The

GAP LABELLING THEOREM

for

APERIODIC SOLIDS

Jean BELLISSARD [1] [2]

Université Paul Sabatier, Toulouse
&
Institut Universitaire de France

Collaborations:

M. ZARROUATI (IRSAMC, Toulouse)

D. HERRMANN (K.U. Nijmegen & T.U. Berlin)

J. KELLENDONK (U. Cardiff)

A. LEGRAND (U. Paul Sabatier, Toulouse)

J.M. GAMBAUDO (U. Dijon)

M. MAERTENS (IBM)

[1] I.R.S.A.M.C., Université Paul Sabatier, 118, route de Narbonne, Toulouse Cedex 04, France
[2] e-mail: jeanbel@irsamc2.ups-tlse.fr

Main References

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).

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).

J. BELLISSARD, J. KELLENDONK, A. LEGRAND, *Gap Labelling for three dimensional aperiodic solids* , submitted to *C.R.A.S.* , September 2000.

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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. A *Delone* set: $\mathcal{L}$ is uniformly discrete and *relatively dense* : $\exists R > 0$ s.t. each ball of radius R contains at least two points of $\mathcal{L}$.
4. A *Meyer* set: $\mathcal{L}$ and $\mathcal{L} - \mathcal{L}$ are Delone sets.

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.

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 $\mathbb{R}^d$:

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

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

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

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

Facts:

1. Ω is compact and $\mathbb{R}^d$ acts by homeomorphisms.
2. If $\omega \in \Omega$, there is a uniformly discrete point set $\mathcal{L}_\omega$ 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 $\mathcal{L}_\omega$'s.

I.3)- Properties

(a) Minimality

Proposition 1 *$\mathbb{R}^d$ acts minimaly on Ω if and only if, for any $\omega \in \Omega$ and $F \subset \Omega$ closed, the subset $\mathcal{L}_\omega^F = \{x \in \mathcal{L}_\omega ; \mathrm{T}^{-x}\omega \in F\}$ is a Delone set.*

(b) Transversal

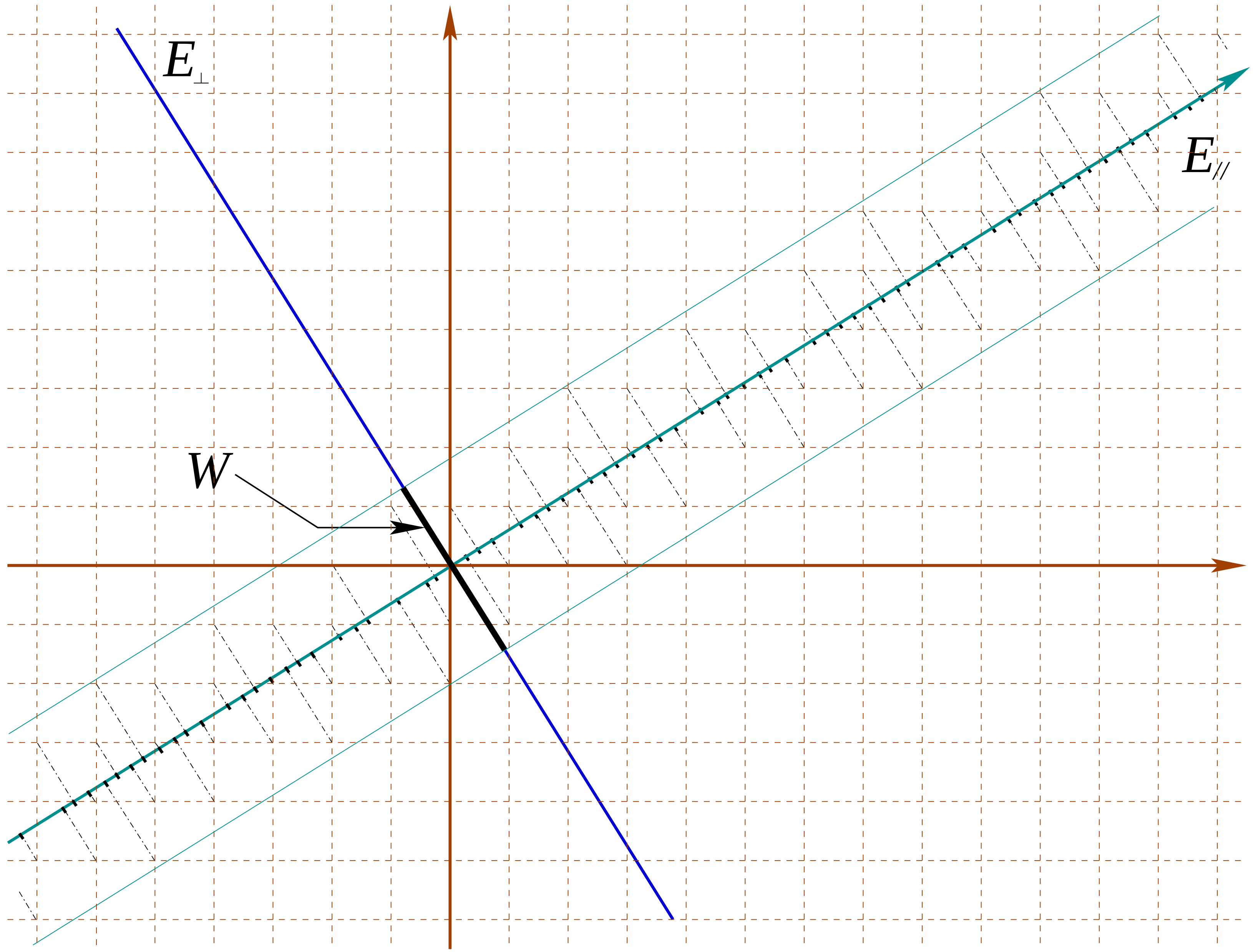
The closed subset $X = \{\omega \in \Omega \ ; \ \nu_\omega(\{0\}) = 1\}$ is called the *canonical transversal*. Let G be the subgroupoid of $\Omega \rtimes \mathbb{R}^d$ induced by X.

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

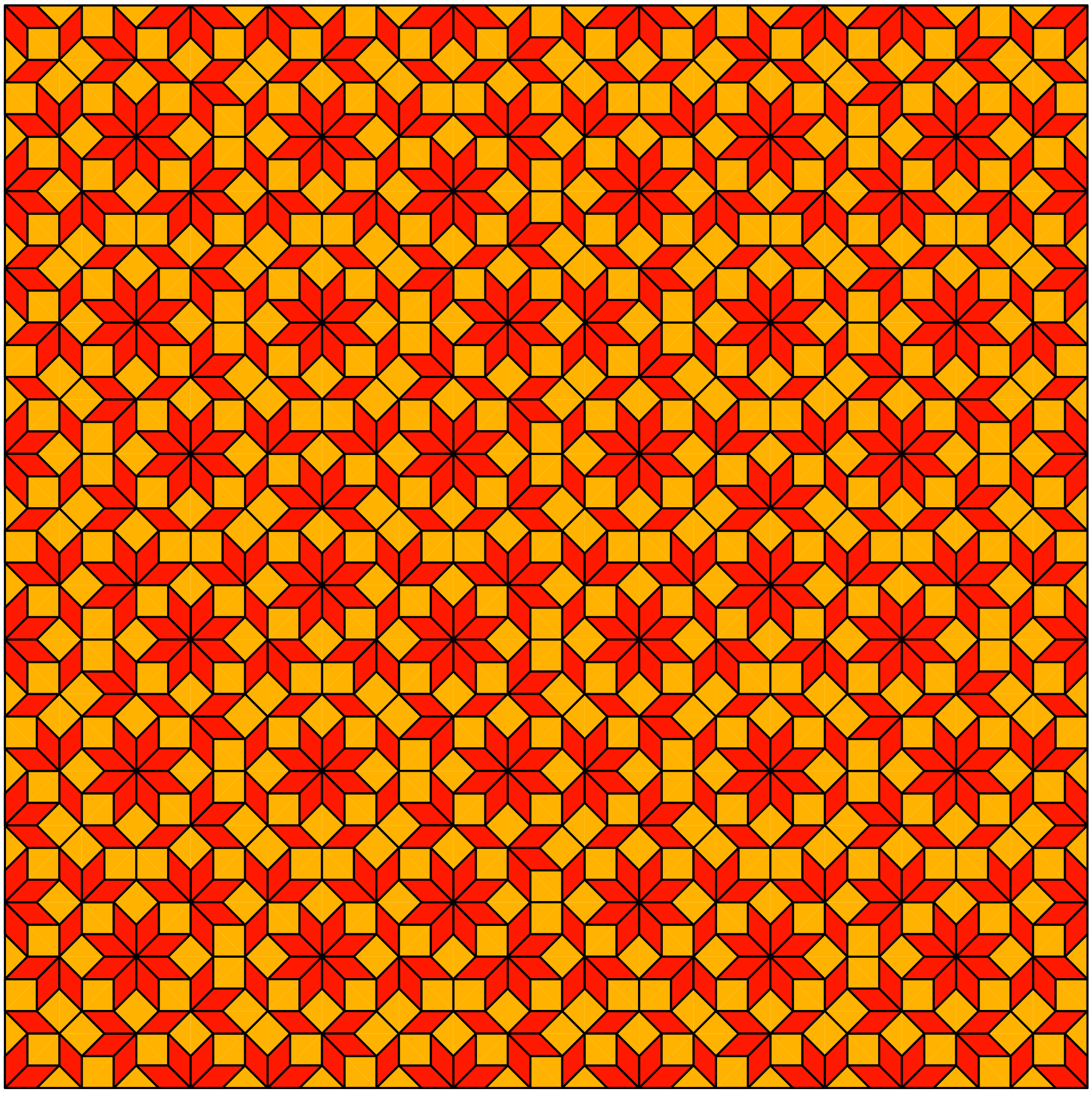
(c) Cantorian Transversal

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

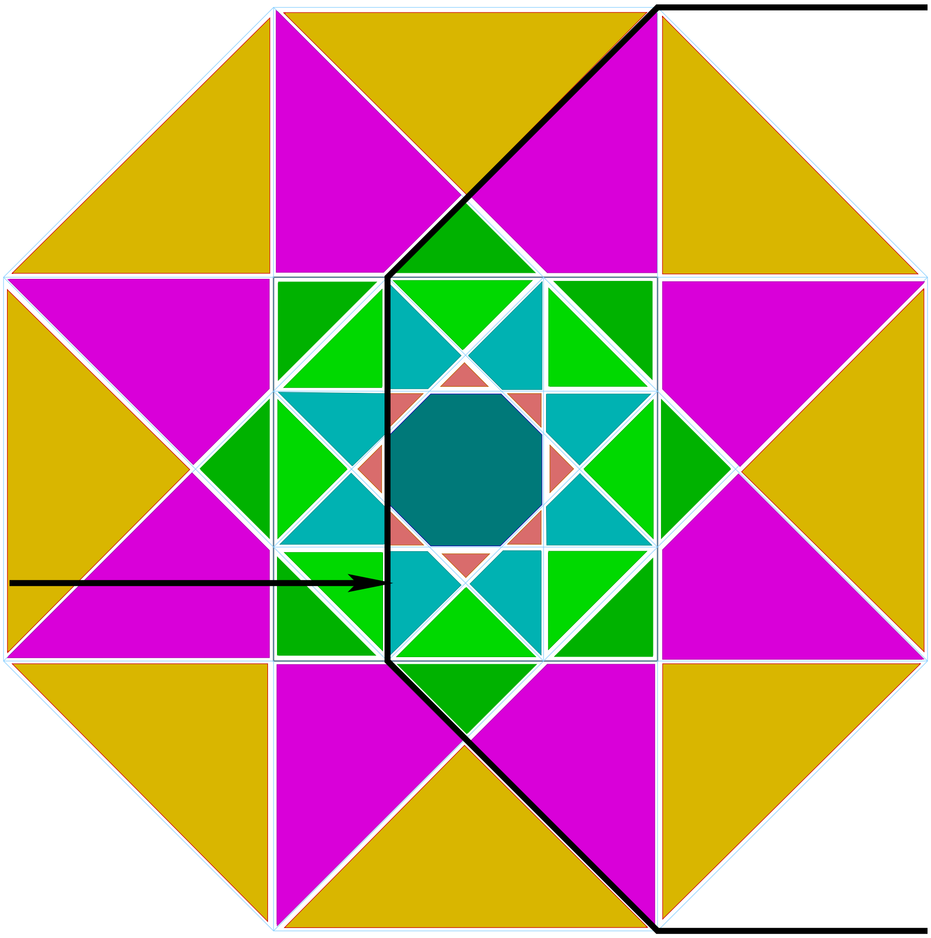
II - Examples: Quasicrystals

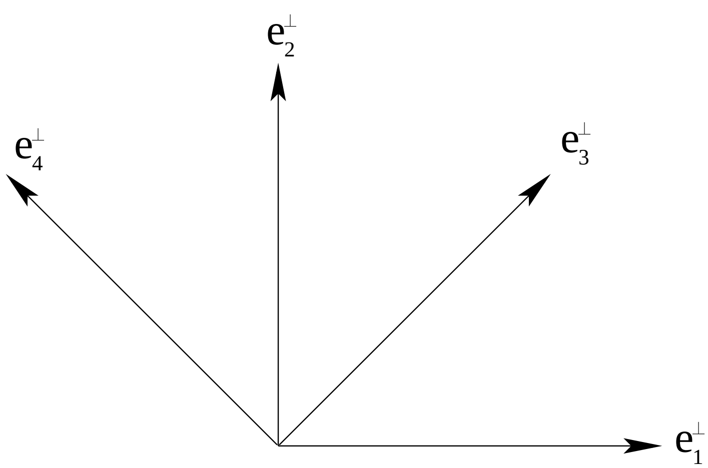


– The cut–and–project construction –



- The octagonal tiling -





- The transversal of the Octagonal Tiling -

- is completely disconnected -

III - Gap Labelling and K-theory

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).

III.1)- Algebra

Let $\mathcal{A}_0 = \mathcal{C}_c(\Omega \times \mathbb{R}^d)$ be seen as a dense subalgebra of $\mathcal{A} = \mathcal{C}(\Omega) \rtimes \mathbb{R}^d$. For any $\omega \in \Omega$, let π_ω be the left regular representation on $\mathcal{H} = L^2(\mathbf{R}^d)$ defined by:

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

.and $\psi \in \mathcal{H}$.

If $\mathbb{P}$ is an $\mathbb{R}^d$-invariant ergodic probability measure on Ω, let $\mathcal{T}_{\mathbb{P}}$ be the trace on $\mathcal{A}$ defined by

$$\mathcal{T}_{\mathbb{P}}(A) \;=\; \int_{\Omega} \mathbb{P}(d\omega) \; A(\omega, 0)) \, ,$$

for $A \in \mathcal{A}_0$

III.2)- Hamiltonian

Schrödinger's equation (ignoring interactions)

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

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*.

Proposition 3 *There is $R(z) \in \mathcal{A}$, such that, for every $\omega \in \Omega$ and $z \in \mathbb{C} \setminus \mathbb{R}$*

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

If $\Sigma_{\mathrm{H}} = \bigcup_{\omega\in\Omega} \mathrm{Sp}(H_\omega)$, then $R(z)$ is holomorphic in $z \in \mathbb{C} \setminus \Sigma_H$.

The bounded connected components of $\mathbb{R}\backslash\Sigma_{\mathrm{H}}$ are called *spectral gaps*.

III.3)- Density of States

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

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

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

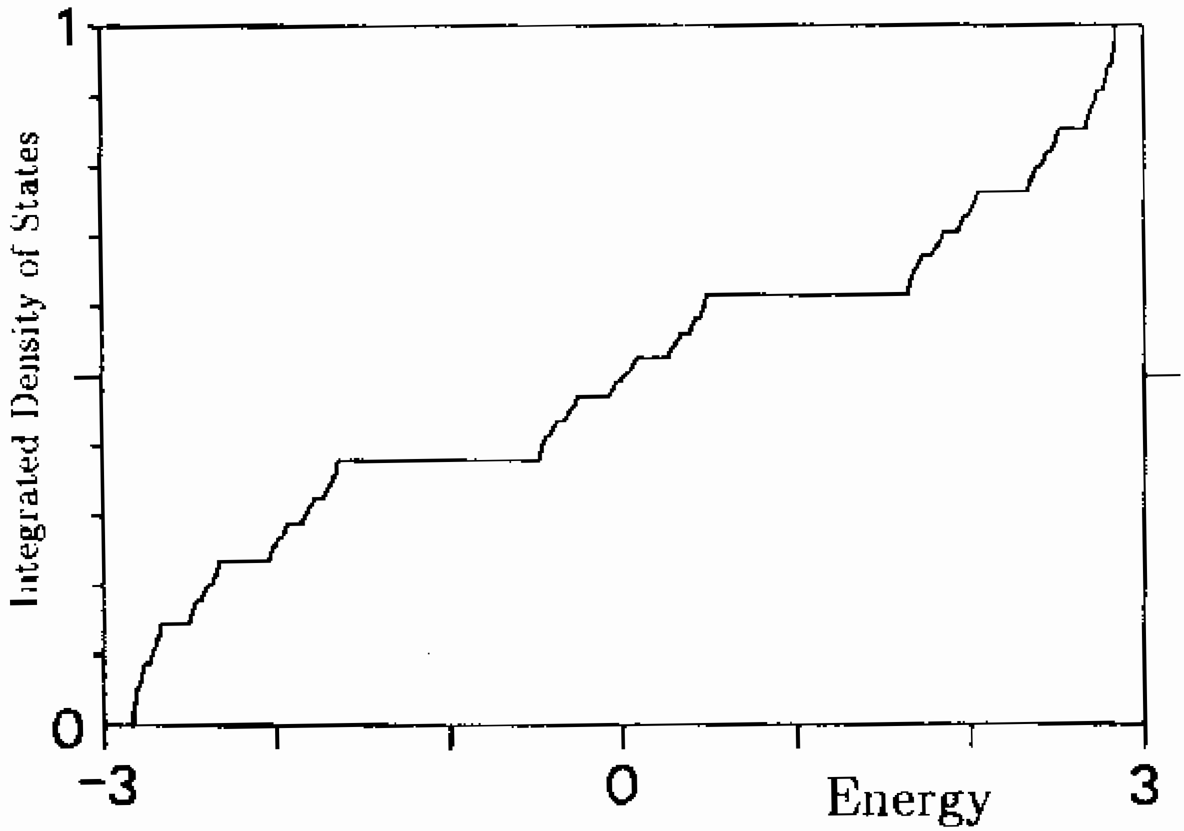
- The limit above exists $\mathbb{P}$-almost surely and

$$\mathcal{N}(E) = \mathcal{T}_{\mathbb{P}}(\chi(H \leq E)) \qquad \textit{(Shubin, '76)}$$

$\chi(H \leq E)$ 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 -

III.4)- 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* $\mathcal{A}$ *!*

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

Theorem 1 (**Abstract gap labelling 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***).*

- *Let* $\lambda \in [0,1] \mapsto H(\lambda) \in \mathcal{A}$ *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***).*

IV - Computing Gap Labels

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).

A. van Elst, *Rev. Math. Phys.*, **6**, (1994), 319-342.

J. Bellissard, J. Kellendonk, A. Legrand, *Gap Labelling for three dimensional aperiodic solids* submitted to *C.R.A.S.*, (2000).

IV.1)- The Main Conjecture

Conjecture 1 *If the transversal X of $(\Omega, \mathbb{R}^d)$ is completely disconnected, then*

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

where $\mathbb{P}_{tr}$ is the transverse measure induced by $\mathbb{P}$ on X.

In many cases, including Quasicrystals, the groupoid of the transversal is Morita equivalent to a $\mathbb{Z}^d$-action.

Theorem 2 *If X is Cantor with a topologically transitive $\mathbb{Z}^d$-action, the conjecture holds true for $\mathcal{A} = \mathcal{C}(X) \rtimes \mathbb{Z}^d$ provided $d = 1, 2, 3$.*

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 $d \geq 3$ one must use spectral sequences instead.

IV.2)- Computing $K_0(\mathcal{A})$

A.H. Forrest & J.R. Hunton, *Erg. Th & Dyn. Syst.* **19**, (1999), 611-625.

Let X be Cantor with a topologically transitive $\mathbb{Z}^d$-action α. If $\mathcal{B} = \mathcal{C}(X)$, the *mapping torus* is

$$M_\alpha \mathcal{B} \;=\; \{f : \mathbb{R}^d \mapsto \mathcal{B} \mid f(x+a) = \alpha_a f(x),\; a \in \mathbb{Z}^d\}$$

Then

$$K_i\left(\mathcal{B} \rtimes_\alpha \mathbb{Z}^d\right) \;\simeq\; K_{i-d}\left(M_\alpha \mathcal{B}\right) \;,$$

and

Theorem 3 (Forrest & Hunton)

$$K_i\left(M_\alpha \mathcal{B}\right) \;\simeq\; \bigoplus_n H^{i+2n}\left(\mathbb{Z}^d, \mathcal{C}(X,\mathbb{Z})\right) \;.$$

IV.3)- Trace and d-trace

M.V. Pimsner, in *Lecture Notes in Math* **1132**, (1983), 374-408.

A $\mathbb{Z}^d$-invariant ergodic probability measure $\mathbb{P}$ on X, induces a trace $\mathcal{T}_{\mathbb{P}}$ on $\mathcal{B} \rtimes \mathbb{Z}^d$ and a d-trace $\mathcal{T}_{\mathrm{d}}$ on $M_\alpha \mathcal{B}$ given by

$$\mathcal{T}_{\mathrm{d}}(f_0, \cdots, f_d) =$$

$$\sum_{\sigma \in Perm(d)} sgn(\sigma) \int dt_1 \cdots dt_d \, \mathcal{T}_{\mathbb{P}} \left(f_0 \frac{\partial f_1}{\partial t_{\sigma(1)}} \cdots \frac{\partial f_d}{\partial t_{\sigma(d)}} \right)$$

Theorem 4 (Pimsner)

$$\langle [\mathcal{T}_d], K_d (M_\alpha \mathcal{B}) \rangle = \langle [\mathcal{T}_{\mathbb{P}}], K_0 \left(\mathcal{B} \rtimes_\alpha \mathbb{Z}^d \right) \rangle .$$

The restriction of this d-trace to the *suspension* $S^d \mathcal{B}$ gives ,

$$\langle [\mathcal{T}_{\mathrm{d}}], K_d \left(S^d \mathcal{B} \right) \rangle = \langle [\mathbb{P}], \mathcal{C}(X, \mathbb{Z}) \rangle .$$

proving theorem 2 if the mapping torus can be replaced by the suspension.

IV.4)- Spectral sequence

1. Let I_n be the ideal of $f \in M_\alpha\mathcal{B}$ vanishing on n-faces of $[0,1]^d$.
2. set $F_n = M_\alpha\mathcal{B}/I_n$, giving a co-filtration:

$$M_\alpha\mathcal{B} = F_d \stackrel{\pi}{\to} F_{d-1} \stackrel{\pi}{\to} \cdots \stackrel{\pi}{\to} F_0 \simeq \mathcal{B}$$

3. Let $Q_n = (S^n\mathcal{B})^{\binom{d}{n}}$ induces exact sequences

$$0 \to Q_n \stackrel{i}{\to} F_n \stackrel{\pi}{\to} F_{n-1} \to 0$$

   where i is defined canonically.
4. Summing up over n and applying the functor K gives an *exact pair*

$$\begin{array}{ccccc} & & K(Q) & & \\ & \partial \nearrow & & \searrow \imath_* & \\ K(F) & & \stackrel{\pi_*}{\longleftarrow} & & K(F) \end{array}$$

   underlying a spectral sequence.

5. The n-th degree cohomology of the differential complex $(K(Q), d_1 = \partial \circ \imath_*)$ is isomorphic to the right-hand side of the Forrest-Hunton formula.
6. The Hunton-Forrest theorem expresses that the spectral sequence converges at page 2.
7.

$$\begin{array}{ccccccccccc}
K(S^d\mathcal{B}) & & K(Q_{d-1}) & \cdots & K(Q_2) & \stackrel{d_1}{\longleftarrow} & K(Q_1) & \stackrel{d_1}{\longleftarrow} & K(\mathcal{B}) & & \\
\imath_* \downarrow & \nwarrow \partial & \imath_* \downarrow & \cdots & \imath_* \downarrow & \nwarrow \partial & \imath_* \downarrow & \nwarrow \partial & \imath_* \downarrow & & \\
K(M_\alpha\mathcal{B}) & \stackrel{\pi_*}{\to} & K(F_{n-1}) & \cdots & K(F_2) & \stackrel{\pi_*}{\to} & K(F_1) & \stackrel{\pi_*}{\to} & K(\mathcal{B}) & \to & 0
\end{array}$$

8. For each element of $\imath_* H_{d_1}(K_i(Q_n))$, for $n = 0, 1$, admits a lift in $K_i(M_\alpha\mathcal{B})$ which lies in the kernel of $\mathcal{T}_{\rm d}$. This lift is explicit.
9. For $d \leq 3$ this is sufficient to show that the only contribution to $\langle [\mathcal{T}_{\rm d}], K_d\,(M_\alpha\mathcal{B})\rangle$ comes from $\langle [\mathcal{T}_{\rm d}], K_d\left(S^d\mathcal{B}\right)\rangle$, proving the theorem 2.

V - Prospects

1. Extension of this theorem to $d \geq 4$ seems possible (J.B., Kellendonk, Legrand *in progress*)

2. There is an homological approach to this theorem (J.B., Gambaudo *in progress*).
   It then applies to the case for which the groupoid of the transversal is not Morita equivalent to a $\mathbb{Z}^d$-action.

3. The homological approach also permits to compute the set of all invariant measures and the entropy of the atomic tiling.