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

Main References


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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 \( \phi \) per unit cell, they satisfy

\[ U_1U_2U_1^{-1}U_2^{-1} = e^{2i\pi\phi/\phi_0} \]
- Magnetic translations: \( \phi_0 = \frac{h}{e} \) 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 $\omega_i$'s satisfy a diophantine condition

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

They found evidence (without proof) that the spectrum was a Cantor set.
I.3)- Moser’s Result


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

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 \textit{simple discrete unbounded spectrum} \( \text{Sp}(H) = \{\lambda_0 < \lambda_1 < \cdots < \lambda_n < \cdots\} \).

\textbf{Theorem[Liouville]} Let \( \varphi \) be a real solution of \(-\varphi''(x) + q(x)\varphi(x) = \lambda \varphi(x)\). If \( \lambda_{n-1} < \lambda \leq \lambda_n \), the function \( \varphi \) 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 $\lambda$ 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 $N(\lambda)$ (IDS) are defined by (if the limit exists)

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

Then

$$\rho(\lambda) = \pi N(\lambda)$$
$N(\lambda)$ is constant on the spectral gaps
II.2) The Johnson-Moser Gap Labeling Theorem


If \( q : \mathbb{R} \rightarrow \mathbb{R} \) 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 \( \omega \)'s. The frequency module of \( q \) is the group generated by the \( \omega \)'s.

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

\[ N(\lambda) \text{ belongs to the the frequency module of } q. \]
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 $\lambda$ per unit volume.

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

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

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

$\mathcal{T}$ is called the **Trace per Unit Volume**.
II.4)- K-theory: the Harper Model


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

Let $g = (E, E')$ 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 $P_g = f(H)$ is a *spectral projection* such that

$$P_g \in \mathcal{A}_\alpha$$

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** $\tau$ induces a group homomorphism $\tau_* : K_0(\mathcal{A}_\alpha) \mapsto \mathbb{R}$. The image is the countable subgroup $\mathbb{Z} + \alpha\mathbb{Z} \subset \mathbb{R}$. Moreover, $\tau$ 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.

III - Solids and Tilings

J. C. Lagarias, Geometric Models for Quasicrystals:

Constructing a Voronoi cell
III.1)- Periodic Crystals

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

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

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

$$\mathcal{B} = \mathbb{R}^d^*/G^\perp \cong G^*$$

$\mathcal{B}$ 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, ...) on a random Poissonian sublattice.

4. **Quasicrystals:** ex.: $\text{Al}_{62.5} \text{Cu}_{25} \text{Fe}_{12.5}$ or $\text{Al}_{70} \text{Pd}_{21} \text{Re}_9$ in the icosahedral phase.

5. **Others:** amorphous, glasses, liquids, etc..
III.3)- Point Sets

1. $\mathcal{L}$ is \textit{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 \textit{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 \textit{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 \textit{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 $\mathcal{M}(\mathbb{R}^d)$ be the space of Radon measures on $\mathbb{R}^d$ endowed with the \textit{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 \textit{Hull} $\Omega$ of $\mathcal{L}$ is the closure of the $\mathbb{R}^d$-orbit of $\nu_{\mathcal{L}}$. Its \textit{transversal} $\Xi$ 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 \(p = (\mathcal{L} - x) \cap B(0, R), \ x \in \mathcal{L}\).

\(\mathcal{L}\) 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)*.
A Delone set $\mathcal{L}$ is called *repetitive* whenever, given a patch $p$ and $\varepsilon > 0$, 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 $\varepsilon$ (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

$$a \in \mathbb{R}^d \quad \& \quad \mathcal{L} + a = \mathcal{L} \quad \Rightarrow \quad a = 0$$
IV - The Non-commutative Brillouin Zone
IV.1)- The $\mathcal{C}^*$-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 $\mathcal{C}^*$-algebra generated by the space of continuous functions on $\Omega$ and the action of $\mathbb{R}^d$ submitted to the commutation rules (for $f \in C(\Omega)$)

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

1. For a crystal $\Omega = \mathcal{V}$, $\mathbb{R}^d$ acts by quotient action.

2. $C(\mathcal{V}) \rtimes_{\tau} \mathbb{R}^d \simeq C(\mathbb{B}) \otimes \mathcal{K}$, 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 $A_0 = C_c(\Omega \times \mathbb{R}^d)$ will be endowed with (here $A, B \in A_0$)

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

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

- A faithfull family of representations in $\mathcal{H} = L^2(\mathbb{R}^d)$ (here $A \in A_0, \psi \in \mathcal{H}$)

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

- A $C^*$-norm $\|A\| = \sup_{\omega \in \Omega} \|\pi_\omega(A)\|$. 

**Definition 1** The $C^*$-algebra $\mathcal{A}$ is the completion of $A_0$ under this norm.
IV.3)- Calculus

• Integration

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

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

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

$$\mathcal{T}_\mathbb{P}(A) = \lim_{\Lambda \uparrow \mathbb{R}^d} \frac{1}{|\Lambda|} \text{Tr}(\pi_\omega(A) \uparrow \Lambda) \quad \mathbb{P}\text{-a.e. } \omega$$
A commuting set of ∗-derivations is given by

\[ \partial_i A(\omega, x) = ix_i A(\omega, x) \]

developed on \( \mathcal{A}_0 \). Then

\[ \pi_\omega(\partial_i A) = -𝑖[𝑋_𝑖, 𝜋_\omega(A)] \]

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

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

**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 $N_P$ on $\mathbb{R}$ defined by

$$\int_{\mathbb{R}} \frac{dN_P(E)}{z - E} = \mathcal{T} (R(z))$$

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

$$N_P(E) = \lim_{\Lambda \uparrow \mathbb{R}^d |\Lambda|} \frac{1}{|\Lambda|} \# \{\text{eigenvalues of } H_\omega \upharpoonright_{\Lambda} \leq E\}$$
The support of \( N_P \) is contained in the algebraic spectrum \( \Sigma \). If 
\( g = (E_-, E_+) \) is a spectral gap, let \( P_g \) be the spectral projection of \( H \) on \( (-\infty, E_-] \), so that

\[
  n_g = \mathcal{N}_P(E_- + 0) = \mathcal{N}_P(E_+ - 0) = \mathcal{T}(P_g) = \mathcal{T}^\ast([P_g])
\]

**Fact:** \( P_g \) 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


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.