The NON COMMUTATIVE GEOMETRY of APERIODIC SOLIDS

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Main Reference:

J. Bellissard, D. Herrmann, 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).

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I - The HULL of an APERIODIC SOLID

Aperiodic Solids :

1. $2D$ electrons in a uniform magnetic field:
   the magnetic fields breaks the translation invariance at quantum level.

2. Superlattices:
   superposition of two types of semiconductors

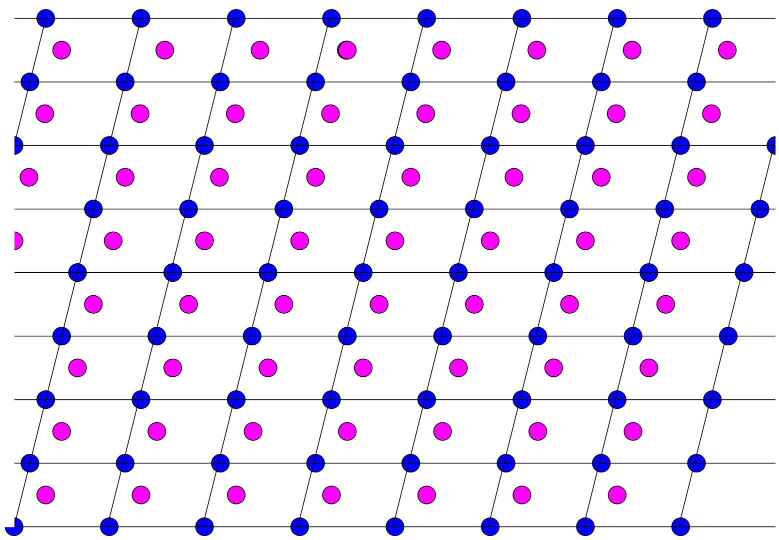
3. Lightly doped compensate semiconductors at low temperature:
   ex.: Si or $AsGa$ on a diamond lattice,
   doping atoms $(P, Al, Ga.As, In, \cdots)$
   on a random Poissonian sublattice.

4. Quasicrystals:
   ex.: $Al_{62.5}\,Cu_{25}\,Fe_{12.5}$ or $Al_{70}\,Pd_{21}\,Re_9$
   in the icosahedral phase.

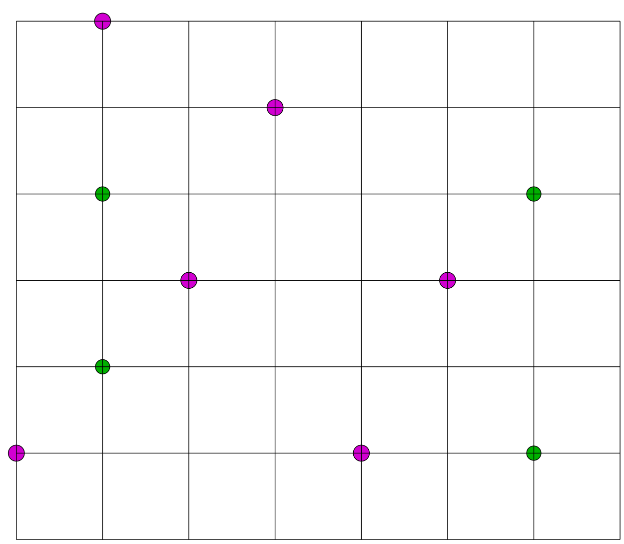
5. Others: amorphous, glasses, liquids, etc..

Array of Atomic Positions :

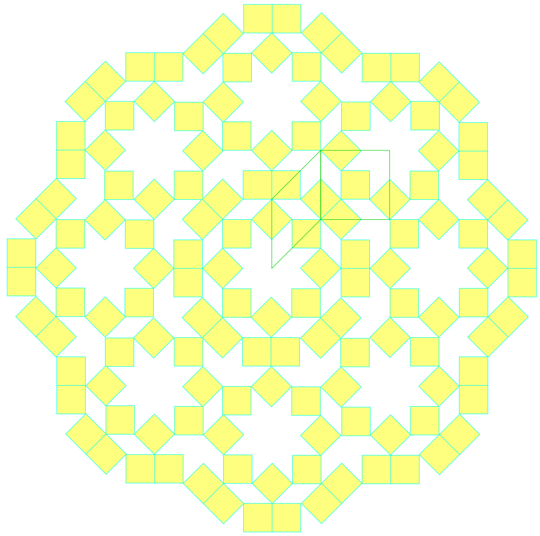
The ideal equilibrium positions of atomic nuclei sit on a discrete subset $\mathcal{L}$ of $\mathbb{R}^d$ ($d = 1, 2, 3$ in practice).



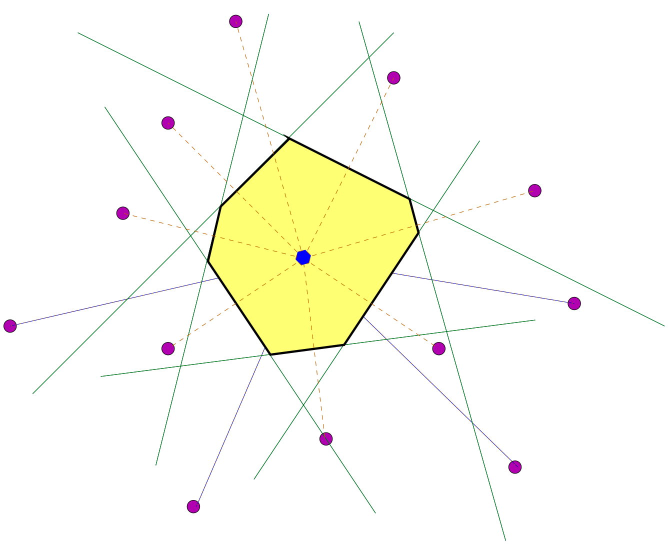
- A periodic array of atomic nuclei -



- A random array of atomic nuclei -



- A quasiperiodic array of atomic nuclei -



- Construction of VORONOI*'s tiling -*

Brillouin Zone of a Crystal :

If $\mathcal{L}$ is periodic with period group $\mathbb{G}$, the Voronoi cell can be identified with

$$\mathbb{V} = \mathbb{R}^d/\mathbb{G}$$

The orthogonal group $\mathbb{G}^\perp$ of $\mathbb{G}$ in the dual space $\mathbb{R}^{d\,*}$ is *the reciprocal lattice*. By Pontryagin duality

$$\mathbb{G}^\perp \simeq \mathbb{V}^*$$

The corresponding Voronoi cells are called *Brillouin zones*. They can also be identified with the quotient

$$\mathbb{B} = \mathbb{R}^{d\,*}/\mathbb{G}^\perp \simeq \mathbb{G}^*$$

$\mathbb{B}$ is topologically a torus $\mathbb{T}^d$.
It represents the *momentum space* of the crystal.

Point Sets in $\mathbb{R}^d$:

1. $\mathcal{L}$ is *uniformly discrete* if there is $r > 0$ such that each (open) ball of radius r meets $\mathcal{L}$ on one point at most.

   Then $\mathcal{L}$ is called r-discrete.

2. $\mathcal{L}$ is *relatively dense* if there is $R > 0$ such that each (closed) ball of radius R meets $\mathcal{L}$ on one point at least.

   Then $\mathcal{L}$ is called R-dense.

3. $\mathcal{L}$ is *Delone* (or *Delaunay*) whenever it is both uniformly discrete and relatively dense.

   Then $\mathcal{L}$ will be called (r, R)-Delone if it is r-discrete and R-dense.

4. $\mathcal{L}$ is *Meyer* whenever both $\mathcal{L}$ and $\mathcal{L} - \mathcal{L}$ are Delone.

   Then $\mathcal{L}$ will be called $(r, R; r', R')$-Meyer if $\mathcal{L}$ is (r, R)-Delone and $\mathcal{L} - \mathcal{L}$ is (r', R')-Delone. .

Array and Measures on $\mathbb{R}^d$:

Let $\mathfrak{M}(\mathbb{R}^d)$ be the space of Radon measures on $\mathbb{R}^d$ endowed with the *vague topology* (*Namely the weak topology over the space $\mathcal{C}_c(\mathbb{R}^d)$ of continuous functions with compact support*).

Associate with $\mathcal{L}$ the Radon measure $\nu_{\mathcal{L}}$:

$$\nu_{\mathcal{L}} = \sum_{x \in \mathcal{L}} \delta(\,\cdot\, - x)$$

1. $UD_r(\mathbb{R}^d)$ is the set of Radon measures $\nu_{\mathcal{L}}$ with $\mathcal{L}$ being r-discrete. Set $UD(\mathbb{R}^d) = \bigcup_{r>0} UD_r(\mathbb{R}^d)$.

2. $Del_{(r,R)}(\mathbb{R}^d)$ is the set of Radon measures $\nu_{\mathcal{L}}$ with $\mathcal{L}$ being (r,R)-Delone. Set $Del(\mathbb{R}^d) = \bigcup_{0<r\leq R} Del_{(r,R)}(\mathbb{R}^d)$.

3. $Mey_{(r,R;r',R')}(\mathbb{R}^d)$ is the set of Radon measures $\nu_{\mathcal{L}}$ with $\mathcal{L}$ being $(r,R;r',R')$-Meyer.

4. $QD(\mathbb{R}^d)$ is the closure of $UD(\mathbb{R}^d)$. An element of QD is called a *quasidiscrete set*.

Theorem 1 *(i) UD_r, $Del_{(r,R)}$ and $Mey_{(r,R;r',R')}$ are compact subsets of $\mathfrak{M}$ for all $0 < r \leq R$ and $0 < r' \leq R'$.*
(ii) A Radon measure μ belongs to QD iff there is a discrete point set $\mathcal{L}$ such that

$$\mu = \sum_{x \in \mathcal{L}} n_x \, \delta(\cdot - x)$$

where $n_x \in \mathbb{N}_*$ for all $x \in \mathcal{L}$.

Thus a *quasidiscrete set* can be seen as a discrete subset of $\mathbb{R}^d$ with finitely many atoms on top of each other at each site.

The Hull of a Point Set :

$\mathbb{R}^d$ acts on $\mathfrak{M}$ by translation.

If $\mu \in \mathfrak{M}$, $a \in \mathbb{R}^d$, $\tau^a \mu$ denote the a-translated of μ.

Theorem 2 *QD, UD_r, $Del_{(r,R)}$ and $Mey_{(r,R;r',R')}$ $\mathbb{R}^d$-invariant subsets of $\mathfrak{M}$.*

Consequently given $\nu_{\mathcal{L}} \in UD_r$, $(r > 0)$, its *Hull*

$$\Omega_{\mathcal{L}} = \overline{\{\tau^a \nu_{\mathcal{L}}\,; a \in \mathbb{R}^d\}}$$

is a compact metrizable space.

The Hull is a compactification of all possible finite samples found in $\mathcal{L}$.

The *canonical transversal* is the closed subspace $\Upsilon_{\mathcal{L}}$

$$\Upsilon_{\mathcal{L}} = \{\omega \in \Omega_{\mathcal{L}}\,; \omega\{0\} = 1\}$$

namely those point sets in the Hull with one point at the origin.

Gibbs Measures :

Gibbs measures are basic tools in Thermodynamics and describe the equilibrium states of the atomic array. They have the following properties:

1. An atomic Gibbs measure is a probability measure $\mathbb{P}$ on $QD(\mathbb{R}^d)$ (*Note that* $QD(\mathbb{R}^d)$ *is a polish space*).

2. Whenever unique, $\mathbb{P}$ is $\mathbb{R}^d$-invariant and ergodic. (*Non-uniqueness means coexistence of phases*).

3. To describe a solid, $\mathbb{P}$ is expected to give probability one to $UD(\mathbb{R}^d)$ (*or even to* $Del(\mathbb{R}^d)$).
   The $\mathbb{P}$ is called *uniformly discrete* (*resp. Delone*).

From now on $\mathbb{P}$ will be an $\mathbb{R}^d$-invariant ergodic uniformly discrete probability measure on $QD(\mathbb{R}^d)$.

Theorem 3 *If $\mathbb{P}$ is a $\mathbb{R}^d$-invariant ergodic uniformly discrete probability measure on $QD(\mathbb{R}^d)$, then:*
(i) There is $r > 0$ unique such that $\mathbb{P}\{UD_r\} = 1$ and for every $r' > r$, $\mathbb{P}\{UD_{r'}\} = 0$.
(ii) for $\mathbb{P}$-almost all $\nu \in QD(\mathbb{R}^d)$, the Hull of ν is compact and given by the topological support of $\mathbb{P}$.

Thus a Gibbs measure $\mathbb{P}$ determines the Hull $\Omega_{\mathbb{P}}$ with probability one.

Diffraction Measure :

For Λ a ball in $\mathbb{R}^d$, the *diffraction measure* associated to $\nu_{\mathcal{L}} \in UD$ is given by the density

$$\rho_\Lambda^{(\mathcal{L})}(k) = \frac{1}{|\Lambda|} \left| \sum_{x \in \mathcal{L} \cap \Lambda} e^{\imath k \cdot x} \right|^2$$

Theorem 4 *If $\mathbb{P}$ is a $\mathbb{R}^d$-invariant ergodic uniformly discrete probability measure on $QD(\mathbb{R}^d)$, then for $\mathbb{P}$-almost every $\nu \in QD$ the family $\left(\rho_\Lambda^{(\mathcal{L})}\right)_{\Lambda \subset \mathbb{R}^d}$ converges as $\Lambda \uparrow \mathbb{R}^d$ to a measure $\rho_{\mathbb{P}} \in \mathfrak{M}(\mathbb{R}^{d*})$ such that:*
(i) $\rho_{\mathbb{P}}$ is positive,
(ii) its Fourier transform is positive and supported by the closure of $\mathcal{L} - \mathcal{L}$.

Thus the diffraction picture seen by an experimentalist depends only upon the Gibbs measure describing the atomic equilibrium.

II - The NC BRILLOUIN ZONE

The C^*-algebra of the Hull :

$(\Omega, \mathbb{R}^d, \tau)$ 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 $f \in \mathcal{C}(\Omega)$)

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

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.

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

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

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

3. A faithfull family of representations in $\mathcal{H} = L^2(\mathbb{R}^d)$
$$\pi_\omega(A)\,\psi(x) = \int_{\mathbb{R}^d} d^{\mathrm{d}}y\; A(\tau^{-x}\omega, y - x) \cdot \psi(y)$$
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.*

Calculus on $\mathcal{A}$:

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

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

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

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

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

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 $X = (X_1, \cdots, X_d)$ are the coordinates of the position operator.

The Electronic Hamiltonian :

The Schrödinger Hamiltonian for an electron submitted to atomic forces (for one species of atoms and ignoring interactions) is given by

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

It acts on $\mathcal{H} = L^2(\mathbb{R}^d)$ and v is the atomic potential.

Theorem 5 *For any $z \in \mathbb{C}\setminus\mathbb{R}$ there is $R(z) \in \mathcal{A}$ such that*

$$\pi_\omega(R(z)) \;=\; \frac{1}{z\;-\;H_\omega}$$

The *algebraic spectrum* of H is defined by

$$\Sigma \;=\; \bigcup_{\omega\in\Omega} \sigma(H_\omega) \;\;\Leftrightarrow\;\; \sigma(R(z)) \;=\; \frac{1}{z-\Sigma}$$

The Density of States :

The Density of States (DOS) is the positive measure $\mathcal{N}_{\mathbb{P}}$ on $\mathbb{R}$ defined by

$$\int_{\mathbb{R}} \frac{d\mathcal{N}_{\mathbb{P}}(E)}{z - E} = \mathcal{T}_{\mathbb{P}}(R(z))$$

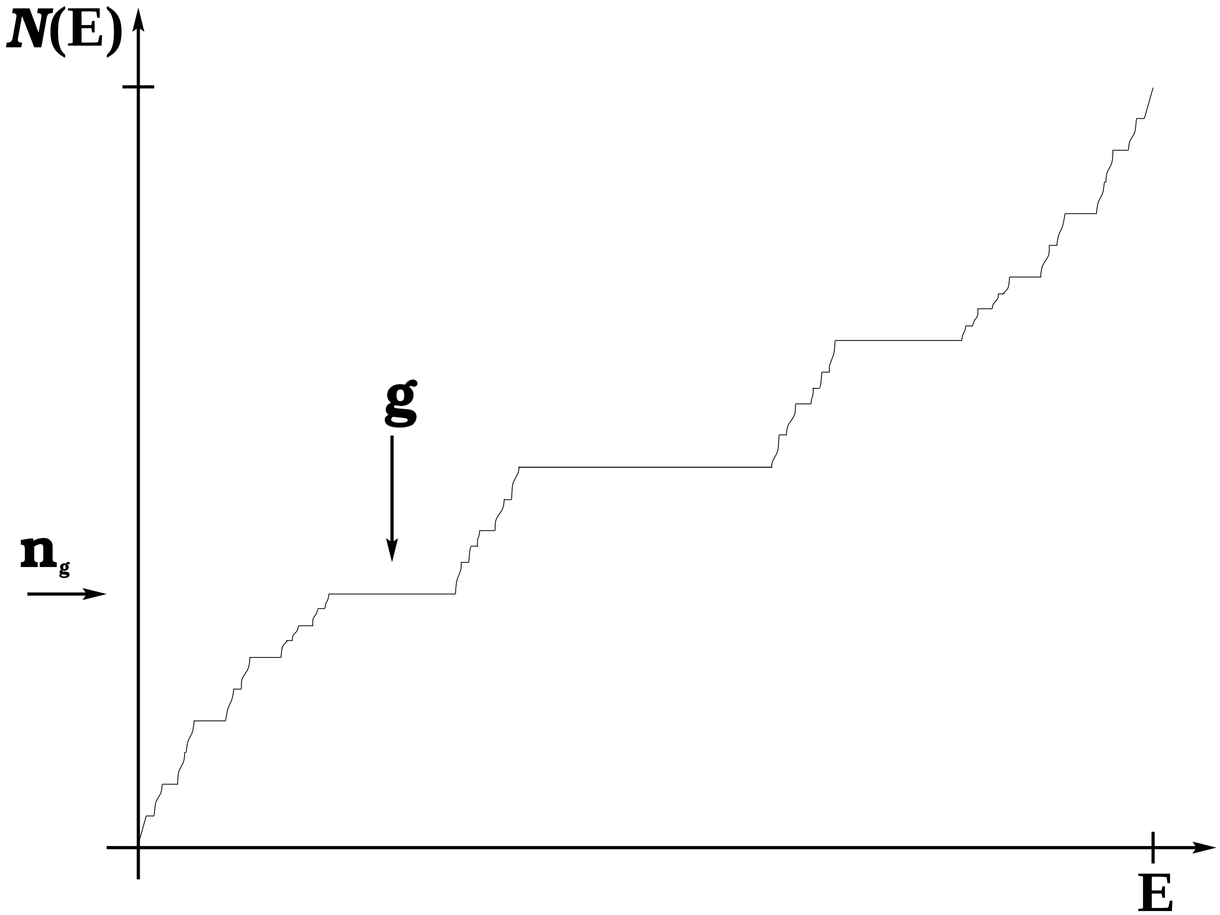
Set $\mathcal{N}_{\mathbb{P}}(E) = \int_{-\infty}^{E} d\mathcal{N}_{\mathbb{P}}$. If E is a continuity point of $\mathcal{N}_{\mathbb{P}}$, *Shubin's formula* holds $\mathbb{P}$-almost all ω's:

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

The *support* of $\mathcal{N}_{\mathbb{P}}$ is contained in Σ. If $\mathfrak{g} = (E_-, E_+)$ is a spectral gap, let $P_{\mathfrak{g}}$ be the spectral projection of H on $(-\infty, E_-]$, so that

$$n_{\mathfrak{g}} = \mathcal{N}_{\mathbb{P}}(E_- + 0) = \mathcal{N}_{\mathbb{P}}(E_+ - 0) = \mathcal{T}_{\mathbb{P}}(P_{\mathfrak{g}})$$

Fact: $P_{\mathfrak{g}}$ is a projection belonging to $\mathcal{A}$!!



- An example of DOS -

K-Theory & Gap Labelling :

Very roughly:

1. $K_0(\mathcal{A})$ is the set of (unitary) equivalence classes of projections in $\mathcal{A}$.
2. It is a countable abelian group if endowed with the direct sum

$$[P] + [Q] = [P \oplus Q]$$

3. The trace $\mathcal{T}_{\mathbb{P}}$ induces a group homomorphism $\tau_* : K_0(\mathcal{A}) \mapsto \mathbb{R}$ such that

$$\tau_*([P]) = \mathcal{T}_{\mathbb{P}}(P)$$

4. The values $n_{\mathfrak{g}}$ of $\mathcal{N}_{\mathbb{P}}$ on gaps, *the gap labels*, belong to the countable subgroup $\tau_*(K_0(\mathcal{A}))$ of $\mathbb{R}$.

Problem: *Prove or disprove that if the Hull Ω is totally disconnected transversally to the $\mathbb{R}^d$-action*

$$\tau_*(K_0(\mathcal{A})) = \int_{\Omega} d\mathbb{P}\ \mathcal{C}(\Omega, \mathbb{Z})$$

Gap Labelling Theorems :

1. The abstract Gap Labelling Theorem:

   J. Bellissard, in *Lecture Notes in Physics*, **153**, pp. 356-363, (1982).
   J. Bellissard, in *Lecture Notes in Physics*, **257**, pp. 99-156, (1986).

2. Gap labelling theorems and explicit computation in dimension $d = 1$. The problem has a positive answer.

   J. Bellissard, A. Bovier, J. M. Ghez., *Rev. Math. Phys.*, **4**, pp. 1-38, (1992).
   J. Bellissard, *Gap labelling theorems for Schrödinger operators* in *From Number Theory to Physics*, eds. M. Waldschmidt, P. Moussa, J. M. Luck and C. Itzykson, Berlin (1993), pp. 539-630. (1993).

3. Proof of the conjecture in $d = 2$

   A. van Elst, , *Rev. Math. Phys.*, **6**, 319-342, (1994).
   J. Bellissard, E. Contensou, A. Legrand, , *C.R.A.S.*, **327**, pp. 197-200, (1998).
   M. Zarrouati, Ph. D. Thesis, June 2000.

4. Computation of the K-groups for transversally completely disconnected Hulls. Application to quasi-crystals in dimension $d = 2, 3$ and codimension $n = 2, 3$.

   A. H. Forrest and J. R. Hunton,, *Erg. Th. & Dyn. Syst.*, **19**, 611-625, (1999).
   A. H. Forrest, J. R. Hunton, J. Kellendonk, , *Cohomology of canonical projection tilings*, preprint (1999).
   A. H. Forrest, J. Kellendonk, , work in progress for $d = 3$.

Conclusions :

1. The Gibbs measure for atomic positions $\mathbb{P}$ defines uniquely the Hull $(\Omega, \mathbb{R}^d, \tau)$. It defines uniquely the diffraction pattern.
2. The Hull defines the Noncommutative Brillouin zone (NCBZ) through the C^*-algebra $\mathcal{A} = \mathcal{C}(\Omega) \rtimes_{\tau} \mathbb{R}^d$.
3. $\mathcal{A}$ contains the one-particles electronic observables. $\mathbb{P}$ defines a trace $\mathcal{T}_{\mathbb{P}}$ on $\mathcal{A}$ which in turns gives the electronic DOS.
4. A similar construction holds for *phonons*.
5. The K-theory characterizes the Noncommutative topology of the NCBZ. The trace $\mathcal{T}_{\mathbb{P}}$ gives rise to a canonical *gap labelling*. NC Geometry is described by higher order traces (*cyclic cohomology*).
6. Results in transport theory available, together with second quantization (D. Spehner, Ph. D. Th., March 2000).
7. **Prospect and problems:**
   (a) Prove or disprove the gap labelling conjecture.
   (b) Physical interpretation of the K-groups ?
   (c) Is *measurement* of K-groups possible ?