TILING
APERIODIC MEDIA
and their
NONCOMMUTATIVE GEOMETRY

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Main References


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Aperiodic Solids

1. *Perfect crystals* in $d$-dimensions: translation and crystal symmetries. Translation group $\mathcal{T} \simeq \mathbb{Z}^d$.

2. *Quasicrystals*: no translation symmetry, but icosahedral symmetry. Ex.:
   (a) $\text{Al}_{62.5}\text{Cu}_{25}\text{Fe}_{12.5}$;
   (b) $\text{Al}_{70}\text{Pd}_{22}\text{Mn}_8$;
   (c) $\text{Al}_{70}\text{Pd}_{22}\text{Re}_8$;

3. *Amorphous media*: short range order
   (a) Glasses;
   (b) Silicium in amorphous phase;

4. *Disordered media*: random atomic positions
   (a) Normal metals (with defects or impurities);
   (b) Doped semiconductors ($\text{Si}$, $\text{AsGa}$, . . .).
I - The Hull as a Dynamical System

J. Bellissard, D. Hermann, M. Zarrouati, Hull of Aperiodic Solids and Gap Labelling Theorems
I.1)- Point Sets

Equilibrium positions of atomic nuclei make up a point set $\mathcal{L} \subset \mathbb{R}^d$ the set of lattice sites. $\mathcal{L}$ may be:

1. **Discrete**.

2. **Uniformly discrete**: $\exists r > 0$ s.t. each ball of radius $r$ contains at most one point of $\mathcal{L}$.

3. **Relatively dense**: $\exists R > 0$ s.t. each ball of radius $R$ contains at least one point of $\mathcal{L}$.

4. A **Delone** set: $\mathcal{L}$ is uniformly discrete and relatively dense.

5. **Finite type Delone** set: $\mathcal{L} - \mathcal{L}$ is discrete.

6. **Meyer** set: $\mathcal{L}$ and $\mathcal{L} - \mathcal{L}$ are Delone.

**Examples:**

1. A random Poissonian set in $\mathbb{R}^d$ is almost surely discrete but not uniformly discrete nor relatively dense.

2. Due to Coulomb repulsion and Quantum Mechanics, lattices of atoms are always uniformly discrete.

3. Impurities in semiconductors are not relatively dense.

4. In amorphous media $\mathcal{L}$ is Delone.

5. In a quasicrystal $\mathcal{L}$ is Meyer.
The ideal equilibrium positions of atomic nuclei sit on a discrete subset $\mathcal{L}$ of $\mathbb{R}^d$ ($d = 1, 2, 3$ in practice).

- A periodic array of atomic nuclei -

- A random array of atomic nuclei -
- A quasiperiodic array of atomic nuclei -

- Construction of Voronoi’s tiling -
I.2)- Point Measures

\( \mathcal{M}(\mathbb{R}^d) \) is the set of Radon measures on \( \mathbb{R}^d \) namely the dual space to \( \mathcal{C}_c(\mathbb{R}^d) \) (continuous functions with compact support), endowed with the weak* topology.

For \( \mathcal{L} \) a uniformly discrete point set in \( \mathbb{R}^d \):

\[
\nu := \nu^\mathcal{L} = \sum_{y \in \mathcal{L}} \delta(x - y) \quad \in \mathcal{M}(\mathbb{R}^d) .
\]

The \textit{Hull} is the closure in \( \mathcal{M}(\mathbb{R}^d) \)

\[
\Omega = \overline{\{ T^a \nu^\mathcal{L}; a \in \mathbb{R}^d \}} ,
\]

where \( T^a \nu \) is the translated of \( \nu \) by \( a \).

\textbf{Results:}

1. \( \Omega \) is compact and \( \mathbb{R}^d \) acts by homeomorphisms.

2. If \( \omega \in \Omega \), there is a uniformly discrete point set \( \mathcal{L}_\omega \) in \( \mathbb{R}^d \) such that \( \omega \) coincides with \( \nu_\omega = \nu^\mathcal{L}_\omega \).

3. If \( \mathcal{L} \) is \textit{Delone} (resp. \textit{Meyer}) so are the \( \mathcal{L}_\omega \)'s.
I.3)- Properties

(a) Minimality

\( \mathcal{L} \) is *repetitive* if for any finite patch \( p \) there is \( R > 0 \) such that each ball of radius \( R \) contains an \( \epsilon \)-approximant of a translated of \( p \).

**Proposition 1** \( \mathbb{R}^d \) acts minimaly on \( \Omega \) if and only if \( \mathcal{L} \) is repetitive.

(b) Transversal

The closed subset \( X = \{ \omega \in \Omega ; \nu_\omega(\{0\}) = 1 \} \) is called the *canonical transversal*. Let \( G \) be the subgroupoid of \( \Omega \rtimes \mathbb{R}^d \) induced by \( X \).

A Delone set \( \mathcal{L} \) has *finite type* if \( \mathcal{L} - \mathcal{L} \) is closed and discrete.

(c) Cantorian Transversal

**Proposition 2** If \( \mathcal{L} \) has finite type, then the transversal is completely discontinuous (Cantor).
II - Building Hulls

II.1)- Examples

1. **Crystals**: \( \Omega = \mathbb{R}^d/\mathcal{T} \cong \mathbb{T}^d \) with the quotient action of \( \mathbb{R}^d \) on itself. (Here \( \mathcal{T} \) is the translation group leaving the lattice invariant. \( \mathcal{T} \) is isomorphic to \( \mathbb{Z}^D \).)

   The transversal is a finite set (number of point per unit cell).

2. **Quasicrystals**: \( \Omega \cong \mathbb{T}^n, \ n > d \) with an irrational action of \( \mathbb{R}^d \) and a completely discontinuous topology in the transverse direction to the \( \mathbb{R}^d \)-orbits. The transversal is a Cantor set.

3. **Impurities in Si**: let \( \mathcal{L} \) be the lattices sites for Si atoms (it is a Bravais lattice). Let \( \mathcal{A} \) be a finite set (alphabet) indexing the types of impurities. The transversal is \( X = \mathcal{A}^{\mathbb{Z}^d} \) with \( \mathbb{Z}^d \)-action given by shifts.

   The Hull \( \Omega \) is the mapping torus of \( X \).
- The Hull of a Periodic Lattice -
II.2) Quasicrystals

Use the *cut-and-project* construction:

\[
\mathbb{R}^d \sim \mathcal{E}_\parallel \quad \longleftrightarrow \quad \mathbb{R}^n \xrightarrow{\pi_\perp} \mathcal{E}_\perp \sim \mathbb{R}^{n-d}
\]

\[
\mathcal{L} \quad \overset{\pi_\parallel}{\leftarrow} \quad \tilde{\mathcal{L}} \quad \overset{\pi_\perp}{\rightarrow} \quad W
\]

Here

1. \(\tilde{\mathcal{L}}\) is a *lattice* in \(\mathbb{R}^n\),
2. the *window* \(W\) is a compact polytope.
3. \(\mathcal{L}\) is the induced *quasilattice* in \(\mathcal{E}_\parallel\).
– The cut–and–project construction –
- The octagonal tiling -
II.3)- Hull of Quasicrystals

1. Let $\mathcal{F}$ be the family of affine hyperplanes in $\mathbb{R}^n$ with projections on $\mathcal{E}_\perp$ containing the maximal faces of $W$. Endow $\mathbb{R}^n$ with the topology such that for any $F \in \mathcal{F}$ and $a \in \tilde{\mathcal{L}}$, the two half spaces separated by the affine hyperplane $F + a$ are both closed and open. Let $\mathbb{R}^n_{\mathcal{F}}$ be the completion of $\mathbb{R}^n$ with this topology.

2. By construction, for $a \in \tilde{\mathcal{L}}$, the map $\tilde{x} \in \mathbb{R}^n \mapsto \tilde{x} + a \in \mathbb{R}^n$ extends to $\mathbb{R}^n_{\mathcal{F}}$ by continuity. Let then $T^n_{\mathcal{F}} = \mathbb{R}^n_{\mathcal{F}}/\tilde{\mathcal{L}}$ be the corresponding pseudo torus.

3. By construction, for $x \in \mathcal{E}_\parallel$, the map $\tilde{x} \in \mathbb{R}^n \mapsto \tilde{x} + x \in \mathbb{R}^n$ extends also by continuity to $\mathbb{R}^n_{\mathcal{F}}$ and commutes with $\tilde{\mathcal{L}}$. Thus it defines an $\mathbb{R}^d$ action on $T^n_{\mathcal{F}}$.

**Theorem 1** $\mathcal{L}$ is a Meyer set. Its Hull is conjugate to $T^n_{\mathcal{F}}$ endowed with its canonical $\mathbb{R}^d$-action. This Hull is uniquely ergodic.
III - Tilings & Point Sets


III.1)- Voronoi Cells

For $\mathcal{L}$ Delone and $x \in \mathcal{L}$, the Voronoi cell of $x$ is

$$V_x = \{ y \in \mathbb{R}^d ; |y - x| < |y - x'|, \forall x' \in \mathcal{L} \setminus \{x\} \}$$

- Building a Voronoi Cell -

The $V_x$’s are open polyhedrons with uniformly bounded diameter. They are mutually disjoint and their closure cover $\mathbb{R}^d$: it is a tiling of $\mathbb{R}^d$. 

III.2)- The Finite Pattern Condition

A *patch* is the set of tiles of $\mathcal{T}$ contained in some ball. A tiling $\mathcal{T}$ fulfills the *finite pattern condition* (FPC) if the number of patches of radius smaller than $R$ *modulo translations* is finite for all $R$’s.

*Then the transversal is a Cantor set.*

- The octagonal tiling is FPC -
- The pinwheel tiling is NOT FPC! -
III.3)- Branched Oriented Flat Manifolds

Step 1:

1. $X$ is the disjoint union of all prototiles;

2. glue prototiles $T_1$ and $T_2$ along a face $F_1 \subseteq T_1$ and $F_2 \subseteq T_2$ if $F_2$ is a translated of $F_1$ and if there are $x_1, x_2 \in \mathbb{R}^d$ such that $x_i + T_i$ are tiles of $\mathcal{T}$ with $(x_1 + T_1) \cap (x_2 + T_2) = x_1 + F_1 = x_2 + F_2$;

3. after identification of faces, $X$ becomes a branched oriented flat manifold (BOF) $B_0$.

- The branching process -
- Vertex branching for the octagonal tiling -
Step 2:

1. Choose an increasing sequence \( \{R_n\}_{n>0} \) of positive real numbers with \( R_n \uparrow \infty \);

2. for each \( n \geq 1 \) consider all patches of diameter less than \( R_n \);

3. add to each patch in \( \mathcal{T} \), the tiles touching it from outside along its frontier. Call such a patch *modulo translation* a *colored patch*;

4. proceed then as in Step 1 by replacing prototiles by colored patches to get the BOF-manifold \( B_n \).
Step 3:

1. Define a **BOF-submersion** $f_n : B_{n+1} \hookrightarrow B_n$ by identifying patches of order $n$ in $B_{n+1}$ with the prototiles of $B_n$;

2. call $\Omega$ the *projective limit* of the sequence

$$\cdots \xrightarrow{f_{n+1}} B_{n+1} \xrightarrow{f_n} B_n \xrightarrow{f_{n-1}} \cdots$$

3. there are commuting vector fields $X_1, \cdots X_d$ on $B_n$ generating local translations and giving rise to a $\mathbb{R}^d$ action $\tau$ on $\Omega$.

**Theorem 2** The dynamical system

$$(\Omega, \mathbb{R}^d, \tau) = \lim_{\leftarrow}(B_n, f_n)$$

obtained as inverse limit of branched oriented flat manifolds, is conjugate to the Hull of the Delone set of the tiling $\mathcal{T}$ by an homomorphism.
IV - NC Brillouin Zone

IV.1)- Algebra

$(\Omega, \mathbb{R}^d, \tau)$ is a topological dynamical system. One orbit at least is dense. The crossed product

$$\mathcal{A} = \mathcal{C}(\Omega) \rtimes_{\tau} \mathbb{R}^d$$

is (almost) the smallest $C^*$-algebra containing both the space of continuous functions on $\Omega$ and the action of $\mathbb{R}^d$ submitted to the commutation rules (for $f \in \mathcal{C}(\Omega)$)

$$T(a)fT(a)^{-1} = f \circ \tau^{-a}$$

1. For a crystal $\Omega = \mathbb{V}$, $\mathbb{R}^d$ acts by quotient action.

2. $\mathcal{C}(\mathbb{V}) \rtimes_{\tau} \mathbb{R}^d \simeq \mathcal{C}(\mathbb{B}) \otimes \mathcal{K}$, where $\mathcal{K}$ is the algebra of compact operators and $\mathbb{B}$ is the dual of the period group of $\mathcal{L}$. $\mathbb{B}$ is called the Brillouin zone.

$\mathcal{A}$ is the Noncommutative version of the space of $\mathcal{K}$-valued function over the Brillouin zone.
IV.2)- Construction of $\mathcal{A}$

Endow $\mathcal{A}_0 = C_c(\Omega \times \mathbb{R}^d)$ with (here $A, B \in \mathcal{A}_0$):

1. Product

$$A \cdot B(\omega, x) = \int_{y \in \mathbb{R}^d} d^d y \, A(\omega, y) \, B(\tau^{-y}\omega, x - y)$$

2. Involution

$$A^*(\omega, x) = \overline{A(\tau^{-x}\omega, -x)}$$

3. A faithful family of representations in $\mathcal{H} = L^2(\mathbb{R}^d)$

$$\pi_\omega(A) \psi(x) = \int_{\mathbb{R}^d} d^d y \, A(\tau^{-x}\omega, y - x) \cdot \psi(y)$$

if $A \in \mathcal{A}_0$, $\psi \in \mathcal{H}$.

4. $C^*$-norm

$$\|A\| = \sup_{\omega \in \Omega} \|\pi_\omega(A)\| .$$

**Definition 1** The $C^*$-algebra $\mathcal{A}$ is the completion of $\mathcal{A}_0$ under this norm.
IV.3)- Calculus

**Integration:** Let $\mathbb{P}$ be an $\mathbb{R}^d$-invariant ergodic probability measure on $\Omega$. Then set (for $A \in \mathcal{A}_0$):

$$\mathcal{T}_\mathbb{P}(A) = \int_{\Omega} d\mathbb{P} A(\omega, 0) = \langle 0 | \pi_\omega(A) 0 \rangle^{dis.}$$

Then $\mathcal{T}_\mathbb{P}$ extends as a *positive trace* on $\mathcal{A}$.

**Trace per unit volume:** thanks to Birkhoff’s theorem:

$$\mathcal{T}_\mathbb{P}(A) = \lim_{\Lambda \uparrow \mathbb{R}^d} \frac{1}{|\Lambda|} \text{Tr}(\pi_\omega(A) \mathbb{1}_\Lambda) \text{ a.e. } \omega$$

**Differential calculus:** A commuting set of $*$-derivations is given by

$$\partial_i A(\omega, x) = i x_i A(\omega, x)$$

defined on $\mathcal{A}_0$. Then $\pi_\omega(\partial_i A) = -i [X_i, \pi_\omega(A)]$ where $X = (X_1, \cdots, X_d)$ are the coordinates of the position operator.
IV.4)- Electrons

Schrödinger’s equation (ignoring interactions) on \( \mathbb{R}^d \)

\[
H_\omega = -\frac{\hbar^2}{2m} \Delta + \sum_{y \in \mathcal{L}_\omega} v(\cdot - y),
\]

acting on \( \mathcal{H} = L^2(\mathbb{R}^d) \). Here \( v \in L^1(\mathbb{R}^d) \) is real valued, decays fast enough, is the atomic potential.

Lattice case (tight binding representation)

\[
\tilde{H}_\omega \psi(x) = \sum_{y \in \mathcal{L}_\omega} h(\tau^{-x} \omega, y - x) \psi(y),
\]

Proposition 3

1. There is \( R(z) \in \mathcal{A} \), such that, for every \( \omega \in \Omega \) and \( z \in \mathbb{C} \setminus \mathbb{R} \)

\[
(z - H_\omega)^{-1} = \pi_\omega(R(z)).
\]

2. There is \( \tilde{H} \in C^*(\Gamma_{tr}) \) such that \( \tilde{H}_\omega = \pi_\omega(\tilde{H}) \).

3. If \( \Sigma_H = \bigcup_{\omega \in \Omega} \text{Sp}(H_\omega) \), then \( R(z) \) is holomorphic in \( z \in \mathbb{C} \setminus \Sigma_H \). The bounded components of \( \mathbb{R} \setminus \Sigma_H \) are called spectral gaps (same with \( \tilde{H} \)).
IV.5)- Density of States

- Let \( \mathbb{P} \) be an invariant ergodic probability on \( \Omega \). Let

\[
\mathcal{N}(E) = \lim_{\Lambda \uparrow \mathbb{R}^d} \frac{1}{|\Lambda|} \# \{\text{eigenvalues of } H_\omega|_\Lambda \leq E\}
\]

It is called the **Integrated Density of states** or **IDS**.

- The limit above exists \( \mathbb{P} \)-almost surely and

\[
\mathcal{N}(E) = \mathcal{T}_\mathbb{P}(\chi(H \leq E)) \quad (Shubin, '76)
\]

\( \chi(H \leq E) \) is the eigenprojector of \( H \) in \( \mathcal{L}^\infty(\mathcal{A}) \).

- \( \mathcal{N} \) is non decreasing, non negative and constant on gaps. \( \mathcal{N}(E) = 0 \) for \( E < \inf \Sigma_H \). For \( E \to \infty \), \( \mathcal{N}(E) \sim \mathcal{N}_0(E) \) where \( \mathcal{N}_0 \) is the IDS of the free case (namely \( v = 0 \)).

- **Gaps can be labelled by the value the IDS takes on them**
- An example of IDS -
1. Phonons are *acoustic waves* produced by small displacements of the atomic nuclei.

2. These waves are polarized with $d$-directions of polarization: $d - 1$ are *transverse*, one is *longitudinal*.

3. The nuclei motion is approximatively harmonic and quantized according to the *Bose-Einstein* statistics.

4. The charged nuclei interact with electrons, leading to an *electron-phonon interaction*.
1. For identical atoms with \textit{harmonic motion},
the classical equations of motion are:

\[
M \frac{d^2 \vec{u}_{(\omega, x)}}{dt^2} = \sum_{x \neq y \in \mathcal{L}_\omega} K_\omega(x, y) (\vec{u}_{(\omega, y)} - \vec{u}_{(\omega, x)})
\]

where \(M\) is the atomic mass, \(\vec{u}_{(\omega, x)}\) is its classical displacement vector and \(K_\omega(x, y)\) is the matrix of \textit{spring constants}.

2. \(K_\omega(x, y)\) decays fast in \(x - y\), uniformly in \(\omega\).

3. Covariance gives

\[
K_\omega(x, y) = k(\tau^{-x}\omega, y - x)
\]

thus

\[
k \in C^*(\Gamma_{tr}) \otimes M_d(\mathbb{C})
\]

4. Then the spectrum of \(k/M\) gives the \textit{eigenmodes} propagating in the solid. Its density (DPM) is given by Shubin’s formula again.
V - Gap labels and $K$-theory


V.1)- $K$-group

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

1. A projection is $P \in \mathcal{A}$ with $P = P^* = P^2$.

2. Two projections $P$ and $Q$ are equivalent if there is $U \in \mathcal{A}$ such that $P = UU^*$, $Q = U^*U$. $[P]$ denotes the equivalent class of $P$.

3. Two projections $P$ and $Q$ are orthogonal if $PQ = QP = 0$. Then $P + Q$ is a projection called the direct sum $P \oplus Q$.

4. If $\mathcal{K} = \bigcup_n M_n(\mathbb{C})^* \|\cdot\|$, then $\mathcal{A}$ is stable if $\mathcal{A} \simeq \mathcal{A} \otimes \mathcal{K}$. In a stable $C^*$-algebra for any pair $P, Q$ of projections, there are $P' \sim P$, $Q' \sim Q$ with $P'Q' = Q'P' = 0$.

Thus $[P] + [Q] = [P' \oplus Q']$ is well defined.

5. $K_0(\mathcal{A})$ is the group generated by the $[P]$’s with the previous addition.

6. $[P]$ is invariant by homotopy.
V.2)- K-group labels

• If $E$ belongs to a gap $g$, the characteristic function $E' \in \mathbb{R} \mapsto \chi(E' \leq E)$ is continuous on the spectrum of $H$. Thus:

$$P_g = \chi(H \leq E) \text{ is a projection in } \mathcal{A}!$$

• $N(E) = T_P(P_g) \in T_P^*(K_0(\mathcal{A}))!$

Theorem 3 (Abstract gap labeling theorem)

• $S \subset \Sigma_H \text{ clopen, } n_S = [\chi_S(H)] \in K_0(\mathcal{A})$. If $S_1 \cap S_2 = \emptyset$ then $n_{S_1 \cup S_2} = n_{S_1} + n_{S_2}$ (additivity).

• Gap labels are invariant under norm continuous variation of $H$ (homotopy invariance).

• For $\lambda \in [0, 1] \mapsto H(\lambda) \in \mathcal{A}$ continuous, if $S(\lambda) \subset \Sigma_H \text{ clopen, continuous in } \lambda$ with $S(0) = S_1 \cup S_2, S(1) = S'_1 \cup S'_2$ and $S_1 \cap S_2 = \emptyset = S'_1 \cap S'_2$ then $n_{S_1} + n_{S_2} = n_{S'_1} + n_{S'_2}$ (conservation of gap labels under band crossings).
Theorem 4  If $\mathcal{L}$ is an finite type Delone set in $\mathbb{R}^d$ with Hull $(\Omega, \mathbb{R}^d, T)$, then, for any $\mathbb{R}^d$-invariant probability measure $\mathbb{P}$ on $\Omega$

$$
\mathcal{T}_\mathbb{P}^* (K_0(A)) = \int_X d\mathbb{P}_{tr} \ C(X, \mathbb{Z}).
$$

if $A = C(\Omega) \rtimes \mathbb{R}^d$, $X$ is the canonical transversal and $\mathbb{P}_{tr}$ the transverse measure induced by $\mathbb{P}$.

Main ingredient for the proof

*the Connes measured index theorem for foliated spaces*

V.3)- History

For $d = 1$ this result follows from the Pimsner & Voiculescu exact sequence \((Bellissard, '92)\).

For $d = 2$, a double use of the Pimsner & Voiculescu exact sequence provides the result \((van Elst, '95)\).

For $d \geq 3$ whenever \((\Omega, \mathbb{R}^d, \tau)\) is Morita equivalent to a $\mathbb{Z}^d$-action, using spectral sequences \((Hunton, Forrest)\) this theorem was proved for $d = 3$ \((Bellissard, Kellendonk, Legrand, '00)\).

The theorem has also been proved for all $d$’s recently and independently by
- \((Bellissard, Benedetti, Gambaudo, 2001)\),
- \((Benameur, Oyono, 2001)\),
- \((Kaminker, Putnam, 2002)\).