The GAP LABELING THEOREM *then and now*

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This topics is owing a lot to Alain Connes who has inspired most of it

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Content

I - Cantor Spectra

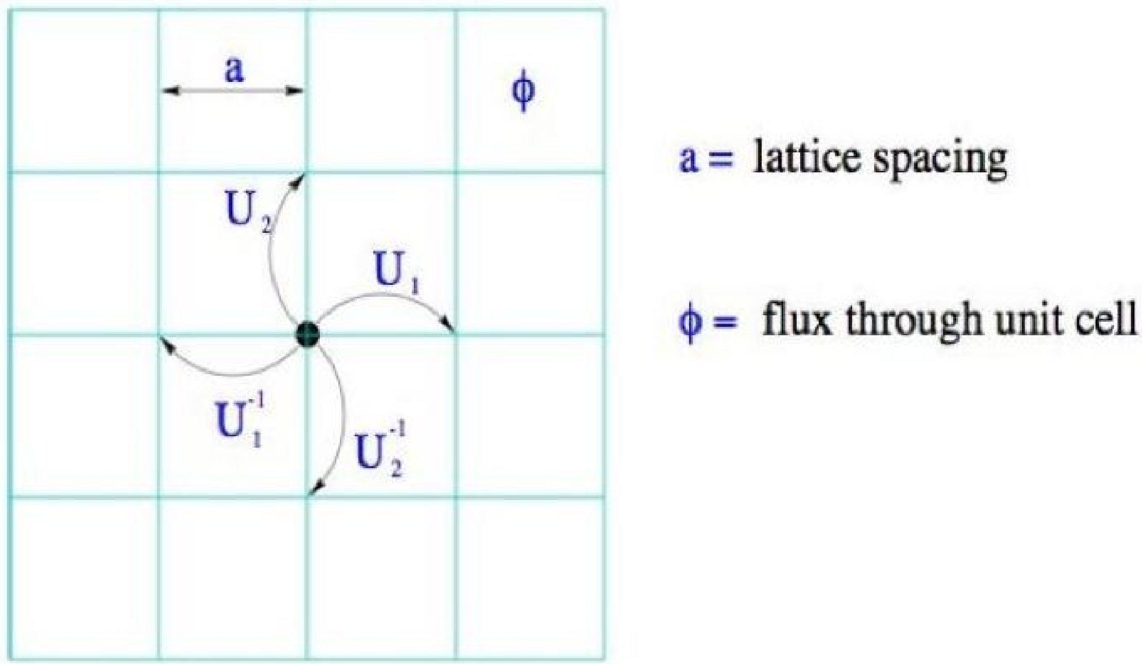
I.1)- Electrons in Magnetic Field

The study of crystal electrons in a uniform magnetic field goes back to Landau (1930) and Peierls (1933). No Solid State physicists has escaped this difficult problem. In 1955, Harper proposed an effective model to describe a 2D square-lattice electron in a uniform magnetic field

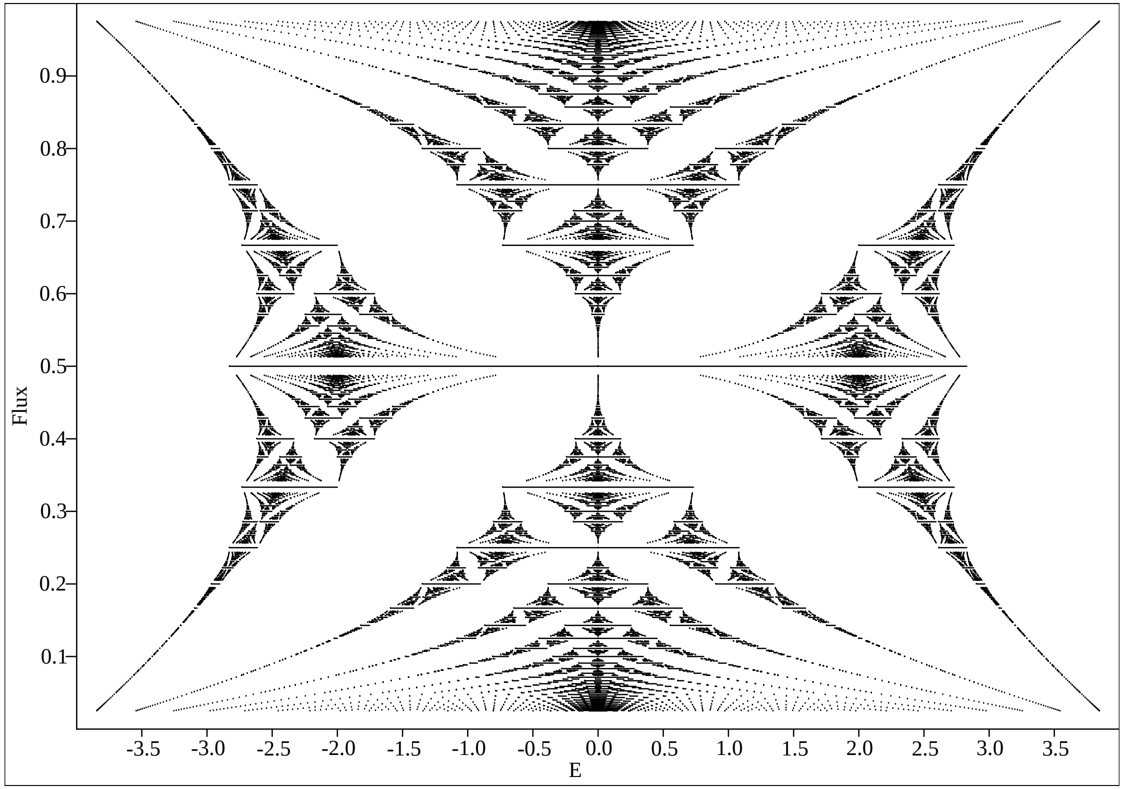
$$H = U_1 + U_1^{-1} + U_2 + U_2^{-1}$$

The U_i's are the operators of translation by one unit along the axis of coordinates. In presence of a magnetic flux ϕ per unit cell, they satisfy

$$U_1 U_2 U_1^{-1} U_2^{-1} = e^{2\imath\pi\phi/\phi_0}$$



- Magnetic translations: $\phi_0 = h/e$ is the flux quantum -



1976 : The Hofstadter Spectrum !

I.2)- Quasi-periodic Potentials

In 1976, *Dinaburg & Sinai* studied the spectrum of

$$H = -\frac{d^2}{dx^2} + V(\omega_1 x, \cdots, \omega_N x)$$

acting on $L^2(\mathbb{R})$, where V is a smooth function on $\mathbb{T}^N$ and the ω_i's satisfy a diophantine condition

$$\left|\sum_{i=1}^{N} n_i \omega_i\right| \geq \frac{C}{(\sum_i |n_i|)^{N+\rho}} \qquad \forall (n_i)_i \in \mathbb{Z}^N$$

They found evidence *(without proof)* that the spectrum was a Cantor set.

I.3)- Moser's Result

J. MOSER, *An example of a Schrödinger equation with almost periodic potential and nowhere dense spectrum*, Comment. Math. Helv., **56**, (1981), 198-224.

In 1981, Moser proved the following theorem

Theorem *Let $q_0(x)$ be a continuous periodic function on $\mathbb{R}$. In any neighborhood of q_0, for the uniform topology, there is a limit-periodic function q such that the Schrödinger operator*

$$H = -\frac{d^2}{dx^2} + q(x)$$

has a nowhere dense spectrum.

I.4)- Harper's Model

The following result took 24 years to get a complete proof !

Theorem *There is a set S of full Lebesgue measure in* $[0,1]$ *such that if* $\alpha = \phi/\phi_0 \in S$ *then the Harper operator has a Cantor spectrum. All gap possible are open but the central one.*

The first result in this direction was proved in 1982. The proof was completed in 2006, thanks to the contributions of many authors

J. Bellissard, B. Simon, *Cantor spectrum for the almost Mathieu equation*, J. Funct. Anal., **48**, (1982), 408-419.
A. Avila, S. Jitomirskaya, *Solving the ten Martini problem*, Lecture Notes in Phys., **690**, Springer (2006).

I.5)- Other Models

Many models of Schrödinger operators in 1D have been designed leading to a Cantor spectrum. Among them, the discrete ones acting on $\ell^2(\mathbb{Z})$

$$H\psi(n) = \psi(n+1) + \psi(n-1) + V_n\,\psi(n)$$

where the V_n's takes on *finitely many values* defined by a *substitution* sequence. For the *Fibonacci, Thue-Morse and period doubling sequences*, the spectrum has been proved to be a Cantor set of zero Lebesgue measure.

In higher dimension in some specific cases, models with Cantor Spectra have been designed (*labyrinth models, C. Sire (1986)*). But the problem is still mostly open.

II - Gap Labeling Theorem

If the spectrum of a self-adjoint operator is a Cantor set, there are infinitely many gaps in each bounded interval.

Question: How can one label these gaps in a way which is robust under perturbation of the operator ?

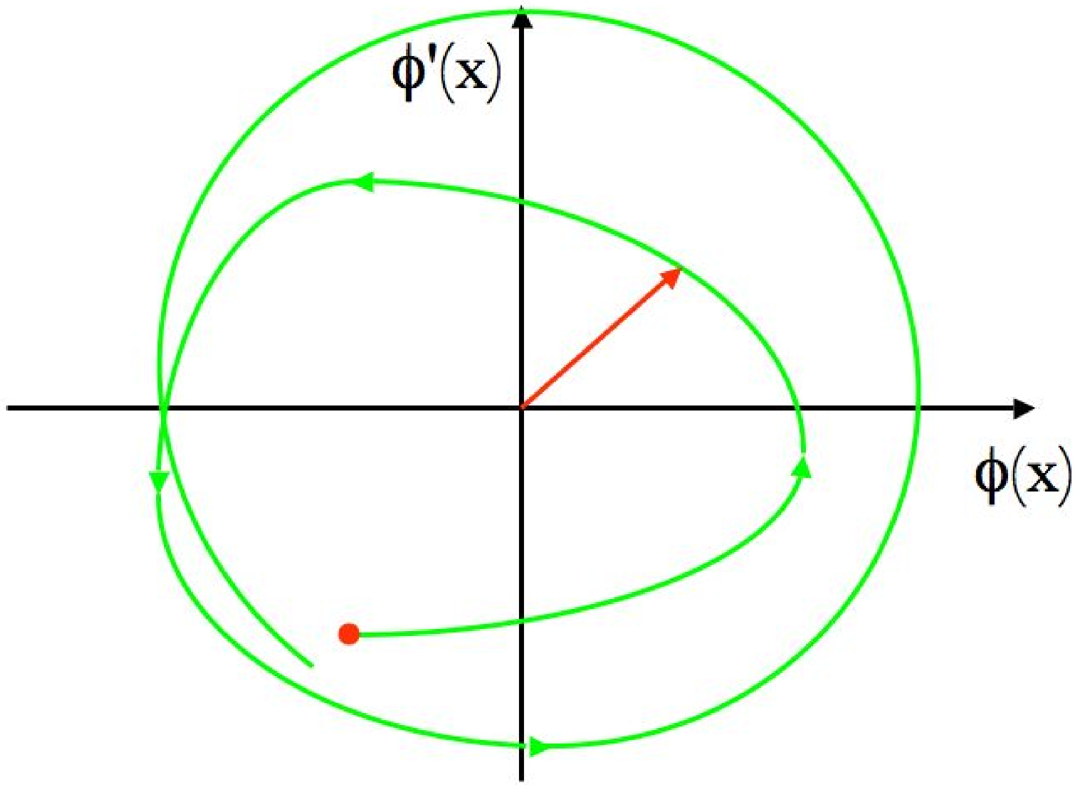
II.1)- Liouville's Theorem

If $q : \mathbb{R} \mapsto \mathbb{R}$ is smooth, then $H = -d^2/dx^2 + q$ restricted to $[-L, L]$ with some boundary condition has a *simple discrete unbounded spectrum* $\mathrm{Sp}(H) = \{\lambda_0 < \lambda_1 < \cdots < \lambda_n < \cdots\}$.

Theorem[Liouville] *Let φ be a real solution of $-\varphi''(x) + q(x)\varphi(x) = \lambda\varphi(x)$. If $\lambda_{n-1} < \lambda \leq \lambda_n$, the function φ has exactly n zeroes in $[-L, L]$.*

Equivalently, the point $\varphi(x) + \imath\varphi'(x) = r(x)e^{\imath\theta(x)} \in \mathbb{C}$ describes a curve around the origin which cuts the vertical axis n times. In particular

$$n\pi \;\leq\; \theta_L(\lambda) \;=\; -\imath \int_{-L}^{L} d\theta(x) \;<\; (n+1)\pi$$



Rotation number

If now $N_L(\lambda)$ denotes the *number of eigenvalues smaller than* λ then

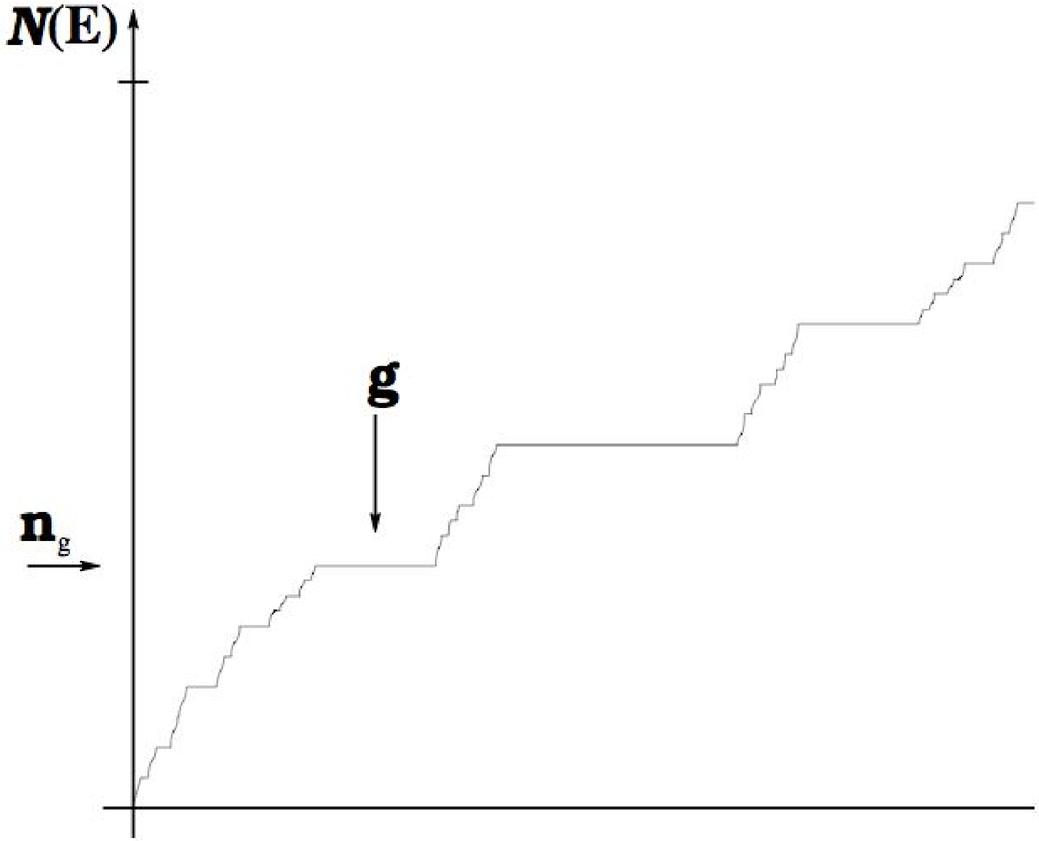
$$\pi N_L(\lambda) \;\leq\; \theta_L(\lambda) \;<\; \pi(N_L(\lambda)+1)$$

Let H act on $L^2(\mathbb{R})$ instead of $[-L, L]$. The *rotation number* $\rho(\lambda)$ and the *Integrated Density of States* $\mathcal{N}(\lambda)$ (IDS) are defined by (*if the limit exists*)

$$\rho(\lambda) = \lim_{L\to\infty} \frac{\theta_L}{2L} \qquad \mathcal{N}(\lambda) = \lim_{L\to\infty} \frac{N_L}{2L}$$

Then

$$\rho(\lambda) \;=\; \pi\mathcal{N}(\lambda)$$



$\mathcal{N}(\lambda)$ **is constant on the spectral gaps**

II.2)- The Johnson-Moser Gap Labeling Theorem

JOHNSON R., MOSER J., *The rotation number for almost periodic potentials*, Comm. Math. Phys., **84, (1982), 403-438**

If $q : \mathbb{R} \mapsto \mathbb{R}$ is almost periodic, the H. Bohr theorem asserts that it is the uniform limit of linear combinations of $e^{\omega x}$ for a countable family of ω's. The *frequency module* of q is the group generated by the ω's.

Theorem *If q is almost periodic, then the rotation number and the IDS exist. Moreover $\mathcal{N}$ is a non-decreasing continuous function and its derivative is a measure supported by the spectrum of H.*
If, in addition, λ belongs to a gap of the spectrum of H, then

$$\mathcal{N}(\lambda) \textit{ belongs to the the frequency module of } q.$$

Since the frequency module of an almost periodic function is a countable subgroup of the real line, a perturbation of the Hamiltonian changing the spectrum only slightly

is not going to change the value of the IDS on the gap !

II.3)- The Shubin Formula

The IDS of a self-adjoint operator H acting on $L^2(\mathbb{R}^d)$ or on $\ell^2(\mathbb{Z}^d)$ is defined in a similar way as the number of eigenvalues less than or equal to λ *per unit volume*.

Theorem [Shubin '76] *The Integrated Density of State $\mathcal{N}(\lambda)$ of H is given by*

$$\mathcal{N}(\lambda) = \lim_{\Lambda \uparrow \mathbb{R}^d} \frac{1}{|\Lambda|} \mathrm{Tr}_{\Lambda}(\chi(H \leq \lambda)) = \mathcal{T}(\chi(H \leq \lambda))$$

where $\chi(H \leq \lambda)$ denotes the spectral projector of H on the part of the spectrum smaller than or equal to λ.

$\mathcal{T}$ is called the *Trace per Unit Volume*.

II.4)- K-theory: the Harper Model

B. Blackadar, *K-theory for operator algebras*, 2nd edition, Cambridge University Press, Cambridge, 1998.

In a C^*-algebra $\mathcal{A}$, two projections P, Q are *equivalent* if there is $S \in \mathcal{A}$ such that $P = S^*S$ and $Q = SS^*$.

Then $P \sim Q$ denotes the equivalence relation and $[P]$ denotes the equivalence class of P.

Theorem *(i) If $\mathcal{A}$ is a separable C^*-algebra, the set of equivalent classes of projections is at most countable.*

(ii) If P, Q are orthogonal projections in $\mathcal{A}$, then $[P \oplus Q]$ depends only upon $[P]$ and $[Q]$ and will be denoted by $[P] + [Q]$.

(iii) If $\mathcal{K}$ denotes the C^*-algebra of compact operators on a separable Hilbert space, then any pair of projections in $\mathcal{A} \otimes \mathcal{K}$ is equivalent to a pair of orthogonal projections. In particular the addition $[P] + [Q]$ is defined everywhere.

(iv) $K_0(\mathcal{A})$ is the Grothendieck group generated by the equivalence classes of projections in $\mathcal{A} \otimes \mathcal{K}$.

Theorem *(i) Let P and Q be two projectors in a C^*-algebra $\mathcal{A}$. If $||P - Q|| < 1$ they are equivalent.*

(ii) if $t \in [0,1] \mapsto P(t)$ is a continuous path in the set of projectors of $\mathcal{A}$, then these projectors are pairwise equivalent. In particular $[P(t)]$ does not depend on t.

J. Bellissard, *Schrödinger's operators with an almost periodic potential: an overview*, Lecture Notes in Phys., **153**, Springer (1982).

The two unitary operators U_1, U_2 such that $U_1 U_2 = e^{2\imath\pi\alpha} U_2 U_1$ generate a C^*-algebra called the *irrational rotation algebra* and denoted by $\mathcal{A}_\alpha$ (*M. Rieffel, 1978*) .

Let $\mathfrak{g} = (E, E')$ be a gap in the spectrum of $H = U_1 + U_1^{-1} + U_2 + U_2^{-1}$.

If $0 \leq f \leq 1$ is a continuous function on $\mathbb{R}$ such that $f(x) = 1$ for $x \leq E$ and $f(x) = 0$ for $x \geq E'$, then $P_\mathfrak{g} = f(H)$ is a *spectral projection* such that

$$P_\mathfrak{g} \in \mathcal{A}_\alpha$$

M. Rieffel, *C^*-algebras associated with irrational rotations*, Pacific J. Math., **93**, (1981), 415-429.
M. Pimsner, D. Voiculescu, *Imbedding the irrational rotation C^*-algebra into an AF-algebra*, J. Operator Theory, **4**, (1980), 201-210.

There is a unique *tracial state* $\tau : \mathcal{A}_\alpha \mapsto \mathbb{C}$ defined by

$$\tau(U_1^{m_1} U_2^{m_2}) \;=\; \delta_{m_1,0}\,\delta_{m_2,0}$$

If P is a projection in $\mathcal{A}_\alpha$ then its trace $\tau(P)$ depends only upon $[P]$. Moreover

Theorem τ *induces a group homomorphism* $\tau_* : K_0(\mathcal{A}_\alpha) \mapsto \mathbb{R}$. *The image is the countable subgroup* $\mathbb{Z} + \alpha\mathbb{Z} \subset \mathbb{R}$.
Moroever, τ *coincides with the trace per unit volume and the values of the IDS of the Harper model belong to* $(\mathbb{Z} + \alpha\mathbb{Z}) \cap [0, 1]$.

REMARK: gap labels are *K*-Theoretic invariants (topology), there are NOT Group-Theoretic invariants (frequency module) !!

In 1983, a model was designed with an almost periodic potential, for which the Johnson-Moser gap labeling was violated, while the gap labels where given by the image of the K-group under the trace per unit volume.

J. BELLISSARD, E. SCOPPOLA, Comm. Math. Phys., **85**, (1982), 301-308.

III - Solids and Tilings

J. C. Lagarias, *Geometric Models for Quasicrystals:*
I. Delone Sets of Finite Type, Discrete Comput. Geom., **21**, (1999) 161-191.
II. Local Rules Under Isometries, Discrete Comput. Geom., **21**, (1999) 345-372.

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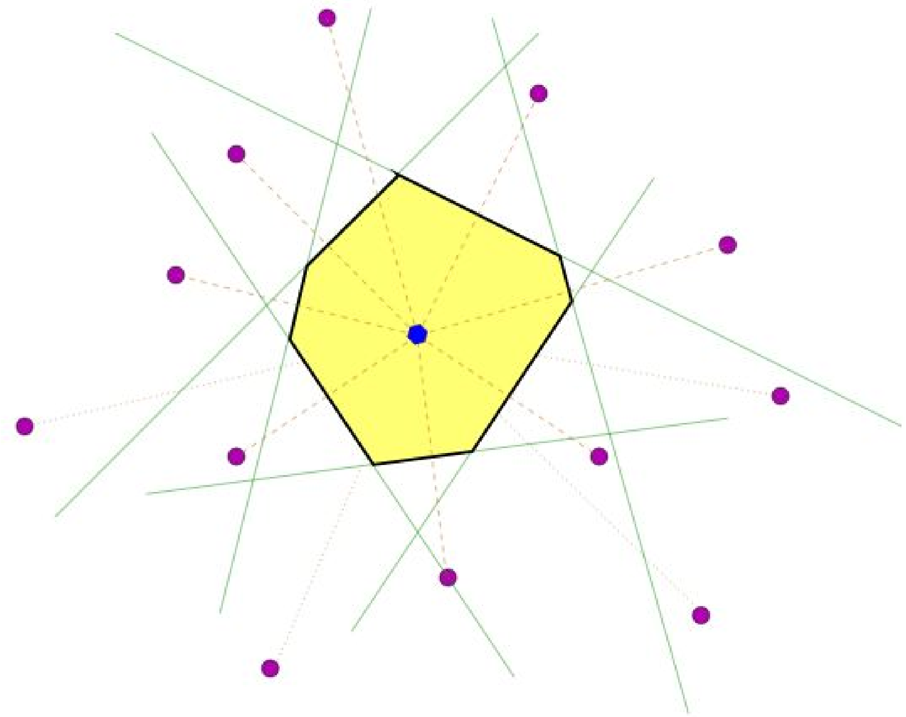


Constructing a Voronoi cell

III.1)- Periodic Crystals

If $\mathcal{L}$ is a periodic discrete subset of $\mathbb{R}^d$, with period group $\mathbb{G}$, the Voronoi cells can be identified with $\mathbb{V} \simeq \mathbb{R}^d/\mathbb{G}$

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.

III.2)- 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:* for instance Si or $AsGa$ on a diamond lattice, with 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..

III.3)- Point Sets

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* whenever it is both uniformly discrete and relatively dense. *(Then $\mathcal{L}$ is 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 $\mathcal{L}$ is called $(r, R; r', R')$-Meyer.)*

III.4)- The Hull

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

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

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

Theorem *The set of Radon measures of the form $\nu_{\mathcal{L}}$ with $\mathcal{L}$ uniformly discrete (resp. Delone, Meyer) is compact and $\mathbb{R}^d$-invariant.*

The *Hull* Ω of $\mathcal{L}$ is the closure of the $\mathbb{R}^d$-orbit of $\nu_{\mathcal{L}}$.
Its *transversal* Ξ is the set of elements $\omega \in \Omega$ with $\omega(\{0\}) > 0$.

III.5)- Tilings

An (r,R)-Delone set $\mathcal{L}$ defines a *tiling* through the Voronoi construction. The tiles are punctured convex polyhedra containing the ball of radius r and are contained in the ball of radius R centered at the puncture.

Conversely, a tiling with tiles punctured and containing the ball of radius r and contained in the ball of radius R centered at the puncture, defines an (r,R)-Delone set.

A *patch* can be seen either as a (connected) finite union of tiles or as a subset of $\mathbb{R}^d$ of the form $p = (\mathcal{L} - x) \cap \overline{B(0,R)}, \quad x \in \mathcal{L}$.

$\mathcal{L}$ has *finite type* whenever $\mathcal{L} - \mathcal{L}$ is *discrete and closed*. Equivalently, given any $R > 0$, the set of patches of radius R is finite. In such a case the tiling is said to have *Finite Local Complexity (FLC)*.

III.6)- Repetitivity, Aperiodicity

A Delone set $\mathcal{L}$ is called *repetitive* whenever, given a patch p and $\epsilon > 0$, there is $R > 0$ such that in any ball of radius R, there is a set coinciding with a translated of p modulo an error smaller than ϵ (measured with the Hausdorff distance).

Theorem . *A Delone set $\mathcal{L}$ is repetitive if and only if the dynamical system defined by the action of $\mathbb{R}^d$ on the Hull is minimal.*

A Delone set $\mathcal{L}$ is called *completely aperiodic* whenever

$$a \in \mathbb{R}^d \quad \& \quad \mathcal{L} + a = \mathcal{L} \qquad \Rightarrow \qquad a = 0$$

IV - The Non-commutative Brillouin Zone

IV.1)- 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 $\mathcal{A} = C(\Omega) \rtimes_\tau \mathbb{R}^d$ is the C^*-algebra generated by the space of continuous functions on Ω and the action of $\mathbb{R}^d$ submitted to the commutation rules (for $f \in C(\Omega)$)

$$T(a) f T(a)^{-1} = f \circ \tau^{-a} \qquad a \in \mathbb{R}^d$$

1. For a crystal $\Omega = \mathbb{V}$, $\mathbb{R}^d$ acts by quotient action.
2. $C(\mathbb{V}) \rtimes_\tau \mathbb{R}^d \simeq C(\mathbb{B}) \otimes \mathcal{K}$, 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*.

IV.2)- Constructing the Crossed Product Algebra

The algebra $\mathcal{A}_0 = C_c(\Omega \times \mathbb{R}^d)$ will be endowed with *(here $A, B \in \mathcal{A}_0$)*

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

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

- A faithfull family of *representations* in $\mathcal{H} = L^2(\mathbb{R}^d)$ *(here $A \in \mathcal{A}_0$, $\psi \in \mathcal{H}$)*

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

- *A 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 $A \in \mathcal{A}_0$))

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

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

Then $\mathcal{T}_{\mathbb{P}}$ is the *trace per unit volume* thanks to Birkhoff's theorem

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

• *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.

IV.4)- Electronic Hamiltonian

The Schrödinger Hamiltonian for an electron submitted to atomic forces *(for one species of atoms and ignoring interactions)* acts on $\mathcal{H} = L^2(\mathbb{R}^d)$ and is given by (v is the *atomic potential*)

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

Theorem 1 *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

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

IV.5)- The Density of States

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

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

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:

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

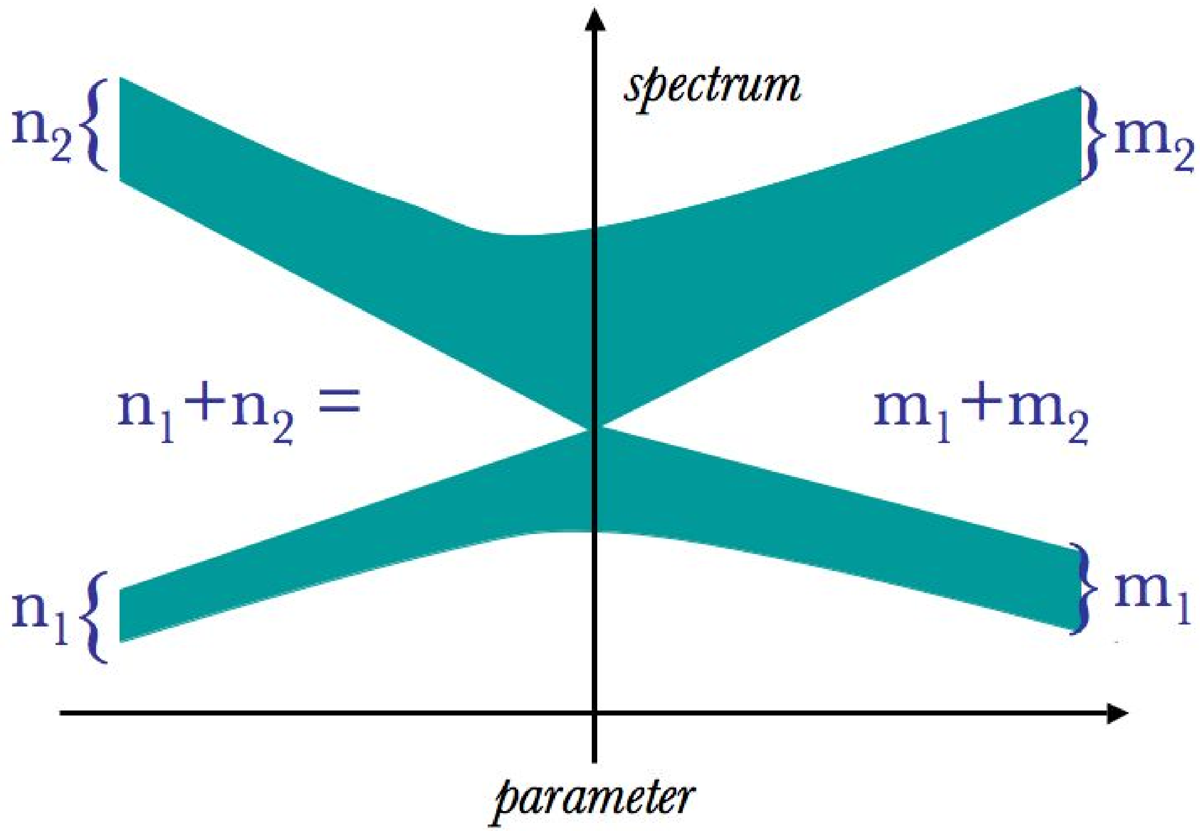
IV.6)- The Gap Labeling Theorem

The *support* of $\mathcal{N}_{\mathbb{P}}$ is contained in the algebraic specrum 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

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

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

Gap Labeling Theorem I. *The set of gap labels, namely the values of the IDS on gaps, belong to the image of the K_0-group of the algebra $C(\Omega) \rtimes \mathbb{R}^d$ by the trace per unit volume.*



- Sum rule for gap labels -

IV.7)- FLC Tilings

M.-T. Benameur, H. Oyono-Oyono, *Gap labeling for quasi-crystals (proving a conjecture by J. Bellissard)*, Operator algebras and mathematical physics (Constanča, 2001), 11-22, Theta, Bucharest, 2003.
J. Kaminker, I.F. Putnam, *A proof of the gap labeling conjecture*, Michigan Math. J., **51**, (2003), 537-546.
J. Bellissard, R. Benedetti, J.-M. Gambaudo, *Spaces of Tilings, Finite Telescopic Approximations and Gap-labeling*, Comm. Math. Phys., **261**, (2006), 1-41.

If the Delone set is repetitive and FLC, more can be said

Gap Labeling Theorem II. *If the Delone set describing the atomic positions is repetitive, completely aperiodic and FLC, then the gap labels are contained in the* $\mathbb{Z}$*-module defined by the occurrence probabilities of finite patches.*

V - Conclusion

- The Gap Labeling Theorem gives a labeling of gaps of self-adjoint operators. It is useful especially if the spectrum is a Cantor set.

- Gap labels are provided by the value of the Integrated Density of States on gaps.

- It is shown that the set of possible labels is model independent. It is given by the K_0-group (topology) of the algebra describing the structure of a solid.

- The labeling of a gap is robust under perturbation of the dynamics thanks to the homotopy invariance of gap labels.

- Sum rules apply thanks to the homotopy invariance of gap labels.