The THEORY of APERIODIC SOLIDS

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Lecture I

STRUCTURAL ASPECTS

and

NONCOMMUTATIVE TOPOLOGY

Content

- 1. The Hull as a Dynamical System
- 2. Building Hulls
- 3. Tilings & Point Sets
- 4. The Noncommutative Brillouin Zone
- 5. Gap labeling and K-theory.

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) $Al_{62.5}Cu_{25}Fe_{12.5};$
 - (b) $\mathbf{Al_{70}Pd_{22}Mn_8};$
 - (c) $\mathbf{Al_{70}Pd_{22}Re_8};$
- 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 (Si, AsGa, ...);

I - The Hull as a Dynamical System

J. BELLISSARD, D. HERMMANN, M. ZARROUATI, Hull of Aperiodic Solids and Gap Labelling Theorems To appear in Directions in Mathematical Quasicrystals, M.B. Baake & R.V. Moody Eds, AMS, (2000).

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 points 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

 $\mathfrak{M}(\mathbb{R}^d)$ 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 :

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

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

$$\Omega = \overline{\left\{ \mathbf{T}^a \boldsymbol{\nu}^{\mathcal{L}}; a \in \mathbb{R}^d \right\}} \;,$$

where $T^{a}\nu$ is the translated of ν by a.

Results:

- 1. Ω is compact and \mathbb{R}^d acts by homeomorphisms.
- 2. If $\omega \in \Omega$, there is a uniformly discrete point set \mathcal{L}_{ω} in \mathbb{R}^d such that ω coincides with $\nu_{\omega} = \nu^{\mathcal{L}_{\omega}}$.
- 3. If \mathcal{L} is *Delone* (resp. *Meyer*) so are the \mathcal{L}_{ω} '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 ϵ -approximant of a translated of p.

Proposition 1 \mathbb{R}^d acts minimaly on Ω 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

J. BELLISSARD, R. BENEDETTI, J.-M. GAMBAUDO, Spaces of Tilings, Finite Telescopic Approximations and Gap-Labelling, preprint August (2001).

II.1)- Examples

1. Crystals : $\Omega = \mathbb{R}^d / \mathcal{T} \simeq \mathbb{T}^d$ 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 : $\Omega \simeq \mathbb{T}^n$, 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 \mathfrak{A} be a finite set (alphabet) indexing the types of impurities.

The transversal is $X = \mathfrak{A}^{\mathbb{Z}^d}$ with \mathbb{Z}^d -action given by shifts.

The Hull Ω is the mapping torus of X.

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- The Hull of a Periodic Lattice -

II.2)- Quasicrystals

Use the *cut-and-project* construction:

$$\mathbb{R}^{d} \simeq \mathcal{E}_{\parallel} \xleftarrow{\pi_{\parallel}} \mathbb{R}^{n} \xrightarrow{\pi_{\perp}} \mathcal{E}_{\perp} \simeq \mathbb{R}^{n-d}$$
$$\mathcal{L} \xleftarrow{\pi_{\parallel}} \tilde{\mathcal{L}} \xrightarrow{\pi_{\perp}} W ,$$

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 -



- The transversal of the Octagonal Tiling -

- is completely disconnected -

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 $\mathbf{T}^n_{\mathcal{F}} = \mathbb{R}^n_{\mathcal{F}}/\tilde{\mathcal{L}}$ 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 $\mathbf{T}^n_{\mathcal{F}}$.

Theorem 1 \mathcal{L} is a Meyer set. Its Hull is conjugate to $\mathbf{T}_{\mathcal{F}}^n$ endowed with its canonical \mathbb{R}^d -action. This Hull is uniquely ergodic.

III - Tilings & Point Sets

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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 $F_1 \subset T_1$ and $F_2 \subset T_2$ 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 $n \ge 1$ 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 *a colored patch*;
- 4. proceed then as in Step 1 by replacing prototiles by colored patches to get the BOF-manifold B_n .



- A colored patch -

Step 3:

- 1. Define a *BOF-submersion* $f_n : B_{n+1} \mapsto B_n$ by identifying patches of order n in B_{n+1} with the prototiles of B_n ;
- 2. call Ω 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 $X_1, \dots X_d$ on B_n generating local translations and giving rise to a \mathbb{R}^d action T on Ω .

Theorem 2 The dynamical system $(\Omega, \mathbb{R}^d, \mathbf{T}) = \lim_{\leftarrow} (B_n, f_n)$

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 homemorphism.

IV - NC Brillouin Zone

J. BELLISSARD, The Gap Labelling Theorems for Schrödinger's Operators, in From Number Theory to Physics, pp. 538-630, Les Houches March 89, Springer, J.M. Luck, P. Moussa & M. Waldschmidt Eds., (1993).

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 Ω 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 $\mathcal{A}_0 = \mathcal{C}_c(\Omega \times \mathbb{R}^d)$ 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 faithfull 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 Ω . Then set (for $A \in \mathcal{A}_0$):

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

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

Trace per unit volume: thanks to Birkhoff's theorem:

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

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

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

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

IV.4)- Electrons

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

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

acting on $\mathcal{H} = L^2(\mathbf{R}^d)$. Here $v \in L^1(\mathbb{R}^d)$ is real valued, decays fast enough, is the *atomic potential*. Lattice case (*tight hinding representation*)

Lattice case (*tight binding representation*)

$$\tilde{H}_{\omega}\psi(x) = \sum_{y \in \mathcal{L}_{\omega}} h(\mathbf{T}^{-x}\omega, y - x)\,\psi(y) \;,$$

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 $\Sigma_{\mathrm{H}} = \bigcup_{\omega \in \Omega} \operatorname{Sp}(H_{\omega})$, then R(z) is holomorphic in $z \in \mathbb{C} \setminus \Sigma_{H}$. The bounded components of $\mathbb{R} \setminus \Sigma_{\mathrm{H}}$ are called spectral gaps (same with \tilde{H}).

IV.5)- Density of States

• Let \mathbb{P} be an invariant ergodic probability on Ω . Let

$$\mathcal{N}(E) = \lim_{\Lambda \uparrow \mathbf{R}^d} \frac{1}{|\Lambda|} \# \{ \text{eigenvalues of } H_{\omega} |_{\Lambda} \le E \}$$

It is called the *Integrated Density of states* or *IDS*.
The limit above exists P-almost surely and

$$\mathcal{N}(E) = \mathcal{T}_{\mathbb{P}}\left(\chi(H \le E)\right)$$
 (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 $E < \inf \Sigma_{\mathrm{H}}$. 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 -

IV.6)- Phonons



- 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 *harmonic motion*, the classical equations of motion are:

$$M \, rac{d^2 \, ec{u}_{(\omega, x)}}{dt^2} \, = \, \sum_{x
eq y \in \mathcal{L}_\omega} K_\omega(x, y) \, (ec{u}_{(\omega, y)} - ec{u}_{(\omega, x)})$$

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

- 2. $K_{\omega}(x, y)$ decays fast in x y, uniformly in ω ..
- 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 *eigenmodes* propagating in the solid. Its density (DPM) is given by Shubin's formula again.

V - Gap labels and K-theory

B. BLACKADAR, *K*-Theory for Operator Algebras, Springer, New-York, (1986), 2nd Ed, Cambridge U. Press (1998)

J. BELLISSARD, The Gap Labelling Theorems for Schrödinger's Operators, in From Number Theory to Physics, pp. 538-630, Les Houches March 89, Springer, J.M. Luck, P. Moussa & M. Waldschmidt Eds., (1993).

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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 classe 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 $\mathcal{K} = \overline{\bigcup_n M_n(\mathbb{C})}^{\|\cdot\|}$, 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 \mathfrak{g} , the characteristic function $E' \in \mathbf{R} \mapsto \chi(E' \leq E)$ is continuous on the spectrum of H. Thus:

 $P_{\mathfrak{g}} = \chi(H \leq E)$ is a projection in \mathcal{A} !

• $\mathcal{N}(E) = \mathcal{T}_{\mathbb{P}}(P_{\mathfrak{g}}) \in \mathcal{T}_{\mathbb{P}}^*(K_0(\mathcal{A}))$!

Theorem 3 (Abstract gap labeling theorem)

- $S \subset \Sigma_{\mathrm{H}}$ 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 $S(\lambda) \subset \Sigma_{\mathrm{H}}$ clopen, continuous in λ 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 $(\Omega, \mathbb{R}^d, \mathbf{T})$, then, for any \mathbb{R}^d -invariant probability measure \mathbb{P} on Ω

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

if $\mathcal{A} = \mathcal{C}(\Omega) \rtimes \mathbb{R}^d$, 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

A. CONNES, Sur la théorie non commutative de l'intégration, Lecture Notes in Math **725**, 19-143, Springer, Berlin (1979).

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 $(\Omega, \mathbb{R}^d, T)$ 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).