1D-Quantum Systems
(1980-1993)
a review

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Main References

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I - The Situation in 1980
The 1D discrete Schrödinger eigenvalue equation
\[ \psi(n + 1) + \psi(n - 1) + V_n \psi(n) = E \psi(n) \]
can be written as
\[ \Phi_{n+1} = \begin{bmatrix} \psi(n + 1) \\ \psi(n) \end{bmatrix} = \begin{bmatrix} E - V_n & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \psi(n) \\ \psi(n - 1) \end{bmatrix} = M_n \Phi_n \]

The matrix \( M_n \) is called the transfer matrix.

If, for instance, \( V_{n+p} = V_n \) is periodic, then the Floquet matrix
\[ F = M_p M_{p-1} \cdots M_1 \]
defines the behaviour of the wave function \( \psi \) at infinity, in terms of the energy \( E \).
Aperiodic Potentials

In 1979, the following potentials were under scrutiny

- the $V_n$’s are *i.i.d. random variables* for which the spectrum is pure point, *(Pastur ’73, Goldsheid-Molchanov-Pastur ’78, Kunz-Souillard ’79)*

- the sequence $(V_n)_{n \in \mathbb{Z}}$ is *quasiperiodic*: at small coupling, the *KAM theorem* applies and gives a large a.c. spectrum *(Dinaburg-Sinai ’75, for the continuum)*

- There is a class of bounded non-decreasing potential leading to a purely s.c. spectrum, *(Jona-Lasinio, Martinelli, Scoppola, ’79)*
The Harper and Almost-Mathieu models

• For the almost-Mathieu equation $V_n = 2\lambda \cos 2\pi n \alpha$, $\alpha \notin \mathbb{Q}$, Aubry’s duality predicts a transition between a.c. spectrum for $|\lambda| < 1$ to p.p. spectrum for $|\lambda| > 1$, (Aubry-André ‘78)

• The Lebesgue measure of the spectrum of the almost-Mathieu equation is $4|\lambda - 1|$, (numerical result of Aubry-André ‘78)

• The spectrum of the Harper equation looks Cantorian, self similar and the gap edges look continuous in $\alpha$ (numerical calculation Hofstadter ‘76)
• The gaps of the Hofstadter spectrum can be labeled by integers
  (Claro-Wannier, ’78),
  (the coloring encoding the labels is due to Osadchy-Avron ’01)
II - Formalism

\[(H_c \psi)(x) = -\psi''(x) + V(x)\psi(x) \quad \text{on} \quad L^2(\mathbb{R})\]

\[(H\psi)(n) = \psi(n + 1) + \psi(n - 1) + V_n\psi(n) \quad \text{on} \quad \ell^2(\mathbb{Z})\]
Tight Binding Representation


• Correspondence between the continuum Schrödinger equation and an equivalent discrete one, through a transfer matrix over some unit length; example of a Krönig-Penney model: the French connection (Bellissard-Formoso-Lima-Testard '81)

• Analogy with the Poincaré section in dynamical system; the inverse operation is called suspension

• Same operation as the tight-binding representation in Solid State Physics

• This can be extended to higher dimension, also in the context of $C^*$-algebras through the notion of Morita equivalence
The Hull

- If the sequence $\xi_0 = (V_n)_{n \in \mathbb{Z}}$ is bounded by $C$, its **Hull** is the closure $\Xi$ of its orbit under the shift $t\xi_0 = (V_{n-1})_{n \in \mathbb{Z}}$, in the compact metrizable space $[-C, C]^\mathbb{Z}$.

- The pair $(\Xi, t)$ is a **topological dynamical system**, a $\mathbb{Z}$-action on $\Xi$ by homeomorphisms.

- There is a **continuous** function $v : \Xi \to \mathbb{R}$ such that $V_n = v(t^{-n}\xi_0)$.

- Any point in the Hull $\xi \in \Xi$ defines a potential $V_\xi(n) = v(t^{-n}\xi)$, which satisfies $T^nV_\xi T^{-n} = V_{T^n\xi}$, ($T$ is the translation operator on $\ell^2(\mathbb{Z})$).
Groupoid

The set $\Gamma_\Xi = \Xi \times \mathbb{Z}$ can be seen as a locally compact groupoid as follows

- **Set of units:** $\Gamma^{(0)} = \Xi$
- **Range and Source:** $r(\xi, n) = \xi$, $s(\xi, n) = T^{-n}\xi$
- **Product:** $(\xi, m) \circ (T^{-m}\xi, n) = (\xi, m + n)$
- **Inverse:** $(\xi, n)^{-1} = (T^{-n}\xi, -n)$
The convolution algebra on the space $C_c(\Xi \times \mathbb{Z})$ of continuous functions with compact support is defined as follows

- **Product:** $fg(\xi, n) = \sum_{m \in \mathbb{Z}} f(\xi, m)g(T^{-m}\xi, n - m)$
- **Adjoint:** $f^*(\xi, n) = f(T^{-n}\xi, -n)$
- **Representation:** on $\ell^2(\mathbb{Z})$

\[
(\pi_\xi(f)\psi)(n) = \sum_{m \in \mathbb{Z}} f(T^{-n}\xi, m - n) \psi(m)
\]

- **Covariance:** $T\pi_\xi(f)T^{-1} = \pi_{T\xi}(f))$
- **$C^*$-norm:** $\|f\| = \sup_{\xi \in \Xi} \|\pi_\xi(f)\|$

The completion is denoted by $\mathcal{A} = C^*(\Gamma_\Xi) = C(\Xi) \rtimes \mathbb{Z}$. 

**$C^*$-algebra**
• **Hamiltonian:** \( h(\xi, n) = \delta_{n,1} + \delta_{n,-1} + \delta_{n,0} \nu(\xi) \)

\[ \pi_\xi(h) = H_\xi \Rightarrow \left( H_\xi \psi \right)(n) = \psi(n + 1) + \psi(n - 1) + V_\xi(n)\psi(n) \]

• **Trace:** if \( \mathbb{P} \) is a \( \mathbb{Z} \)-invariant *ergodic* probability on \( \Xi \), then

\[ T_\mathbb{P}(f) = \int_\Xi f(\xi, 0) \mathbb{P}(d\xi) = \lim_{L \to \infty} \frac{1}{2L} \text{Tr}_{[-L,L]}(\pi_\xi(f)) \quad \mathbb{P}\text{-a.s.} \]

• **Shubin’s formula:** The integrated density of state is given by

\[ \mathcal{N}(E) = T_\mathbb{P}(\chi(h \leq E)) \]
Gap labeling Theorem


• **$K_0$-group:** it is the Grothendieck group generated by (unitary) equivalence classes of projections in $\bigcup_{n \in \mathbb{N}} \mathcal{A} \otimes M_n(\mathbb{C})$ with addition given by the *direct sum*. $K_0$ is *countable abelian*. The equivalence class $[P]$ of a projection is *homotopy invariant*.

• **Gap labels:** The trace on $\mathcal{A}$ induces a group homomorphism $\tau : K_0(\mathcal{A}) \rightarrow \mathbb{R}$. The image $\tau(K_0(\mathcal{A}))$ is the set of *gap labels*.

• **Algebraic spectrum:** $\text{Sp}_\mathcal{A}(h) = \bigcup_{\xi \in \Xi} \text{Sp}(H_\xi) = \text{Sp}(H_{\xi_0})$

• **Spectral gaps:** If $S$ is a clopen subset in $\text{Sp}(h)$ the spectral projection $P_S = \chi(h \in S)$ belongs to $\mathcal{A}$. The IDS on this gap is $\tau([P_S])$.

• **Sum rule:** if $S = S_1 \cup S_2$ with $S_1 \cap S_2 = \emptyset$ and $S_i$ clopen, then $[P_S] = [P_{S_1}] + [P_{S_2}]$. 
The number $\Phi_{\xi}(n) = \psi(n) + i\psi(n - 1)$ does not vanish if $\psi \neq 0$ is a solution of the Schrödinger equation. If $E$ is in a gap, there is a unique solution $\Phi_{\xi,\pm}$ (up to a multiplicative constant) vanishing at $\pm\infty$.

If $\theta_{\xi,\pm}(n)$ is the argument of $\Phi_{\xi,\pm}(n)$

$$N(E) = \tau([P_E]) = \frac{1}{\pi} \int_\Xi \left( \theta_{\xi,\pm}(1) - \theta_{\xi,\pm}(0) \right) P(d\xi)$$

No analog of this formula is available in higher dimension.
III - Cantor Spectra
Moser’s Result

• Cantor spectrum: A limit periodic potential of the form

\[ V(x) = a_0 + \sum_{k \in \mathbb{N}} a_{k,l} \cos\left(\frac{2\pi lx}{2^k}\right) + b_{k,l} \sin\left(\frac{2\pi lx}{2^k}\right) \]

leads to a Cantor spectrum for a generic choice of the Fourier coefficients in the uniform topology.

• Gap Labels: The IDS on the gaps has the form \( l/2^k \), \( l, k \in \mathbb{N} \).

• a.c spectrum: if the Fourier coefficient of \( V \) decay fast enough the spectrum is a.c. (Gordon ‘76)
The Almost-Mathieu model


• For $\lambda \neq 0$ and $\alpha \notin \mathbb{Q}$, the spectrum of the almost-Mathieu Hamiltonian is a Cantor set.

• The Lebesgue measure of the spectrum is $4|\lambda - 1|$ for $\alpha \notin \mathbb{Q}$.

• $\lambda \neq 0$ and $\alpha \notin \mathbb{Q}$ the gap labels are given by $n\alpha - [n\alpha]$ for some $n \in \mathbb{Z}$ and all gaps but for the central one at $E = 0$ are open.

• The gap edges are Lipschitz continuous in $\alpha$ as long as the gap does not close, and are Hölder continuous with exponent $1/2$ otherwise.

• The gap edges are left and right differentiable near any rational $\alpha$ and the two derivatives are distinct and computable explicitly.
1D-quasicrystals


• \( V(n) = \lambda \) if \( n\alpha \in (0, \alpha] \mod 1 \) and \( V(n) = 0 \) otherwise. This leads to two values of the transfer matrix, called \( A, B \)

• For \( \alpha = (\sqrt{5} - 1)/2 \), the transfer matrix can be computed from the substitution \( A \rightarrow BA \), \( B \rightarrow A \).

• Note that \( \det(A) = \det(B) = 1 \).
The three variables $x = \text{Tr}(A), y = \text{Tr}(B), z = \text{Tr}(AB)$ are sufficient to compute the spectrum. Under the substitution, it becomes (trace map)

$$x_{n+1} = z_n, \quad y_{n+1} = x_n, \quad z_{n+1} = x_nz_n - y_n$$

$I(x, y, z) = x^2 + y^2 + z^2 - xyz$ is invariant by substitution.

The spectrum is the set of $E$'s such that $(x_n, y_n, z_n)$ stay bounded.

The spectral measure is purely s.c. for $\lambda \neq 0, \alpha \notin \mathbb{Q}$ and the spectrum has zero Lebesgue measure.

Estimates on the Hausdorff dimension of the spectrum are available (Damanik et al. '10)
Spectrum of the 1D-quasicrystal

Horizontal axis $E$, vertical axis $0 \leq \alpha \leq 1$

(after Ostlundt, Kim '85)
Are there potential that are not almost periodic

leading to a Cantor spectrum?
The Thue-Morse model

J. Bellissard, *Spectral properties of Schrödinger’s operator with a Thue-Morse potential.*

- The Thue-Morse sequence is obtained from the substitution $A \rightarrow BA$, $B \rightarrow AB$ and a trace map.
- The corresponding sequence $(V_n)_{n \in \mathbb{Z}}$ is not almost periodic (Kakutani ’54)
- If $\lambda \neq 0$, the Thue-Morse model has a Cantor spectrum with zero Lebesgue measure. The spectral measure is s.c.
- The gap edges are computable in terms of a nonlinear implicit equation.
- Gap labels: $l/(3 \cdot 2^k)$ for $l, k \in \mathbb{N}$. Gaps with $l = 0 \mod 3$ are closed.
- For gap width behave like $|\lambda|^{\sigma}$, $|\lambda| \downarrow 0$ for some $\sigma > 0$. 
Gap labeling for substitution sequences

- **Data:** a finite alphabet $\mathcal{A}$, the set $\mathcal{W}_k$ of words of length $k$, $\mathcal{W}$, set of finite words, $\mathcal{W}_*$ the set of infinite sequences of letters.

- **Potential:** if $\text{ev} : \mathcal{A} \rightarrow \mathbb{R}$, any sequence $(V_n)_{n \in \mathbb{Z}}$ with $V_n \in \text{ev}(\mathcal{A})$.

- If $\mathbb{P}$ is an ergodic probability of the Hull of the previous $V$, the set of gap labels is the $\mathbb{Z}$-module generated by the occurrence probabilities of all finite words in $V$.

- **Substitution:** $\sigma : \mathcal{A} \rightarrow \mathcal{W}$ extended as a map $\sigma : \mathcal{W}_* \rightarrow \mathcal{W}_*$ by concatenation.

- **Extension:** $\sigma_k$ is the substitution induced by $\sigma$ on the set of words of length $k$. 
• **Regularity:** \( \sigma \) is *regular* if (i) the substitution is primitive, (ii) the length of \( \sigma^n(a) \) diverges as \( n \to \infty \), (iii) there is a letter \( 0 \in \mathcal{A} \) such that \( \sigma(0) = w0w' \) with \( w, w' \) non empty words.

If \( \sigma \) is regular, there is a unique infinite sequence \( \underline{u} \) such that \( \sigma(\underline{u}) = \underline{u} \). Through ev this gives a potential.

• **Matrices:** If \( a, b \in \mathcal{A}_k \) let \( M_{ba}^{(k)} \) be the number of occurrences of \( b \) in \( \sigma_k(a) \). The Perron-Frobenius eigenvalue \( \theta \) of \( M^{(k)} \) is the same for all \( k \)'s. *(Queffelec '87)*

• **Gap Labels:** the set of gap labels for a potential coming from a regular substitution is the \( \mathbb{Z}[\theta^{-1}] \)-module generated by the coordinates of the Perron-Frobenius normalized vectors of \( M \) and \( M^{(2)} \). *(Bellissard '93)*
VI - Open Problems

\[(H_\xi \psi)(n) = \psi(n + 1) + \psi(n - 1) + \lambda V_\xi(n)\psi(n),\]

\[\lambda \geq 0\]
Gap Opening

The $IDS$ at $\lambda = 0$ is

$$N_0(E) = \frac{1}{\pi} \arccos \left( \frac{E}{2} \right) \iff E = 2 \cos \pi N_0(E)$$

The set of *gap labels* give the energies at which values of $E$ a gap may open as $\lambda > 0$.

- **Problem # 1:** find the condition on $V$ for gaps with a given label to open.
- **Problem # 2:** find a theory predicting the *asymptotic gap widths* at $\lambda \downarrow 0$. (Luck ‘89)
Entropy

Let the dynamical system \((\mathcal{X}, \tau)\) have positive topological entropy

- **Problem # 3:** prove or disprove that the Schrödinger operator has only a **finite number of gaps**.

  *(Note: if the set of periodic orbit is dense this is known. What about minimal \(\mathbb{Z}\)-action with positive entropy ?)*

- **Problem # 4:** prove or disprove that the Schrödinger operator has **pure point spectrum**. *(see Simon-Wolf ’86, Damanik & Avila ’10)*

- **Problem # 5:** same problem with algorithmic complexity larger than 1 *(see Levitov ’88)*
For $\lambda = 0$ an expression of the form

$$C(t) = \langle \psi | e^{itH} \psi \rangle = \int_T |\psi(k)|^2 e^{ith(k)} \, dk$$

admits an asymptotic expansion as $t \uparrow \infty$ depending only upon the nature of the local singularities of the Fourier transform $h$ of $H$. Malgrange used the Gauss-Manin connection to derive this expansion systematically.

**Problem #6:** is there an analog of the Gauss-Manin connection liable to predict the asymptotic behavior of $C(t)$ if a potential is added?