q}(n, d, M)$ [**Bel93**].

Let $(\Omega, \mathbb{R}^d)$ be the hull of the corresponding quasilattice $L = \Lambda(M)$. The topology of Ω is given by Theorem 3.8. Let $\mathbb{R}^n$ be the internal space.

THEOREM 4.6. [**BCL**] *The algebras $\mathcal{Q}(n, d, M)$ and $\mathcal{C}(\mathbb{R}^n_M) \rtimes \mathbb{Z}^{n+d}$ are Morita equivalent.*

THEOREM 4.7. *Let Υ be the canonical transversal of $(\Omega, \mathbb{R}^d)$ defined in Proposition 2.2. Then $\mathcal{Q}(n, d, M)$ is isomorphic to $C^*(G_\Upsilon)$, where $C^*(G_\Upsilon)$ is the groupoid C^*-algebra constructed in Section 4.1.*

PROOF: Let be $L = L^{(\nu)} = \Lambda(M)$. We consider $\mathcal{Q}(n, d, M)$ as acting on $\ell^2(L)$. Since L has finite type we know by Corollary 2.1 that Υ is totally disconnected. Furthermore, since $\Omega_R(\nu)$, defined in Proposition 2.3, is finite for every $R > 0$ we conclude that G_Υ is also totally disconnected and therefore $C_c(G_\Upsilon)$ is already

generated by the locally constant functions, i.e. by the characteristic functions of clopen (closed and open) sets. Consider $T \subset \Omega_R(\nu)$ for some $R > 0$ and $x \in T$, then we define the set $A(T, x) = \{(\omega, x) \in G_\Upsilon,\ T \subset L(\omega)\}$ which is clopen (cf. Section 2.6). This type of clopen sets form a basis for the topology of G_Υ. Actually, every clopen set in G_Υ is given by a finite, pairwise disjoint union of such clopen sets. Let $e_T \otimes e_x(\omega, t)$ be the characteristic function of the set $A(T, x)$.
For simplicity we assume $0 \in \Lambda(M) = L$ (we have $\ell^2(L) \cong \ell^2(L(T^x\nu))$ for every $x \in \mathbb{R}^d$). Let Π_ν be the representation given by (4.8). By construction the orbit of ν is dense in Ω_ν and therefore this representation is faithful. Let $a \in \mathcal{R}$ such that $y_a = \pi_1(a) \in L - L$ then

$$S_a = \Pi_\nu(e_{\{0,y_a\}} \otimes e_{y_a}), \qquad \chi_{M\cap(M+a)} = \Pi_\nu(e_{\{0,-y_a\}} \otimes e_0) \tag{4.14}$$

as operators in $B(\ell^2(L))$. For $a \in \mathcal{R}$ with $y_a \notin L - L$ we have $S_a = 0$. On the other hand let $T = \{y_0, ..., y_n\} \subset \Omega_R(\nu)$ for some $R > 0$. Then there exist $a_0, ..., a_n \in \mathcal{R}$ with $y_0 = \pi_1(a_0), ..., y_n = \pi_1(a_n)$ and we have

$$\Pi_\nu(e_T \otimes e_{y_0}) = S^*_{a_n} S_{a_n} \dots S^*_{a_2} S_{a_2} S^*_{a_1} S_{a_1} S_{a_0}. \tag{4.15}$$

Therefore we have $\Pi_\nu(C_c(G_\Upsilon)) = \mathcal{Q}(n, d, M)$. □

EXAMPLE 4.8. Here is the situation for $d = 1$. Then the lattice L is supported by a line in $\mathbb{R}^{1+n}$. Choosing an orientation on it and an origin in L, the points of L can be uniquely labelled in increasing order by integers. Hence $\mathcal{H} = \ell^2(L)$ is isomorphic to $\ell^2(\mathbb{Z})$. In the specific case where $n = 1$, let ω be the slope of the line containing L and let $\alpha = \omega/(\omega+1)$ (see Fig. 1). The acceptance domain M is then given by the projection of the unit square, namely the interval $[-\omega/\sqrt{1+\omega^2}\,,\ 1/\sqrt{1+\omega^2})$. The labelling of points of L can be explicitely computed from the points in the strip $\mathcal{S}$ through the map $a = (m, n) \in \mathcal{S} \to l(a) = m + n - n_0 \in \mathbb{Z}$. The inverse map is then given by $n = n_0 + 1 + [l\alpha - \theta]$ and $m = l - 1 - [l\alpha - \theta]$, provided $\theta = \alpha - (1-\alpha)\eta \in [0, 1]$ (where $[l\alpha - \theta]$ denote the integer part of $l\alpha - \theta$).
Then, setting $T = S_1 + S_2$, T is unitary and is represented by the translation by one in $\mathcal{H}$. On the other hand, it can be checked that $\chi_{M\cap(M-e(2))} = S_2^* S_2$ is represented by the operator $\chi_{\alpha,\theta}$ of multiplication by $\chi_{[1-\alpha,1)}(l\alpha - \theta)$ in $\mathcal{H}$ (where $\chi_{[1-\alpha,1]}$ is the characteristic function of $[1-\alpha, 1))$ on the unit circle. Moreover the algebra $\mathcal{Q}(2, 1, M) = \mathcal{Q}_\alpha$ is generated by T and $\chi_{\alpha,\theta}$. The Abelian C^*-algebra generated by the family $\chi_{\alpha,n} = T^n \chi_{\alpha,\theta} T^{-n}$ is thus isomorphic to the algebra $\mathcal{C}_\alpha$ generated by the characteristic functions $\chi_{[1+(n-1)\alpha, 1+n\alpha)}$ of the interval $[1 + (n-1)\alpha, 1 + n\alpha)$ of the unit circle. $\mathcal{Q}_\alpha$ appears therefore as the crossed product of $\mathcal{C}_\alpha$ by the rotation on the unit circle. In particular, if α is an irrational number, $\mathcal{C}_\alpha$ contains all continuous functions on the unit circle, and consequently, $\mathcal{Q}_\alpha$ contains the irrational rotation algebra $\mathcal{A}_\alpha$.
The Kohmoto model is an archetype of discrete Hamiltonian which belongs to this algebra:

$$H_x\psi(n) = \psi(n+1) + \psi(n-1) + V\chi_{[1-\alpha,1)}(n\alpha - x)\psi(n), \;\; x \in \mathbb{T},\ \psi \in \ell^2(\mathbb{Z}). \tag{4.16}$$

The algebra is generated by the characteristic function $\chi_{[1-\alpha,1)}$ of the interval $[1-\alpha, 1)$ on the torus $\Omega = \mathbb{T}$, with $T = R_\alpha$ the rotation by $\alpha \in [0, 1] \setminus \mathbb{Q}$, and $\mathbb{P}$ is the normalized Lebesgue measure. As an admissible model set $(\mathbb{T}, R_\alpha)$ is uniquely ergodic.

5. General gap labelling theorem

5.1. Integrated density of states and Shubin's formula. Let H be the Schrödinger operator, acting on the Hilbert space $L^2(\mathbb{R}^d)$, given by (2.4), where $V \in L^\infty(\mathbb{R}^d)$ is real. For any rectangular box Λ, let H_Λ denote the restriction of H to Λ with some boundary conditions (*e.g.* Dirichlet or periodic boundary conditions). Since H is elliptic and Λ is compact, the spectrum of H_Λ is discrete and bounded from below. Let $N_\Lambda(E)$ be the number of eigenvalues of H_Λ smaller than or equal to E, counted with their multiplicities. Thanks to the homogeneity of H, $N_\Lambda(E)$ should not vary much as Λ is translated. Moreover, since H connects only nearby regions, $N_\Lambda(E)$ should be additive, namely, if Λ and Λ' are two large non-intersecting boxes, $N_{\Lambda\cup\Lambda'}(E) = N_\Lambda(E) + N_{\Lambda'}(E) + o(|\Lambda \cup \Lambda'|)$. In particular, $N_\Lambda(E)$ should grow proportionally to $|\Lambda|$ as $\Lambda \uparrow \mathbb{R}^d$. This is why the Integrated Density of States (IDOS) is defined as follows:

$$\mathcal{N}(E) = \lim_{\Lambda\uparrow\mathbb{R}^d} \frac{N_\Lambda(E)}{|\Lambda|} \quad \in \mathbb{R}_+ \,, \tag{5.1}$$

where the limit, whenever it exists, is understood in the Følner sense [**Gre**]. The first rigorous work on the IDOS goes back to Benderskii and Pastur [**BePa**], who proved the existence of the limit for a one-dimensional Schrödinger operator on a lattice with random potential, with probability one. Then the existence and smoothness properties of the derivative $d\mathcal{N}$ as a Stieljes-Lebesgue measure were proved by different methods with an increasing degree of generality for the Schrödinger operator with random potential [**Pas, Nak, KiMa**]. The algebraic approach goes back to the work of Shubin [**Shub**] inspired by the index theory [**CMS**]. The extension to more general coefficients is elementary and has been given by one of us in the discrete case [**Bel86**] and in the continuum case [**Bel93**].

Actually, the value $N_\Lambda(E)$ is nothing but the trace of the projection $\chi(H_\Lambda \leq E)$ onto eigenstates of H_Λ with energy less than or equal to E. So the IDOS appears as:

$$\mathcal{N}_{\mathbb{P}}(E) = \lim_{\Lambda\uparrow\mathbb{R}^d} \frac{1}{|\Lambda|} Tr_\Lambda(\chi(H_\Lambda \leq E)). \tag{5.2}$$

The IDOS depends upon the choice of the translation-invariant ergodic probability measure $\mathbb{P}$ on the hull of the Hamiltonian.

This formula is very reminiscent to the formula defining the trace per unit volume $\mathcal{T}_{\mathbb{P}}$ (see Equation (1.12)) of the eigenprojector $\chi(H \leq E)$ of the infinite volume limit. Notice that this projector does not belong, in general, to the C^*-algebra $\mathcal{A}$ generated by H but to the von Neumann algebra $L^\infty(\mathcal{A}, \mathcal{T}_{\mathbb{P}})$ associated to the trace per unit volume by means of the GNS construction.

Definition 5.1. **Shubin's Formula** The Schrödinger operator (2.4) obeys *Shubin's formula*, whenever the IDOS satisfies:

$$\mathcal{N}_{\mathbb{P}}(E) = \mathcal{T}_{\mathbb{P}}(\chi(H \leq E)), \tag{5.3}$$

where $\mathcal{T}_{\mathbb{P}}$ is the trace per unit volume defined in Equation (1.11).

Shubin's formula will follow from showing that $Tr_\Lambda(\chi(H_\Lambda \leq E))/|\Lambda|$ and $Tr_\Lambda(\chi(H \leq E))/|\Lambda|$ as $\Lambda \uparrow \mathbb{R}^d$ have the same limit. Here is a short review of the cases in which Shubin's formula has been established [**Bel93**].

Let $(\Omega, \mathbb{R}^d, T)$ be a dynamical system with Ω a compact space. We suppose $(\Omega, \mathbb{R}^d, T)$ is topologically transitive, namely there is $\omega_0 \in \Omega$ the orbit of which being dense in Ω. Let $U^\infty(\Omega, \mathbb{R}^d)$ be the set of smooth functions f on $\mathbb{R}^d$, such that there is $F \in C(\Omega)$ for which $f(x) = F(T^{-x}\omega_0)$ and that, for all $\omega \in \Omega$, the function $f_\omega(x) = F(T^{-x}\omega)$ has bounded derivatives at all order.

THEOREM 5.2. *Let H_ω be a uniformly elliptic self-adjoint operator of the form*

$$H_\omega = \sum_{|\alpha| \leq m} h_\omega^{(\alpha)}(x) D^\alpha \tag{5.4}$$

with coefficient $h^{(\alpha)} \in U^\infty(\Omega, \mathbb{R}^d)$, $\alpha = (\alpha_1, \cdots, \alpha_d) \in \mathbb{N}^d$ is a multi-index, $|\alpha| = \alpha_1 + \cdots + \alpha_d$ and $D^\alpha = \prod_{1 \leq \mu \leq d}(-\imath\partial_\mu)^{\alpha_\mu}$.
Then there is a $r(z) \in C^*(\Omega \times \mathbb{R}^d)$ such that $\Pi_\omega(r(z)) = \{z - H_\omega\}^{-1}$, for every complex z in the resolvent set of H_ω, and Shubin's formula *holds.*

In the discrete case the situation is technicallly much simpler. Let $\mathbb{G}$ be a countable discrete amenable group [**Gre**] (not necessarily Abelian). By amenable we mean that there exists a Følner sequence in $\mathbb{G}$.

THEOREM 5.3. [**Bel86**] *Let $(\Omega, \mathbb{G}, T)$ be a topological dynamical system with Ω compact and metrizable, and $\mathbb{G}$ discrete countable and amenable. Given any $\mathbb{G}$-invariant ergodic probability measure on Ω, any self-adjoint element of the crossed product $C(\Omega) \rtimes \mathbb{G}$ satisfies Shubin's formula.*

From Shubin's formula it is easy to obtain [**Bel93**]:

PROPOSITION 5.1. *Let H be a homogeneous operator, and let $\mathcal{A}$ be the C^*-algebra generated by H and its translates. Let $\mathcal{T}_\mathbb{P}$ be a translation-invariant trace, for which H obeys Shubin's formula. Then its* IDOS *is a non-negative, non-decreasing function of E, which is constant on each gap of* spec(H).

PROPOSITION 5.2. *Let H be as in Proposition* 5.1. *If $\mathcal{T}_\mathbb{P}$ is faithful, the spectrum of H coincides with the set of points in $E \in \mathbb{R}^d$ in the vicinity of which the* IDOS *is not constant.*

REMARK 5.4. Let H be the Schrödinger operator $H = \Delta + V$ on $L^2(\mathbb{R}^d)$ where V converges to zero at infinity. Then the hull of H is the one-point compactification of $\mathbb{R}^d$. The only translation-invariant ergodic probability measure on the hull $\Omega \cong \mathbb{R}^d \cup \{\infty\}$ is the Dirac measure at ∞. Therefore, the trace per unit volume cannot be faithful. In particular, the IDOS does not take into account the discrete spectrum of H, since the density of such eigenvalues is zero.

PROPOSITION 5.3. *With assumption of Proposition* 5.1*, any discontinuity point of the* IDOS *is an eigenvalue of H with infinite multiplicity.*

5.2. General gap labelling and K_0-group. This section is devoted to a short review of K-theory [**Bla, Weg**] and to the statement of the gap labelling theorem for homogeneous media (all the proofs can be found in [**BBG, Bel93**]).

Let H be a homogeneous selfadjoint operator affiliated to the C^*-algebra $\mathcal{A}$. Let $\mathfrak{g}$ be a spectral gap of H and let $P(\mathfrak{g})$ be the eigenprojection on the spectral interval $(-\infty, E]$ for any $E \in \mathfrak{g}$. Being a smooth function of H, $P(\mathfrak{g}) \in \mathcal{A}$. Now, changing H by a unitary transformation does not modify the spectrum as a set. Therefore, the gap $\mathfrak{g}$ can be labelled by the equivalence class of $P(\mathfrak{g})$ under unitary transformations. In order to take into account the case of non-unital algebras, the following definition of equivalence must be used:

DEFINITION 5.5. Two projections P and Q of a C^*-algebra $\mathcal{A}$ are equivalent if there is $U \in \mathcal{A}$ such that $UU^* = P$ and $U^*U = Q$. The equivalence will be denoted by $P \approx Q$.

The set of equivalence classes of projections in $\mathcal{A}$ will be denoted by $\mathcal{P}(\mathcal{A})$, and the equivalence class of P by $[P]$. Two projections P and Q are orthogonal whenever $PQ = QP = 0$. Then $P + Q$ is a new projection, called the direct sum of P and Q, denoted by $P \oplus Q$.

PROPOSITION 5.4. [**Ped**] *Let $\mathcal{A}$ be a separable C^*-algebra.*

(i) *The set $\mathcal{P}(\mathcal{A})$ of equivalence classes of projections in $\mathcal{A}$ is countable.*
(ii) *Let P and Q be two projections in $\mathcal{A}$. Then the equivalence class of their direct sum, if it exists, depends only upon the equivalence classes of P and of Q. In particular, a sum is defined on the set Θ of pairs $([P],[Q])$ in $\mathcal{P}(\mathcal{A})$, such that there are $P' \approx P$ and $Q' \approx Q$ with $P'Q' = Q'P' = 0$, by $[P]+[Q] = [P' \oplus Q']$. This composition law is commutative and associative.*

The main problem is that the direct sum may not be everywhere defined. To overcome this difficulty, $\mathcal{A}$ is replaced by its *stabilization* $\mathcal{A} \otimes \mathcal{K}$, where $\mathcal{K}$ is the algebra of compact operators. A C^*-algebra $\mathcal{A}$ is *stable* if $\mathcal{A}$ and $\mathcal{A} \otimes \mathcal{K}$ are isomorphic. For any C^*-algebra $\mathcal{A}$, $\mathcal{A} \otimes \mathcal{K}$ is always stable, because $\mathcal{K} \otimes \mathcal{K} \cong \mathcal{K}$. Two C^*-algebras $\mathcal{A}$ and $\mathcal{B}$ are *Morita equivalent* whenever $\mathcal{A} \otimes \mathcal{K}$ is isomorphic to $\mathcal{B} \otimes \mathcal{K}$.

PROPOSITION 5.5. *Given any pair P and Q of projections in $\mathcal{A} \otimes \mathcal{K}$, there is always a pair P', Q' of mutually orthogonal projections in $\mathcal{A} \otimes \mathcal{K}$ such that $P' \approx P$ and $Q' \approx Q$. Therefore the sum $[P]+[Q] = [P' \oplus Q']$ is always defined.*

In this way, if $\mathcal{A}$ is a stable algebra, the set $\mathcal{P}(\mathcal{A})$ of equivalence classes of projections is an Abelian monoid with neutral element given by the class of the zero projection. If $\mathcal{A}$ is not stable, $\mathcal{P}(\mathcal{A})$ will be replaced by $\mathcal{P}(\mathcal{A} \otimes \mathcal{K})$. The Grothendieck construction gives a canonical way to construct a group from such a monoid. This is a direct generalization of the construction of the group of integers $\mathbb{Z}$ from $\mathbb{N}$. The formal difference $[P]-[Q]$ is defined as the equivalence class of pairs $([P],[Q]) \in \mathcal{P}(\mathcal{A} \otimes \mathcal{K}) \times \mathcal{P}(\mathcal{A} \otimes \mathcal{K})$ under the relation

$$([P],[Q]) \,\mathfrak{R}\, ([P'],[Q']) \Leftrightarrow \exists [S] \in \mathcal{P}(\mathcal{A} \otimes \mathcal{K});\;\; [P]+[Q']+[S] = [P']+[Q]+[S]\,.$$

The corresponding quotient is the Abelian group $K_{00}(\mathcal{A}) = \mathcal{P}(\mathcal{A} \otimes \mathcal{K}) \times \mathcal{P}(\mathcal{A} \otimes \mathcal{K})/\mathfrak{R}$. Whenever $\mathcal{A}$ is unital, $K_0(\mathcal{A}) := K_{00}(\mathcal{A})$. Otherwise, $\mathcal{A}$ must be enlarged to $\mathcal{A}^+$ obtained by adjoining a unit, so that $\mathcal{A}$ becomes a two-sided closed ideal of $\mathcal{A}^+$. The quotient map $\pi : \mathcal{A}^+ \to \mathcal{A}^+/\mathcal{A}$ induces a group homomorphism $\pi_* : K_{00}(\mathcal{A}^+) \to K_{00}(\mathcal{A}^+/\mathcal{A})$, the kernel of which being the group $K_0(\mathcal{A})$ (see [**Bla**] for details). It leads to:

PROPOSITION 5.6. *Let $\mathcal{A}$ be a separable C^*-algebra.*

(i) *The set $K_0(\mathcal{A})$ is countable and has a canonical structure of Abelian group.*
(ii) *Any $*$-isomorphism $\varphi : \mathcal{A} \mapsto \mathcal{B}$ between C^*-algebras induces a group homomorphism $\varphi_* : K_0(\mathcal{A}) \mapsto K_0(\mathcal{B})$, so that K becomes a functor from the category of C^*-algebras into the category of Abelian discrete groups.*
(iii) *Any trace $\mathcal{T}$ on $\mathcal{A}$ defines in a unique way a group homomorphism $\mathcal{T}_*$ from $K_0(\mathcal{A})$ to $\mathbb{R}$ such that if P is a projection on $\mathcal{A}$, $\mathcal{T}(P) = \mathcal{T}_*([P])$ where $[P]$ is the class of P in $K_0(\mathcal{A})$.*

(iv) *If $\mathcal{A}$ and $\mathcal{B}$ are two Morita equivalent C^*-algebras then $K_0(\mathcal{A})$ and $K_0(\mathcal{B})$ are isomorphic.*

Putting together Shubin's formula with the last proposition leads to:

THEOREM 5.6. ***Gap Labelling Theorem for homogeneous media***
Let H be a homogeneous self-adjoint operator satisfying Shubin's formula (5.1), let $\mathcal{A}$ be the C^*-algebra generated by H and by its translates and let $\operatorname{spec}(H)$ be its spectrum in $\mathcal{A}$. Then:

(i) *For any gap $\mathfrak{g}$ in the spectrum of H, the value of the IDOS of H on $\mathfrak{g}$ belongs to the countable set of real numbers $\mathcal{T}_*(K_0(\mathcal{A})) \cap [0, \mathcal{T}(\mathbf{1})]$.*
(ii) *The equivalence class $n(\mathfrak{g}) = [P(\mathfrak{g})] \in K_0(\mathcal{A})$, gives a labelling which is invariant under norm perturbations of the Hamiltonian H within $\mathcal{A}$.*
(iii) *If $S \subset \mathbb{R}$ is a closed and open subset in $\operatorname{spec}(H)$, then $n_S = [P_S] \in K_0(\mathcal{A})$ where $[P_S]$ is the eigenprojection of H corresponding to S, is a labelling for each such part of the spectrum.*

Let $t \in \mathbb{R} \to H(t)$ be a continuous family of self-adjoint operators (in the norm of the resolvent) with resolvent in $\mathcal{A}$.

(iv) *(homotopy invariance) The gap edges of $H(t)$ are continuous and the labelling of a gap $\{\mathfrak{g}(t)\}$, is independent of t as long as the gap does not close.*
(v) *(additivity) If for $t \in [t_0, t_1]$, the spectrum of H contains a clopen subset $S(t)$ such that $S(0) = S_+ \cup S_-$ and $S(1) = S'_+ \cup S'_-$ where $S_\pm$ and $S'_\pm$ are clopen sets in $\operatorname{spec}(H(t_0))$ and $\operatorname{spec}(H(t_1))$ respectively, then $n_{S_+} + n_{S_-} = n_{S'_+} + n_{S'_-}$.*

5.3. Higher K-groups and exact sequences. The explicit computation of K-groups can be performed using the methods developed in homological algebra. The main tools are exact sequences and spectral sequences. However, these method require introducing higher order K-groups. Let $\mathcal{A}$ be a C^*-algebra and let $GL_n(\mathcal{A})$ be the group of invertible elements of the algebra $M_n(\mathcal{A})$. (when $\mathcal{A}$ is non-unital, $GL_n(\mathcal{A}) = \{u \in GL_n(\mathcal{A}^+); u \equiv \mathbf{1}_n \mod M_n(\mathcal{A})\}$). $GL_n(\mathcal{A})$ is embedded as a subgroup of $GL_{n+1}(\mathcal{A})$ using

$$\begin{pmatrix} GL_n(\mathcal{A}) & 0_n^* \\ 0_n & 1 \end{pmatrix}$$

(with $0_n = (0...0)$). Let $GL_\infty(\mathcal{A})$ be the inductive limit of $GL_n(\mathcal{A})$, namely the norm closure of their union, and let $[GL_\infty(\mathcal{A})]_0$ be the connected component of the identity in $GL_\infty(\mathcal{A})$. K_1 is defined as follows:

$$K_1(\mathcal{A}) = GL_\infty(\mathcal{A})/GL_\infty(\mathcal{A})_0 = \varinjlim \{GL_n(\mathcal{A})/[GL_n(\mathcal{A})]_0\} \tag{5.5}$$

If $\mathcal{A}$ is separable, then $K_1(\mathcal{A})$ is countable, since nearby invertible elements are in the same component. For $u \in GL_n(\mathcal{A})$, let $[u]$ be its class in $K_1(\mathcal{A})$. The relation $[u][v] = [diag(u, v)]$ defines a product in $K_1(\mathcal{A})$.

PROPOSITION 5.7. [**Bla**] *$K_1(\mathcal{A})$ is an Abelian group.*

The *suspension* of $\mathcal{A}$ is the C^*-algebra $S\mathcal{A}$ of continuous functions $f : \mathbb{R} \to \mathcal{A}$ vanishing at $\pm\infty$, endowed with point-wise addition, multiplication and adjoint, and the sup-norm. Hence $S\mathcal{A} \cong C_0(\mathbb{R}) \otimes \mathcal{A}$. Then

THEOREM 5.7. [**Bla**] *$K_1(\mathcal{A})$ is canonically isomorphic to $K_0(S\mathcal{A})$.*

Therefore we can also define higher K-groups by

$$K_2(\mathcal{A}) = K_1(S\mathcal{A}) = K_0(S^2\mathcal{A}), \dots, K_n(\mathcal{A}) = \dots = K_0(S^n\mathcal{A}).$$

THEOREM 5.8. ***Bott Periodicity*** $K_0(\mathcal{A}) \cong K_2(\mathcal{A})$.
More precisely $K_0(\mathcal{A})$ is isomorphic to the group $\pi_1(GL_\infty(\mathcal{A}))$ of homotopy classes of closed paths in $GL_\infty(\mathcal{A})$. Furthermore, if $\mathcal{T}$ is a trace on $\mathcal{A}$ and if $t \in [0,1] \to U(t)$ is a closed path in $GL_\infty(\mathcal{A})$ [**Co81**]:

$$\mathcal{T}_*([U]) = \frac{1}{2\pi i}\int_{[0,1]} dt\, \mathcal{T}(U(t)^{-1}U'(t)), \tag{5.6}$$

where $\mathcal{T}_*$ is the map induced by $\mathcal{T}$ on $K_0(\mathcal{A})$.

K_i is a covariant functor with the following properties:

THEOREM 5.9. *Let $\mathcal{J}, \mathcal{A}, \mathcal{A}_n, \mathcal{B}$ be C^*-algebras and n, i non-negative integers:*

(i) *If $f : \mathcal{A} \to \mathcal{B}$ is a $*$-homomorphism, then f induces a group homomorphism $f_* : K_i(\mathcal{A}) \to K_i(\mathcal{B})$. Then $id_* = id$, and $(f \circ g)_* = f_* \circ g_*$.*

(ii) $K_i(\bigoplus_n \mathcal{A}_n) \cong \bigoplus_n K_i(\mathcal{A})$

(iii) *If $\mathcal{A}$ is the inductive limit of the sequence $(\mathcal{A}_n)_{n>0}$ of C^*-algebras then $K_i(\mathcal{A})$ is the inductive limit of the groups $K_i(\mathcal{A}_n)$.*

(iv) *If $\phi : \mathcal{J} \to \mathcal{A}$, and $\psi : \mathcal{A} \to \mathcal{B}$ are $*$-homomorphisms such that the sequence*

$$0 \to \mathcal{J} \to \mathcal{A} \to \mathcal{B} \to 0$$

be exact, there is a six-term exact sequence of the form:

$$\begin{array}{ccccc} K_0(\mathcal{J}) & \xrightarrow{\phi_*} & K_0(\mathcal{A})) & \xrightarrow{\psi_*} & K_0(\mathcal{B}) \\ {\scriptstyle Ind}\uparrow & & & & \downarrow{\scriptstyle Exp} \\ K_1(\mathcal{B})) & \xleftarrow{\psi_*} & K_1(\mathcal{A}) & \xleftarrow{\phi_*} & K_1(\mathcal{J}) \end{array} \tag{5.7}$$

In the previous theorem, Ind et Exp are the connection automorphisms defined as follows (whenever $\mathcal{A}$ is unital): let P be a projection in $\mathcal{B}\otimes\mathcal{K}$, and let A be a self-adjoint element of $\mathcal{A}\otimes\mathcal{K}$ such that $\psi\otimes id(A) = P$. Then $\psi\otimes id(e^{2\imath\pi A}) = e^{2\imath\pi P} = \mathbf{1}$, so that $B = e^{2\imath\pi A} \in (\mathcal{J}\otimes\mathcal{K})^+$ and is unitary in $(\mathcal{J}\otimes\mathcal{K})^+$. The class of B gives an element of $K_1(\mathcal{J})$ which is, by definition, $Exp([P])$. In much the same way, let now U be an unitary element of $\mathbf{1} + (\mathcal{B}\otimes\mathcal{K})$. Without loss of generality it is the image under $\psi\otimes id$ of a partial isometry W in $(\mathcal{A}\otimes\mathcal{K})$. Then $Ind([U])$ is the class of $[WW^*] - [W^*W]$ in $K_0(\mathcal{J})$. These definitions actually make sense.

The Connes-Thom isomorphism. The C^*-algebra of a dynamical system introduced in Section 1.4 is a special case of the C^*-crossed product construction. Let $\mathcal{A}$ be a C^*-algebra, $\mathbb{G}$ be a locally compact group, and α be a continuous homomorphism from $\mathbb{G}$ into $\mathrm{Aut}(\mathcal{A})$ (namely the group of $*$-automorphisms of $\mathcal{A}$ endowed with the topology of point-wise norm-convergence). A *covariant representation* of the triple $(\mathcal{A}, \mathbb{G}, \alpha)$ is a pair of representations (Π, ρ) of $\mathcal{A}$ and $\mathbb{G}$ on the same Hilbert space such that $\rho(g)\Pi(a)\rho(g)^* = \Pi(\alpha_g(a))$ for all $a \in \mathcal{A}$ and $g \in \mathbb{G}$. Each covariant representation of $(\mathcal{A}, \mathbb{G}, \alpha)$ gives a representation of the twisted convolution algebra $C_c(\mathbb{G}, A)$ by integration (compare with Section 1.4), and hence a pre-C^*-norm on this $*$-algebra. The supremum of all these norms is a C^*-norm, and the completion of $\mathcal{C}_c(\mathbb{G}, A)$ with respect to this norm is called the *crossed product* of $\mathcal{A}$ by $\mathbb{G}$ under the action α, denoted by $A \rtimes_\alpha \mathbb{G}$. The *-representations of $A \rtimes_\alpha \mathbb{G}$

are in natural one-to-one correspondence with the covariant representations of the dynamical system $(\mathcal{A}, \mathbb{G}, \alpha)$.

THEOREM 5.10. [**Co81**] $K_i(A \rtimes_\alpha \mathbb{R}) \cong K_{1-i}(A)$, *for* $i = 0, 1$.

The Pimsner & Voiculescu exact sequence.

THEOREM 5.11. [**PiVo**] *Let $\mathcal{A}$ be a separable C^*-algebra, and let α be a *-automorphism of $\mathcal{A}$. There exists a six-term exact sequence:*

$$
\begin{array}{ccccc}
K_0(\mathcal{A}) & \xrightarrow{id-\alpha_*} & K_0(\mathcal{A})) & \xrightarrow{j_*} & K_0(\mathcal{A} \rtimes_\alpha \mathbb{Z}) \\
{\scriptstyle Ind}\uparrow & & & & \downarrow{\scriptstyle Exp} \\
K_1(\mathcal{A} \rtimes_\alpha \mathbb{Z})) & \xleftarrow{j_*} & K_1(\mathcal{A}) & \xleftarrow{id-\alpha_*} & K_1(\mathcal{A})
\end{array}
\tag{5.8}
$$

where j is the canonical injection of $\mathcal{A}$ into the crossed product.

6. Results for 1D and 2D quasicrystals

Let $L = \Lambda(M)$ be an admissible model set (see Section 3.4), and $(\Omega, \mathbb{R}^d) = (\mathbb{T}_M^{n+d}, \mathbb{R}^d)$ its hull. Let Υ be its (totally disconnected) transversal, and $C^*(G_\Upsilon)$ be the algebra of the corresponding groupoid. Let $\mathbb{T}_M^n$ be the quotient of $\mathbb{R}_M^n$ by the $\mathbb{Z}^n$-action defined in Section 3.4, In the following M will be a Borel set. According to Theorem 3.8, the Lebesgue measure, denoted here by $\mathbb{P}$, is the unique translation-invariant, ergodic measure on $\Omega = \mathbb{T}_M^{n+d}$. It induces transverse measure, also denoted by $\mathbb{P}$, on Υ.

THEOREM 6.1. $\mathcal{T}_{\mathbb{P}*}(K_0(\mathcal{C}(\mathbb{T}_M^n) \rtimes \mathbb{Z}^d)) = \mathcal{T}_{\mathbb{P}*}(K_0(\mathcal{C}(\Omega) \rtimes \mathbb{R}^d))$

PROOF: Proposition 3.3, Theorems 4.6 and 4.7 insure that the algebras are Morita equivalent. But, for separable algebras $\mathcal{A}$ and $\mathcal{B}$, Morita equivalence implies the existence of a $\mathcal{A}$-$\mathcal{B}$-bimodule [**BGR, Co94**]. Then, not only are the K-groups of these two algebras isomorphic but also their images under the traces coincide [**Bel93**]. □

REMARK 6.2. Kellendonk obtained a similar result in [**Kel1**] by proving that model sets can actually be seen as "decorations" of $\mathbb{Z}^d$.

REMARK 6.3. In the one-dimensional case, the Poincaré first return map insures that the transversal Υ can be endowed with a $\mathbb{Z}$-action. The Pimsner and Voiculescu six-terms exact sequence permits to compute the K-groups and the set of gap labels. For higher dimensions however, the Poincaré map is replaced by the groupoid of the transversal, which is not necessarily identical to a group action. Nevertheless the theorem 6.1 permits to reduce the K-theory problem to a group action.

6.1. Completely disconnected hulls. The following results has been known for a long time (see [**BBG**] for a review).

LEMMA 6.4. *Let Ξ be a totally disconnected compact metrizable space. Then,* $K_1(\mathcal{C}(\Xi)) = 0$

PROOF: Let d be a compatible metric on Ξ, and let r be a positive real number. Since Ξ is totally disconnected, each $\xi \in \Xi$ admits a clopen neighbourhood $\mathcal{O}_\xi$ of diameter less than r. Ξ being compact, a finite covering of Ξ by clopen sets of diameter less than r can be extracted. Since the complement of a clopen set is a clopen set, this covering can be chosen to be a finite partition denoted by $\mathfrak{P}$. Let now f be a $M_n(\mathbb{C})$-valued continuous invertible function on Ξ. To prove the lemma, it is enough to show that f is homotopic to the constant function equal to one. Since Ξ is compact, f is uniformly continuous, so that given any $\epsilon > 0$, there is $r > 0$ such that $d(\xi, \xi') \leq r \Rightarrow \|f(\xi) - f(\xi')\| \leq \epsilon$. For each $\mathcal{O}_k \in \mathfrak{P}$, let $\xi_k \in \mathcal{O}_k$ and χ_k be the characteristic function of $\mathcal{O}_k$. Hence $\chi_k \in \mathcal{C}(\Xi)$. Then if $f_\epsilon = \sum_k f(\xi_k)\chi_k$, $\|f - f_\epsilon\| \leq \epsilon$. Thus f and f_ϵ are homotopic for ϵ small enough. By hypothesis, all the $f(\xi_k)$'s are invertible $n \times n$ matrices, so that there are matrices H_k such that $f(\xi_k) = \exp(H_k)$. Setting $f_\epsilon(\xi, t) = \sum_k \exp(tH_k)\chi_k(\xi)$ gives a homotopy between f_ϵ and 1 in the set of invertible elements of $M_n(\mathcal{C}(\Xi))$. □

Let P be a projection in $\mathcal{C}(\Xi) \otimes \mathcal{K}$. P may be viewed as a continuous mapping from Ξ into $\mathcal{K}$ leading to the map $f_P(\omega) = Tr(P(\omega))$ (where Tr is the usual trace on $M_n(\mathbb{C})$). Let then $f_* : P \mapsto f_P$, so that:

Lemma 6.5. *The map f_* is an isomorphism from $K_0(\mathcal{C}(\Xi))$ to the group $\mathcal{C}(\Xi, \mathbb{Z})$ of integer-valued continuous functions on Ξ.*

Proof: f_P depends only on the equivalence class of P. For indeed, if $P \approx Q$, there is $U \in \mathcal{C}(\Xi) \otimes \mathcal{K}$ such that $UU^* = P$ and $U^*U = Q$. In particular, $f_P(\xi) = Tr(U(\xi)U^*(\xi)) = Tr(U^*(\xi)U(\xi)) = f_Q(\xi)$. Moreover, if $PQ = QP = 0$, then $f_{P\oplus Q}(\xi) = Tr(P(\xi) \oplus Q(\xi)) = Tr(P(\xi)) + Tr(Q(\xi)) = f_P(\xi) + f_Q(\xi)$, and so $f_{P\oplus Q} = f_P + f_Q$. Hence f defines a group homorphism f_* between $K_0(\mathcal{C}(\Xi))$ and $\mathcal{C}(\Xi, \mathbb{Z})$.
f_* is surjective: for if $h \in \mathcal{C}(\Xi, \mathbb{Z})$, let Ξ_n denote the set of $\xi \in \Xi$ such that $h(\xi) = n$. Since h is continuous and integer-valued, the family $\{\Xi_n, n \in \mathbb{N}\}$ gives a finite partition of Ξ in clopen sets. Let χ_n denotes the characteristic function of Ξ_n, and π_n be the n-dimensional projection $1_n \oplus 0$ in $\mathcal{K}$. Then if $P' = \sum_{n>0} \chi_n \otimes \pi_n$ and $Q' = \sum_{n>0} \chi_{-n} \otimes \pi_n$, h can be written as $h = f_{P'} - f_{Q'}$.
f_* is injective: it is sufficient to show that any projection in $\mathcal{C}(\Xi) \otimes \mathcal{K}$ is equivalent to a projection of the same type as P' above. For indeed, $f_P - f_Q = 0$ implies that P and Q admit the same partition $\{\Xi_n, n \in \mathbb{N}\}$ into clopen subsets of Ξ on which their dimension is a fixed integer. So if $P \approx P'$, then $Q \approx P'$ namely $[P] - [Q] = 0$. Let then P be a projection in $\mathcal{C}(\Xi) \otimes \mathcal{K}$. Let $\{\Xi_n, n \in \mathbb{N}\}$ be the partition into clopen subsets on which the dimension of P is n. Proceeding as in the proof of Lemma 6.4, given $0 < \epsilon < 1$, for each $n \in \mathbb{N}$, there is a finite partition $(\Xi_{n,k})_k$ of Ξ_n into clopen subsets, such that, if $\xi_{n,k} \in \Xi_{n,k}$, the projection $P_\epsilon = \sum_{n,k} P(\xi_{n,k})\chi_{n,k}$ satisfies $\|P - P_\epsilon\| \leq \epsilon < 1$. Thus $P \approx P_\epsilon$. Now $P(\xi_{n,k})$ is a fixed projection of dimension n so that there is $S_{n,k}$ in $\mathcal{K}$ such that $P(\xi_{n,k}) = S_{n,k}S_{n,k}^*$ and $\pi_n = S_{n,k}^* S_{n,k}$. Therefore, setting $S = \sum_{n,k} S_{n,k}\chi_{n,k}$, S is an element of $\mathcal{C}(\Xi) \otimes \mathcal{K}$ such that $P_\epsilon = SS^*$ and $P' = S^*S$, establishing the equivalence between P and P'. □

6.2. Gap labelling for 1D quasicrystals.

Definition 6.6. Let $\mathbb{G}$ be an Abelian group and let $T : \mathbb{G} \mapsto \mathbb{G}$ be a group isomorphism. The set $\mathcal{E} = \{g \in \mathbb{G}; \exists h \in \mathbb{G}, g = h - T(h)\}$ is a subgroup. The set $\mathbb{G}^T = \{g \in \mathbb{G}; T(g) = g\}$ is called the group of *invariants* whereas $\mathbb{G}_T = \mathbb{G}/\mathcal{E}$ is called the groups of *co-invariants.*

Theorem 6.7. **[Bel93]** *Let Ξ be a totally disconnected compact metrizable space, endowed with a $\mathbb{Z}$-action T.*

(i) *If T is topologically transitive $K_1(\mathcal{C}(\Xi) \rtimes_T \mathbb{Z})$ is isomorphic to $\mathbb{Z}$.*
(ii) *$K_0(\mathcal{C}(\Xi) \rtimes_T \mathbb{Z})$ is isomorphic to $\mathcal{C}(\Xi, \mathbb{Z})_T$.*
(iii) *Let $\mathbb{P}$ be a T-invariant ergodic probability measure on Ξ, and $\mathcal{T}_{\mathbb{P}}$ be the corresponding trace on $\mathcal{C}(\Xi) \rtimes_T \mathbb{Z}$. Then, the image of $K_0(\mathcal{C}(\Xi) \rtimes_T \mathbb{Z})$ by $\mathcal{T}_{\mathbb{P}*}$ is equal to the countable subgroup $\mathbb{P}(\mathcal{C}(\Xi, \mathbb{Z}))$ of $\mathbb{R}$ (see Theorem 1.16).*

Remark 6.8. In the one-dimensional case, any transversal Υ of $(\Omega, \mathbb{R}, T)$ is canonically endowed with a $\mathbb{Z}$-action. Thus this theorem can be applied to Υ.

Proof: Due to Lemmas 6.4 and 6.5, the Pimsner and Voiculescu six-term exact sequence (5.8) for $\mathcal{A} = \mathcal{C}(\Xi)$ leads to the following exact sequence:
(6.1)

$$0 \to K_1(\mathcal{C}(\Xi) \rtimes_T \mathbb{Z}) \xrightarrow{f_* \circ Ind} \mathcal{C}(\Xi, \mathbb{Z}) \xrightarrow{id - T_*} \mathcal{C}(\Xi, \mathbb{Z}) \xrightarrow{j_* \circ f_*^{-1}} K_0(\mathcal{C}(\Xi) \rtimes \mathbb{Z}) \to 0$$

Since the sequence is exact, it follows that $K_1(\mathcal{C}(\Xi) \rtimes_T \mathbb{Z})$ is isomorphic to the kernel of $id - T_*$. If T is topologically transitive, this kernel is the set of constant functions in $\mathcal{C}(\Xi, \mathbb{Z})$, that is $\mathbb{Z}$ and (i) is proved.
For the same reason, since the sequence is exact, j_* is surjective. Thus $K_0(\mathcal{C}(\Xi) \rtimes \mathbb{Z}) \approx \mathcal{C}(\Xi, \mathbb{Z}) / \ker(j_*) = \mathcal{C}(\Xi, \mathbb{Z})_T$. Since j is the canonical injection from $\mathcal{C}(\Xi)$ into $\mathcal{C}(\Xi) \rtimes_T \mathbb{Z}$, it follows from the definition of the trace given by $\mathbb{P}$ that $\mathcal{T}_{\mathbb{P}} \circ j = \mathbb{P}$. By functoriality, $\mathcal{T}_{\mathbb{P}*} \circ j_* = \mathbb{P}_*$ on the corresponding K_0-groups. Since $\mathbb{P}_*$ is nothing but $\mathbb{P}$ acting on $\mathcal{C}(\Xi, \mathbb{Z})$, and j_* is surjective, (iii) holds. (iii) give a proof of Theorem 1.16 for the case $d = 1$. □

Corollary 6.1. *Let L be a one-dimensional admissible model set with acceptance domain M, M being a Borel set. Let $(\mathbb{T}_M^{n+1}, \mathbb{R})$ be its hull, $\mathbb{T}_M^n$ be the quotient of $\mathbb{R}_M^n$ by the $\mathbb{Z}^n$-action, and $\mathbb{P}$ be the Lebesgue measure on $\mathbb{T}_M^n$ normalized such as the measure of the acceptance domain M be one. Then*

$$\mathcal{T}_{\mathbb{P}*}(K_0(\mathcal{C}(\mathbb{T}_M^{n+1}) \rtimes \mathbb{R})) = \mathcal{T}_{\mathbb{P}*}(K_0(\mathcal{C}(\mathbb{T}_M^n))) = \mathbb{P}(\mathcal{C}(\mathbb{T}_M^n, \mathbb{Z})),$$

and the values on gaps of the IDOS of any Hamiltonians on this one-dimensional quasicrystal belong to $\mathbb{P}(\mathcal{C}(\mathbb{T}_M^n, \mathbb{Z})) \cap [0,1]$.

Proof: Theorem 5.6, Theorem 6.1, Lemma 6.5 and Theorem 6.7. □

In Example 4.8 we introduced one-dimensional quasicrystals obtained with $n = 1$ and with M be a projection of a unit cell of $\mathcal{R}$. In this case, M is $\mathcal{R}$-compatible and we get an explicit label for the gaps.

Theorem 6.9. *The values on gaps of the IDOS of the Kohmoto model (4.16) or of any Hamiltonians belonging to the same algebra belong to $(\mathbb{Z} + \mathbb{Z}\alpha) \cap [0,1]$.*

Remark 6.10. Such a result could be alternatively obtained through the use of the irrational rotation algebra (see Example 4.8 and [**Bel93**]).

Proof: We use Corollary 6.1 and the fact that $\mathcal{C}(\mathbb{T}_M^1, \mathbb{Z})$ is generated by a set of characteristic functions associated with the partition of $\mathbb{T}_M^1$ in polytopes (see the description of the topology induced by M in Section 3.4). Each such one-dimensional model set can be related to an irrational number ω, namely the slope of the physical space relatively to the lattice (see Figure 1 and Example 4.8). Integrating the generic characteristic functions can then be performed by computing the lengths of the segments of the partition of $\mathbb{T}_M^1$. It is easy to convinced oneself that such lengths belong to $\mathbb{Z} + \alpha\mathbb{Z}$, where $\alpha = \omega/(\omega + 1)$, once the Lebesgue measure is normalized such as the measure of the acceptance domain be one. □

6.3. Gap labelling for 2D quasicrystals. Let Ξ be a totally disconnected compact metrizable space, endowed with a $\mathbb{Z}^2$-action, given by two commuting *-automorphisms α_1 and α_2. Let $\mathbb{P}$ be an (α_1, α_2)-invariant ergodic probability measure on Ξ, and let $\mathcal{T}_{\mathbb{P}}$ be the corresponding trace on $\mathcal{C}(\Xi) \rtimes_{\alpha_1\alpha_2} \mathbb{Z}^2$. Following [**vEl**], an iteration of the Pimsner and Voiculescu six-terms exact sequence can be performed, leading to a short exact sequence for $K_0(\mathcal{C}(\Xi) \rtimes_{\alpha_1\alpha_2} \mathbb{Z}^2)$. Let $\mathcal{A} = \mathcal{C}(\Xi)$ and let $\mathcal{B} = \mathcal{A} \rtimes_{\alpha_1} \mathbb{Z}$. Then α_2 induces a *-automorphism on $\mathcal{B}$ so that $\mathcal{B} \rtimes_{\alpha_2} \mathbb{Z}$ be isomorphic to $\mathcal{C}(\Xi) \rtimes_{\alpha_1\alpha_2} \mathbb{Z}^2$. Theorem 5.11 leads to:

$$\begin{array}{ccccc} K_0(\mathcal{B}) & \xrightarrow{id-\alpha_{2*}} & K_0(\mathcal{B})) & \xrightarrow{j_*} & K_0(\mathcal{B} \rtimes_{\alpha_2} \mathbb{Z}) \\ {\scriptstyle Ind_2}\uparrow & & & & \downarrow{\scriptstyle Exp_2} \\ K_1(\mathcal{B} \rtimes_{\alpha_2} \mathbb{Z}) & \xleftarrow{j_*} & K_1(\mathcal{B}) & \xleftarrow{id-\alpha_{2*}} & K_1(\mathcal{B}) \end{array} \tag{6.2}$$

Moreover, the exact sequence (6.1) gives:

$$0 \to K_1(\mathcal{B}) \xrightarrow{f_* \circ Ind_1} \mathcal{C}(\Xi, \mathbb{Z}) \xrightarrow{id-\alpha_1*} \mathcal{C}(\Xi, \mathbb{Z}) \xrightarrow{j_1 * \circ f_*^{-1}} K_0(\mathcal{B}) \to 0. \tag{6.3}$$

That is, $K_1(\mathcal{B}) \approx \mathcal{C}(\Xi, \mathbb{Z})^{\alpha_1}$ and $K_0(\mathcal{B}) \approx \mathcal{C}(\Xi, \mathbb{Z})_{\alpha_1}$. Then (6.2) gives

$$0 \to K_0(\mathcal{A})_{\alpha_1\alpha_2} \xrightarrow{j_{2*} \circ j_{1*} \circ f_*^{-1}} K_0(\mathcal{A} \rtimes \mathbb{Z}^2) \xrightarrow{f_* \circ Ind_1 \circ Exp_2} K_0(\mathcal{A})^{\alpha_1\alpha_2} \to 0. \tag{6.4}$$

If the dynamical system $(\Xi, \mathbb{Z}^2)$ is minimal (which is the case for admissible model sets, see Theorem 3.8), the class of identity is the only non-trivial element in $K_0(\mathcal{A})^{\alpha_1\alpha_2}$. Let $\xi_{\mathbf{1}}$ be a lift of the identity $[\mathbf{1}] \in K_0(\mathcal{A})^{\alpha_1\alpha_2}$ in $K_0(\mathcal{A} \rtimes \mathbb{Z}^2)$, then:

Lemma 6.11. [**vEl**] $\mathcal{T}_{\mathbb{P}}(\xi_{\mathbf{1}}) = 1 \in \mathcal{T}_{\mathbb{P}}(K_0(\mathcal{A}))$.

Remark 6.12. There is an alternative method to get (6.4) [**FoHu**], but Lemma 6.11 cannot be established just by considerations of isomorphims because Ind_1 and Exp_2 must be computed explicitely.

Now, it is enough to notice that, because of trace invariance under α_1 and α_2, $\mathcal{T}_{\mathbb{P}}(K_0(\mathcal{A})_{\alpha_1\alpha_2}) = \mathcal{T}_{\mathbb{P}}(K_0(\mathcal{A}))$ to obtain

Theorem 6.13. [**vEl**] $\mathcal{T}_{\mathbb{P}}(K_0(\mathcal{C}(\Xi) \rtimes_{\alpha_1\alpha_2} \mathbb{Z}^2)) = \mathcal{T}_{\mathbb{P}}(K_0(\mathcal{C}(\Xi)))$.

Using Theorem 5.6, Theorem 6.1, Lemma 6.5 and Theorem 6.7, we get as a corollary the main result of this section

Corollary 6.2. *Let L be a two-dimensional admissible model set with acceptance domain M, M being a Borel set, let $(\mathbb{T}_M^{n+2}, \mathbb{R}^2)$ be its hull, $\mathbb{T}_M^n$ be the quotient of $\mathbb{R}_M^n$ by the $\mathbb{Z}^n$-action, and $\mathbb{P}$ be the Lebesgue measure on $\mathbb{T}_M^n$ normalized such as the measure of the acceptance domain M be one. Then*

$$\mathcal{T}_{\mathbb{P}*}(K_0(\mathcal{C}(\mathbb{T}_M^{n+2}) \rtimes \mathbb{R}^2)) = \mathcal{T}_{\mathbb{P}*}(K_0(\mathcal{C}(\mathbb{T}_M^n))) = \mathbb{P}(\mathcal{C}(\mathbb{T}_M^n, \mathbb{Z}))\,,$$

and the IDOS of Hamiltonians on two-dimensional quasicrystals takes values in the set $\mathbb{P}(\mathcal{C}(\mathbb{T}_M^n, \mathbb{Z})) \cap [0, 1]$.

Example 6.14. **The Octagonal Tiling**

In the following, only model sets with $n = d = 2$ are considered, with $\mathcal{R} = \mathbb{Z}^4$. Moreover, the acceptance domain M is given by the π_2-projection of the unit hypercube of $\mathbb{R}^4$ with sides given by the canonical basis $\varepsilon_1, \cdots, \varepsilon_4$. Let $e_i = \pi_2(\varepsilon_i)$ for $i = 1, \cdots, 4$. Let $\mathbb{T}_M^2$ denote the quotient of $\mathbb{R}_M^2$ by the $\mathbb{Z}^2$-action. Given any $f \in \mathcal{C}(\mathbb{T}_M^2, \mathbb{Z})$, for $n \in \mathbb{N}$ the set $f^{-1}(\{n\})$ is both closed and open. Thus f is a

finite $\mathbb{Z}$-linear combination of characteristic functions of clopen sets. Therefore the set of gap labels will be the $\mathbb{Z}$-module generated by the Lebesgue measure of clopen sets, provided the Lebesgue measure is normalized as to give measure one to M.
Let $\mathcal{F}$ be the family of affine hyperplanes in $\mathbb{R}^2 \times \mathbb{R}^2$ given by $\{F_i +;\ a \in \mathcal{L} = \pi_2(\mathbb{Z}^4)\}$ where the F_i's are the hyperplanes parallel to the maximal faces of $\mathbb{R}^2 \times M$. For each i let u_i be a unit vector in $\mathbb{R}^2$ perpendicular to F_i. As underlined at the end of the subsection 3.4, the M-topology can be equivalently defined as the coarsest topology for which the open half-planes $\{x \in \mathbb{R}^2; \langle u_i | x - a\rangle > 0\}$ (with $a \in \mathcal{L}$) are closed. $\mathbb{R}^2_M$ is nothing but the completion of $\mathbb{R}^2$ for this topology.
We present here a method to determine such elementary tiles which can directely be extended to higher dimensions [**Kel2**]. Let the set $\{F_{ij}(a,b) = (F_i + a) \cap (F_j + b); i,j \in [1,\ldots,4], a,b \in \mathbb{Z}^4\}$. By projection on $\mathbb{R}^2$, this define a family of points $\mathcal{F}^{(1)}$ endowed with an action of $\mathbb{Z}^4$. Thus, we consider $\mathcal{F}_{(0)} = \mathcal{F}^{(1)}/\mathbb{Z}^4$. This gives exactly the points we need to built elementary tiles in $\mathbb{T}^2_M$.

Now one study the *octagonal quasicrystal* [**Soc**]. It is obtained with $e_1 = (1,0)$, $e_2 = (0,1)$, $e_3 = (-\sqrt{2}/2, -\sqrt{2}/2)$, $e_4 = (\sqrt{2}/2, -\sqrt{2}/2)$ and with normalization $\|e_i\| = 1$. The acceptance zone is a regular octagonal. A combinatorial computation gives for this tiling: $\mathcal{F}_{(0)} = \{0, e_1/\sqrt{2}, e_3/\sqrt{2}\}$. This defines three types of intersection points. The last two types share the property of being intersection points of orthogonal lines only. Thus they generate *rectangles* and *triangles* as elementary tiles. Since $\mathcal{F}_{(0)}$ is not trivial, there are intersection points which are not projections of the lattice $\mathbb{Z}^4$. This is the reason why we cannot perform a triangulation of this tiling.

We only need to compute the measure of each of the rectangles and triangles, obtained by combining these three types of intersection points, to get

THEOREM 6.15. [**BCL**] *Let $\mathcal{A}_{oc}$ be the C^*-algebra associated to the octagonal quasicrystal. Let us denote by $\mathcal{T}_{\mathbb{P}}$ the trace associated to the Lebesgue measure on $\mathbb{R}^2$ and normalized such that the measure of the acceptance zone is* 1. *Then,*

$$\begin{aligned} \mathcal{T}_{\mathbb{P}*}\Big(K_0(\mathcal{A}_{oc})\Big) &= \frac{1/4\ \mathbb{Z} + \sqrt{2}/2\ \mathbb{Z}}{2(1+\sqrt{2})} \\ &= \left\{ \frac{m + n\sqrt{2}}{8} \in \frac{\mathbb{Z} + \sqrt{2}\ \mathbb{Z}}{8} \quad \text{such that } m+n \text{ is even} \right\}. \end{aligned}$$

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