The NONCOMMUTATIVE GEOMETRY of APERIODIC SOLIDS

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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).

D. Spehner, *Contributions à la théorie du transport électronique, dissipatif dans les solides apériodiques*, Thèse, 13 mars 2000, Toulouse.

J. Bellissard, D. Herrmann, M. Zarrouati, *Hull of Aperiodic Solids and Gap Labelling Theorems*, In *Directions in Mathematical Quasicrystals*, CRM Monograph Series, Volume **13**, (2000), 207-259, M.B. Baake & R.V. Moody Eds., AMS Providence.

J. Bellissard, J. Kellendonk, A. Legrand, *Gap Labelling for three dimensional aperiodic solids* , C. R. Acad. Sci. (Paris), **t.332**, Série I, p. 521-525, (2001).

J. Bellissard, R. Benedetti, J. M. Gambaudo, *Spaces of Tilings, Finite Telescopic Approximations, and Gap-Labelling, math.DS/0109062*, (2001).

Content

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) $\mathbf{Al_{62.5}Cu_{25}Fe_{12.5}}$;
   (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.

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.

Results:

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

$\mathcal{L}$ 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

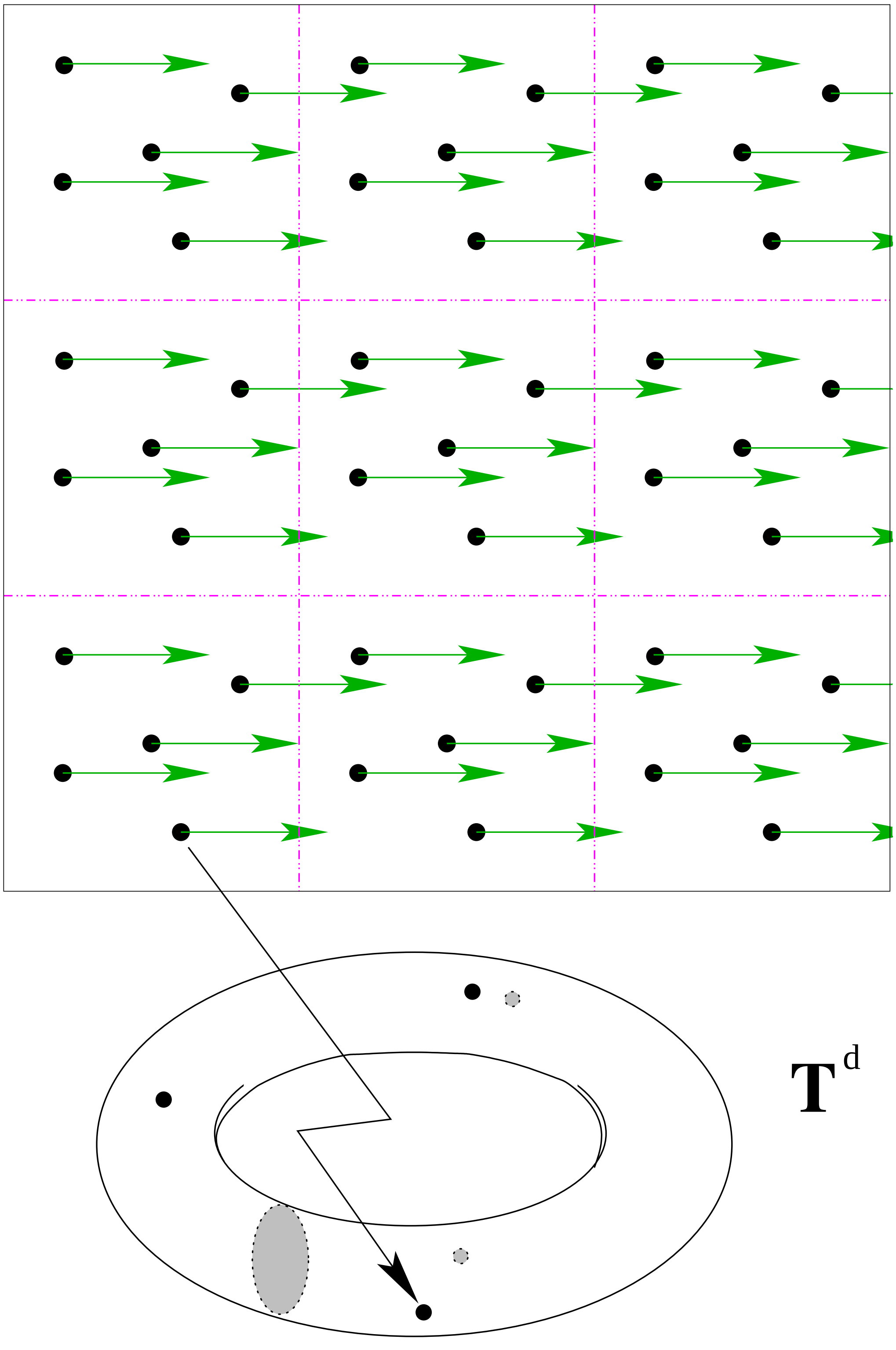
J. Bellissard, R. Benedetti, J.-M. Gambaudo, *Spaces of Tilings, Finite Telescopic Approximations and Gap-Labelling*, preprint August (2001).

II.1)- Examples

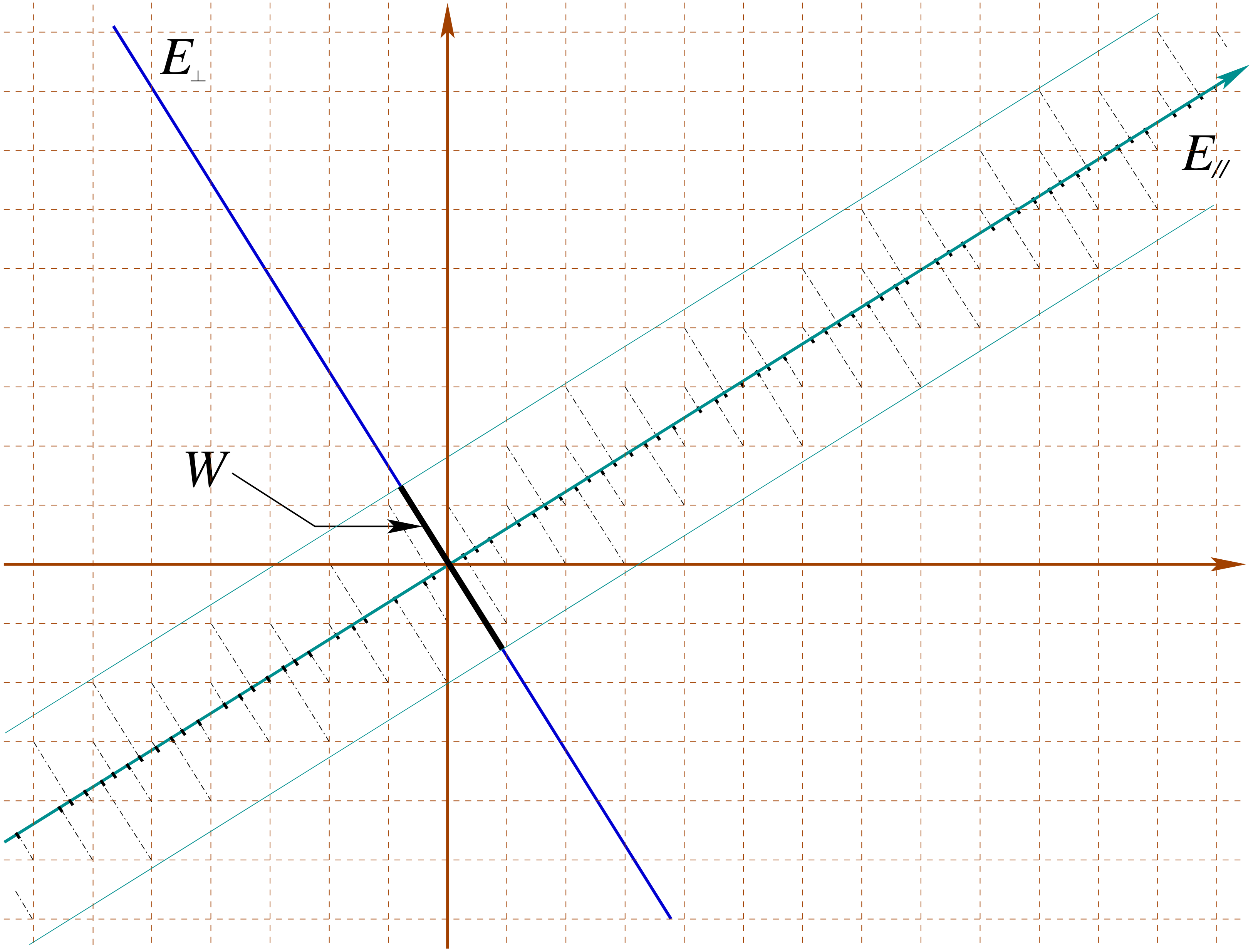
1. *Crystals :* $\Omega = \mathbb{R}^d/\mathcal{T} \simeq \mathbb{T}^d$ with the quotient action of $\mathbb{R}^d$ on itself. (Here $\mathcal{T}$ is the translation group leaving the lattice invariant. $\mathcal{T}$ is isomorphic to $\mathbb{Z}^D$.)

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.

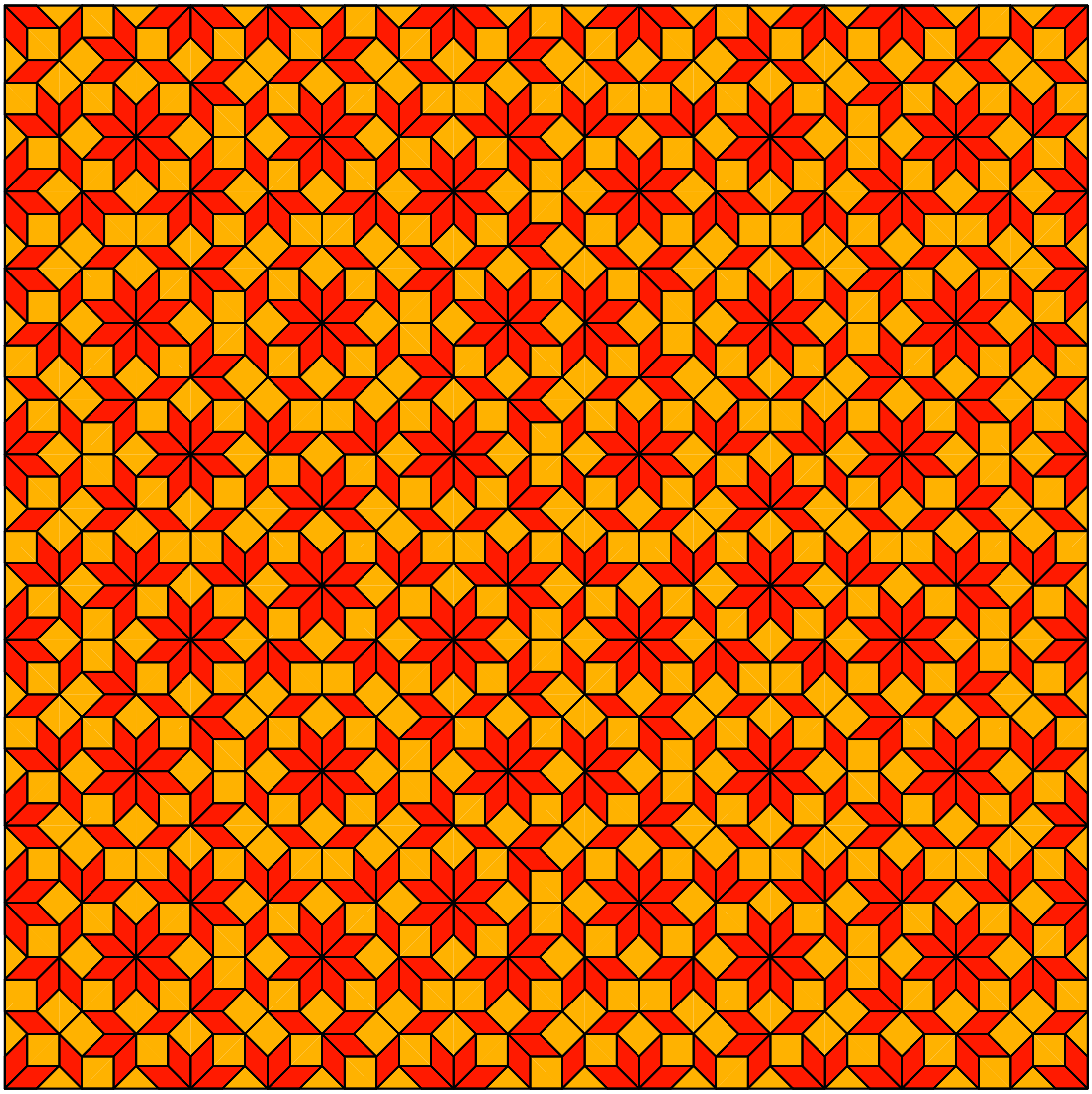
3. *Impurities in* **Si** *:* let $\mathcal{L}$ be the lattices sites for Si atoms (it is a Bravais lattice). Let $\mathfrak{A}$ be a finite set (alphabet) indexing the types of impurities. One sets $\tilde{\Omega} = \mathfrak{A}^{\mathbb{Z}^d}$ with $\mathbb{Z}^d$-action given by shifts. Then Ω is the mapping torus of $\tilde{\Omega}$.



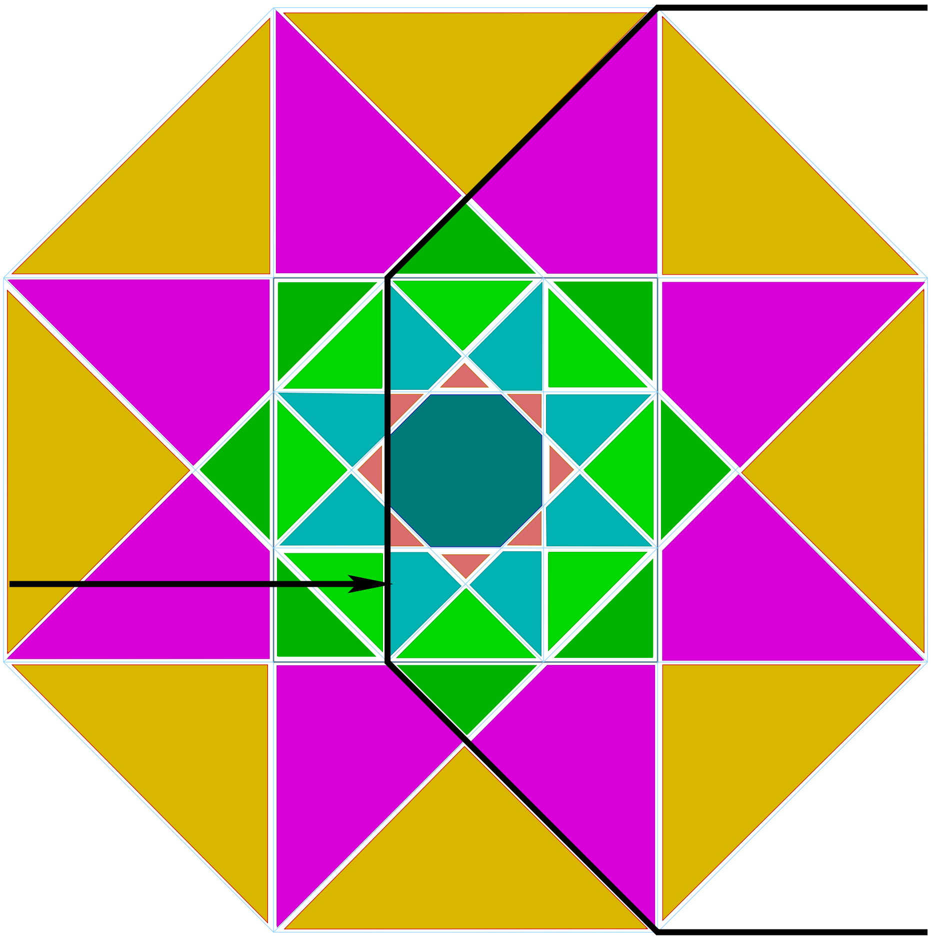
- The Hull of a Periodic Lattice -

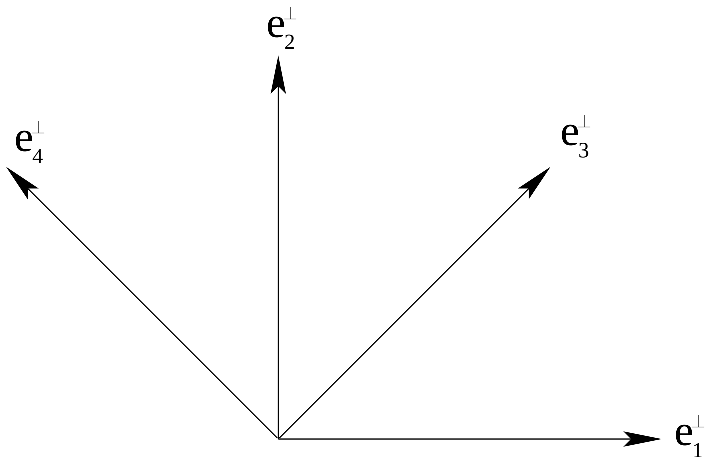


– The cut–and–project construction –



- The octagonal tiling -





- The transversal of the Octagonal Tiling -

- is completely disconnected -

II.2)- Finite Type Tilings

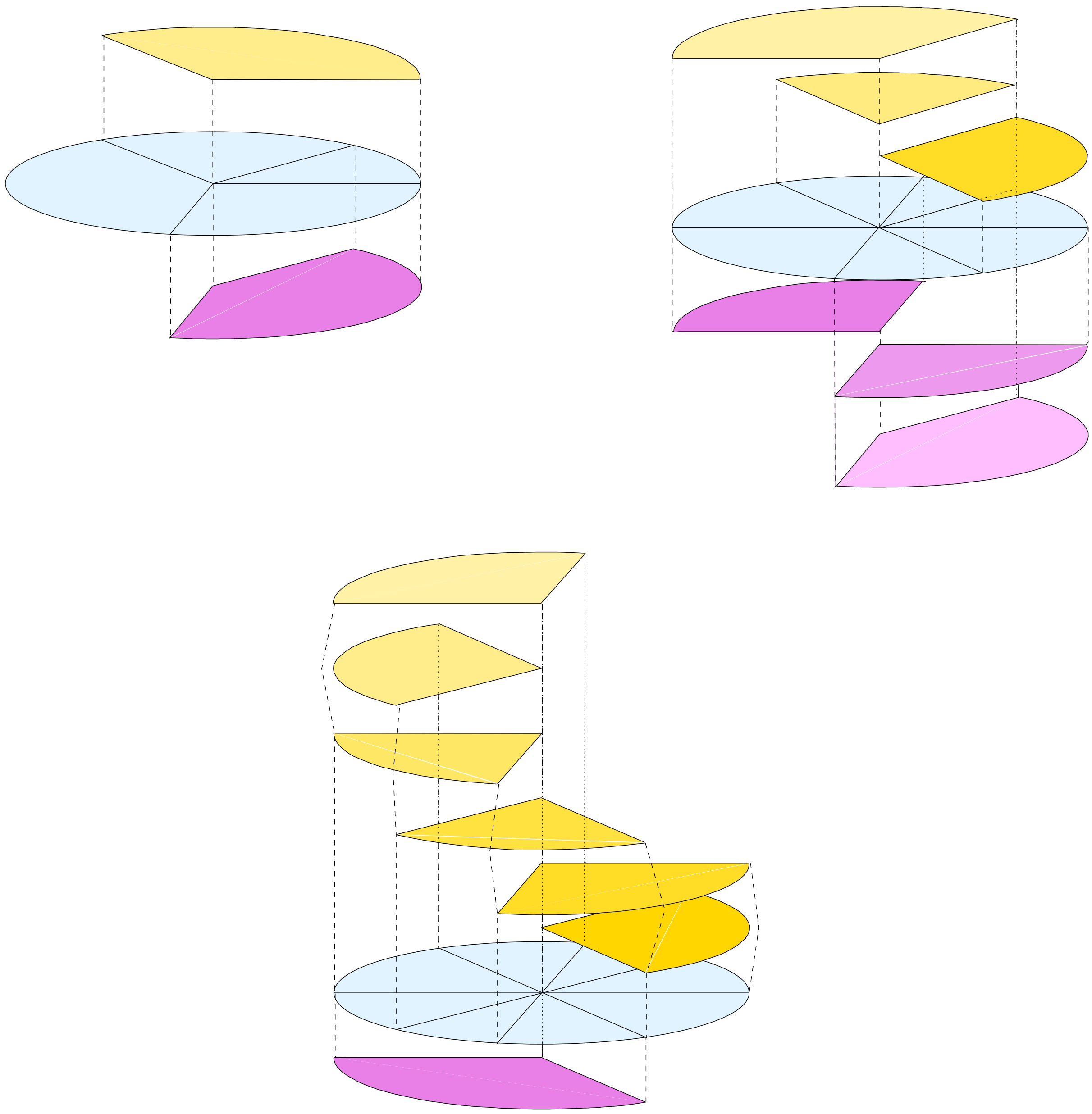
Let $\mathcal{L}$ be a finite type Delone set, and let $\mathcal{T}$ be its *Voronoi* tiling. Then

Theorem 1 *The dynamical system*

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

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.

1. A *Branched Oriented Flat manifold* (BOF) is a family of *colored* tiles glued on their edges.
2. As $n \to \infty$ the tiles of B_n cover more and more of $\mathcal{T}$.
3. *BOF-submersion* $f_n : B_{n+1} \mapsto B_n$ such that $Df_n = \mathbf{1}$. Each tile in B_{n+1} is tiled by tiles of B_n : f_n identifies them.
4. call Ω the *projective limit* of the sequence
$$\cdots \stackrel{f_{n+1}}{\rightarrow} B_{n+1} \stackrel{f_n}{\rightarrow} B_n \stackrel{f_{n-1}}{\rightarrow} \cdots$$
5. *parallel transport* of constant vector fields on B_n, generates the infinitesimal $\mathbb{R}^d$-action on Ω.



- *Vertex branching for the octagonal tiling* -

III - 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).

III.1)- Algebra

Set $\mathcal{A} = \mathcal{C}(\Omega) \rtimes \mathbb{R}^d$. For any $\omega \in \Omega$, let π_ω be the left regular representation on $\mathcal{H} = L^2(\mathbf{R}^d)$:

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

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 (for $A \in \mathcal{C}_c(\Omega \times \mathbb{R}^d)$)

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

In much the same way, $C^*(\Gamma_{tr})$ is the C^*-algebra of the transversal, endowed with the induced trace $\mathcal{T}_{\mathbb{P}}^{tr}$.

Theorem 2 *If $\mathcal{L}$ is $\mathbb{G}$-periodic in $\mathbb{R}^d$, with Brillouin zone $\mathbb{B} = \mathbb{R}^{d\,*}/\mathbb{G}^\perp = \mathbb{G}^*$ then :*

1. *$\mathcal{A}$ is isomorphic to $\mathcal{C}(\mathbb{B}) \otimes \mathcal{K}$,*
2. *$C^*(\Gamma_{tr})$ is isomorphic to $\mathcal{C}(\mathbb{B}) \otimes M_n$ if $n = |\mathcal{L}/\mathbb{G}|$.*

III.2)- 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 binding representation*)

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

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 $\Sigma_{\mathrm{H}} = \bigcup_{\omega\in\Omega}\mathrm{Sp}(H_\omega)$, 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 $\tilde{H}$).

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*.

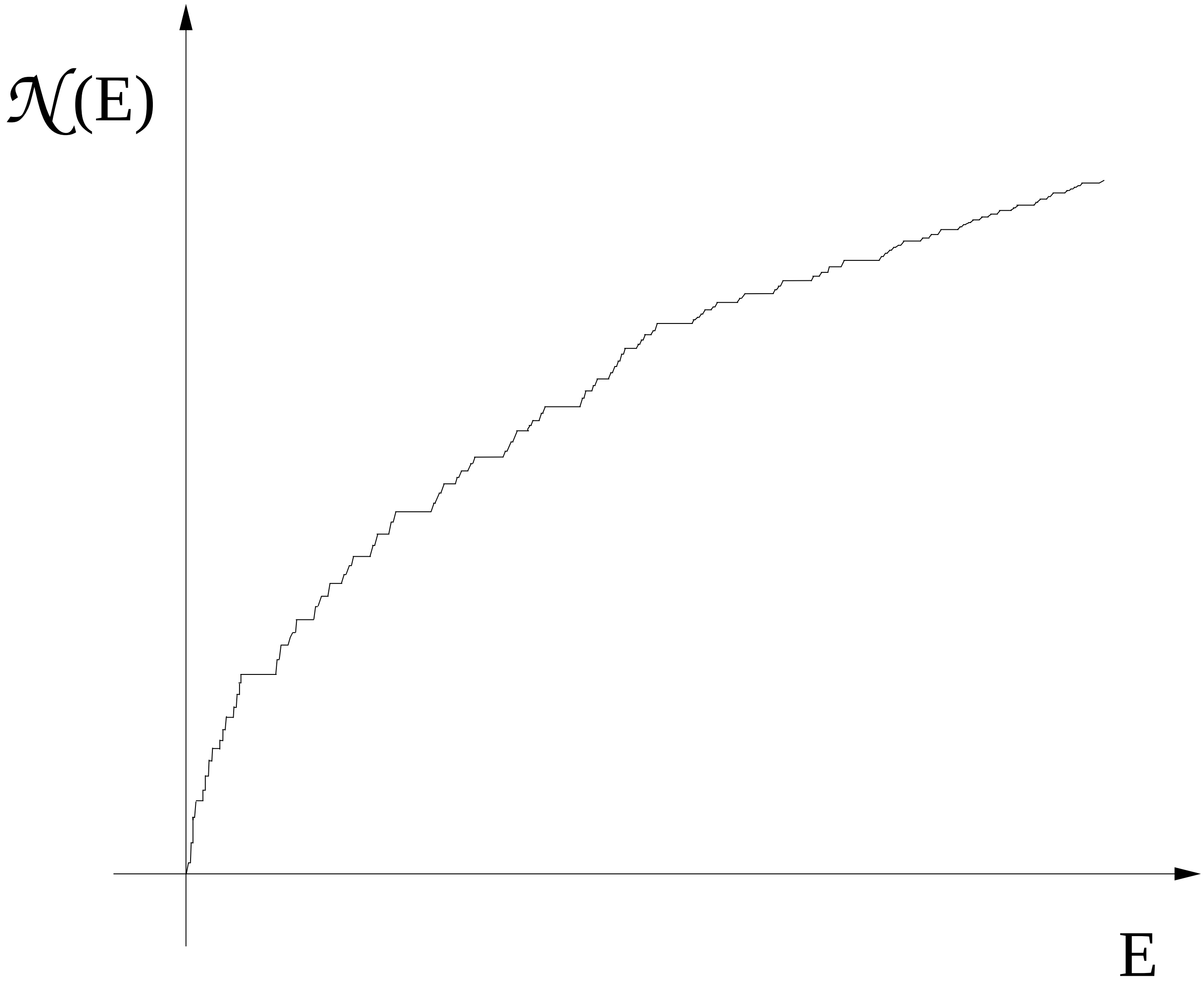
- The limit above exists $\mathbb{P}$-almost surely and

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

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

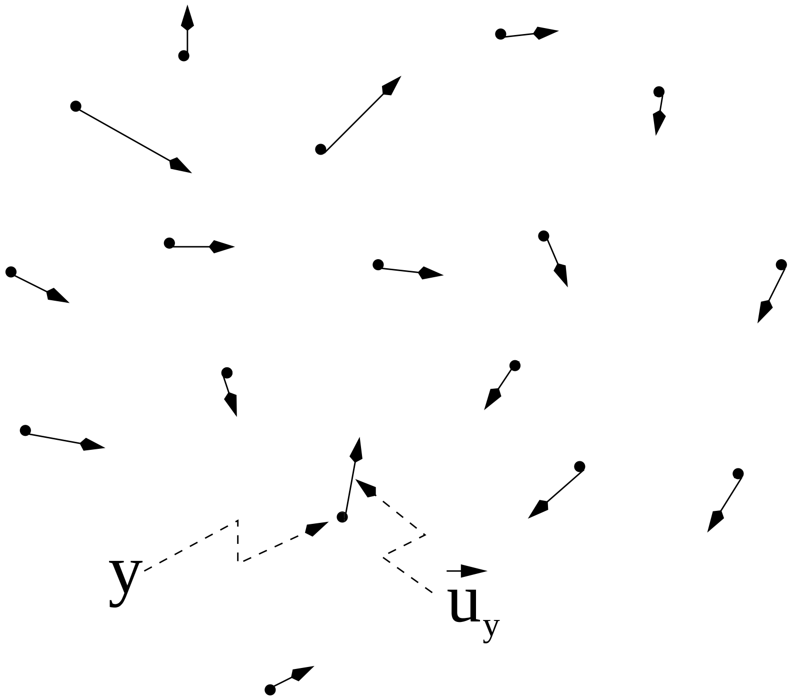
- $\mathcal{N}$ is non decreasing, non negative and constant on gaps. $\mathcal{N}(E) = 0$ for $E < \inf \Sigma_{\mathrm{H}}$. For $E \to \infty$, $\mathcal{N}(E) \sim \mathcal{N}_0(E)$ where $\mathcal{N}_0$ is the IDS of the free case (namely $v = 0$).

- *Gaps can be labelled by the value the IDS takes on them*



- An example of IDS -

III.4)- 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:

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

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

III.5)- 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 3 (**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**).*

- *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 $(\Omega, \mathbb{R}^d, \mathrm{T})$, then, for any $\mathbb{R}^d$-invariant probability measure $\mathbb{P}$ on Ω*

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

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 space

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

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 $(\Omega, \mathbb{R}^d, \mathrm{T})$ 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 *(Benameur, Oyono, 2001)* *(Kaminker, Putnam, 2001)* and *(Bellissard, Benedetti, Gambaudo, 2001)*.

IV - NC Fermi Surface

D. Spehner, *Contributions à la théorie du transport électronique, dissipatif dans les solides apériodiques*, Thèse, 13 mars 2000, Toulouse.

IV.1)- Quasilocal Algebra

Here $\mathcal{L}$ is a Delone set, electrons are described in the tight binding representation.
X denotes its transversal. Then $\mathcal{A} = C^*(\Gamma_{tr})$.

1. For $\omega \in X$, with each site $x \in \mathcal{L}_\omega$ are associated *creation-annihilation* operators for electrons *(fermions)* and phonons *(bosons)*.
2. These operators generate a *quasilocal algebra* $\mathfrak{A}_\omega$. The translation $\gamma = (\omega, a)$ in Γ_{tr} allows to generate a *-isomorphism $\alpha_\gamma : \mathfrak{A}_{\mathrm{T}^{-a}\omega} \mapsto \mathfrak{A}_\omega$.
3. The second quantized Hamiltonian with electron-phonon interactions, generates a dynamics *(Bratteli, Robinson, '72)* $\eta_\omega(t) \in Aut(\mathfrak{A}_\omega)$ that is *covariant*. Adding the various Lagrange multipiers (chemical potential,...) gives a *KMS-dynamics* ϕ in much the same way.
4. The field $\mathfrak{A} = (\mathfrak{A}_\omega)_{\omega \in X}$ becomes *continuous* and *covariant*.
5. The crossed product $\mathfrak{B} = \mathfrak{A} \rtimes_\alpha \Gamma$ is well-defined *(Renault, '86)*. The dynamics induced by η, ϕ give corresponding automorphism groups of $\mathfrak{B}$.

IV.2)- Bimodule over the NC Brillouin Zone

1. $\mathfrak{B}$ is generated by continuous funtions

$$\gamma \in \Gamma \mapsto A(\gamma) \in \mathfrak{A}_\omega$$

   if $\omega = r(\gamma)$, with compact support.

2. The product is given by

$$(AB)(\gamma) = \sum_{\gamma' \in \Gamma^\omega} A(\gamma')\alpha(\gamma')B(\gamma'^{-1} \circ \gamma)$$

3. the adjoint by:

$$A^*(\gamma) = \alpha(\gamma)A(\gamma^{-1})^*$$

4. The (reduced) norm is obtained through covariant representations.

5. $\mathfrak{B}$ is also a $C^*(\Gamma)$-*bimodule*.

IV.3)- Covariant States & GNS Representation

1. A *covariant state* on $\mathfrak{A}$ is a continuous family Φ_ω of states on $\mathfrak{A}_\omega$ such that
$$\Phi_\omega \circ \alpha(\gamma) = \Phi_{\omega'} \quad \textit{if} \quad \gamma : \omega' \mapsto \omega$$

2. A Hilbert C^*-module structure over $C^*(\Gamma)$ is defined on $\mathfrak{B}$ by:
$$\langle A|B\rangle(\gamma) = \Phi_\omega\left(A^* B(\gamma)\right)$$
After quotienting and completion we get a Hilbert C^*-module $\mathcal{F}$.

3. In particular
   (a) $\langle A|B\rangle \in C^*(\Gamma)$,
   (b) If $h \in C^*(\Gamma)$ then $\langle A|Bh\rangle = \langle A|B\rangle h$.
   (c) $\langle A|B\rangle^* = \langle B|A\rangle$.
   (d) $\langle A|CB\rangle = \langle C^* A|B\rangle$

4. So that the left multiplication by an element of $\mathfrak{B}$ defines an *endomorphisms* of $\mathcal{F}$, giving rise to the *GNS representation* of $\mathfrak{B}$ in $\mathcal{F}$.

IV.4)- Ground State

1. If Φ is η-invariant, η^t is implemented by a one parameter group $U(t)$ of unitary endomorphisms of $\mathcal{F}$:

$$\langle A|U(t)B\rangle = \langle A|\eta^t(B)\rangle$$

2. If, in addition, Φ is a *ground state* for η, then the generator $H = -\imath U(t)^{-1}dU/dt$ is *positive*, namely

$$\langle A|HA\rangle \geq 0 \qquad\qquad \forall A \in \mathcal{F}$$

3. This construction applies to the case of the electron-phonon dynamics in an aperiodic solid: a ground state is specified by the *Fermi level* E_F.
The Hilbert C^*-module $\mathcal{F}_F$ obtained in this way, plays the rôle of a fiber bundle over the Noncommutative Brillouin zone defined by $C^*(\Gamma)$, *fixing the geometry of the Fermi surface*. Hence :

Definition 1 *The Noncommutative Fermi surface associated with the dynamics defined by the total Hamiltonian H, and with the Fermi energy E_F is the NC fiber bundle above the NC Brillouin zone associated with the Hilbert C^*-module $\mathcal{F}_F$ constructed above.*

Conclusion

1. An aperiodic solid gives rise to a canonical dynamical system, its Hull, representing the configurations of *lack of periodicity*.
2. The C^*-algebra associated with the Hull can be interperted as the *Noncommutative Brillouin Zone*.
3. Electrons and phonons are affiliated to this algebra.
4. The topology of the NCBZ can be computed via its K-theory. The *Gap Labelling Theorem* is a special example of application.
5. Interactions lead to a NC description of the *Fermi surface*, through a Hilbert C^*-bimodule over the NCBZ.
6. The NC Geometry can be described through the Cyclic Cohomology of the NCBZ.
   We conjecture that it plays a rôle in non dissipative transport
   (ex.: the Integer Quantum Hall Effect).