1*D*-Quantum Systems

(1980-1993)

a review

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Main References

M. Kohmoto, L.P. Kadanoff, C. Tang,
Localization problem in one dimension: mapping and escape,
Phys. Rev. Lett., **50**, (1983), 1870-1872.

S. Ostlund, R. Pandit, D. Rand, H.J. Schellnhuber, E.D Siggia,
One dimensional Schrödinger equation with an almost periodic potential,
Phys. Rev. Lett., **50**, (1983), 1873-1877.

J. Bellissard,
Gap Labeling 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).

Content

1. History: the situation in 1980.
2. Formalism
3. Cantor Spectra
4. Open Problems

I - The Situation in 1980

Transfer Matrix

L. Brillouin, J. Phys. Radium **7**, (1926), 353-368.

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 ψ 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)*

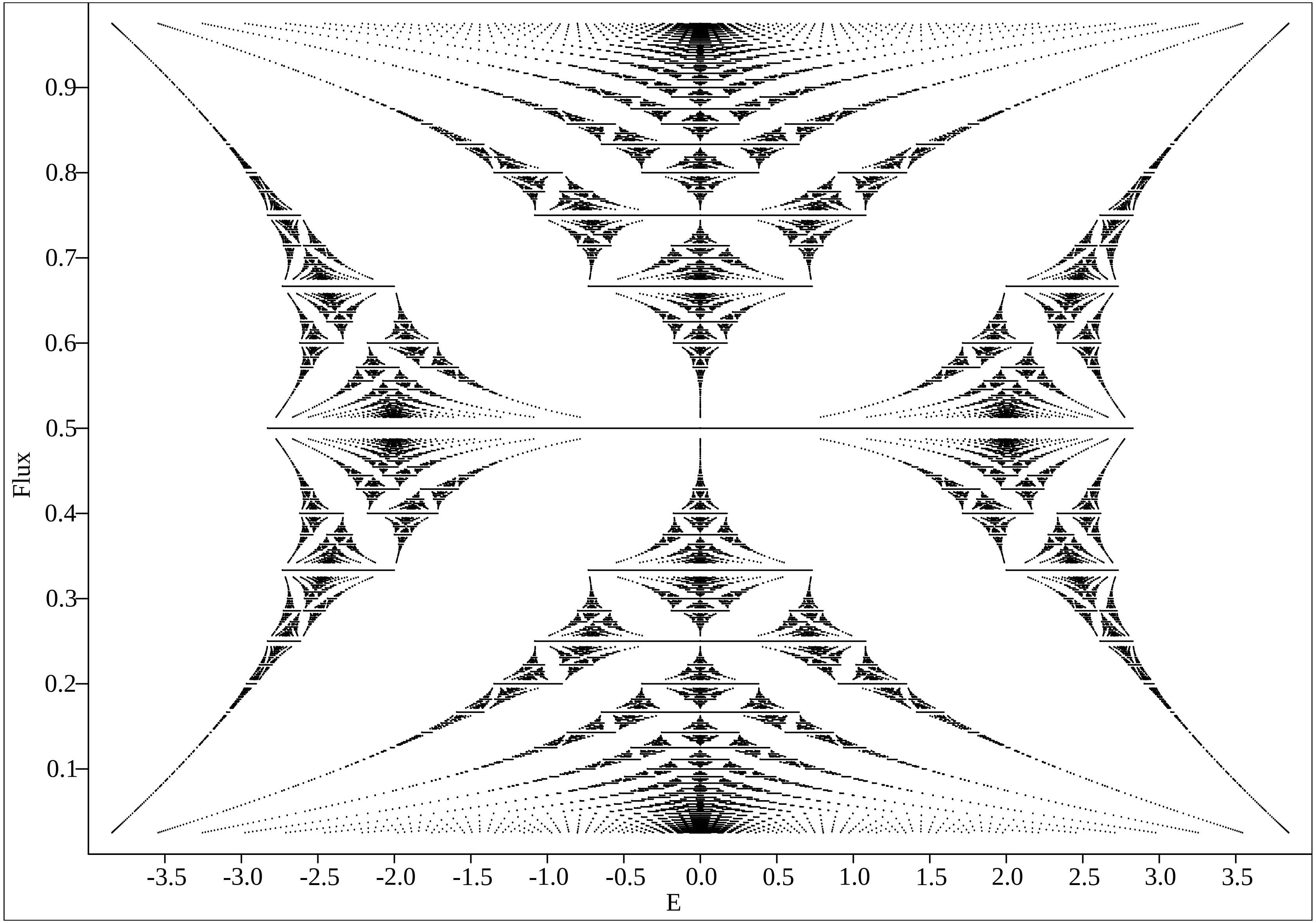
The Harper and Almost-Mathieu models

- 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 α

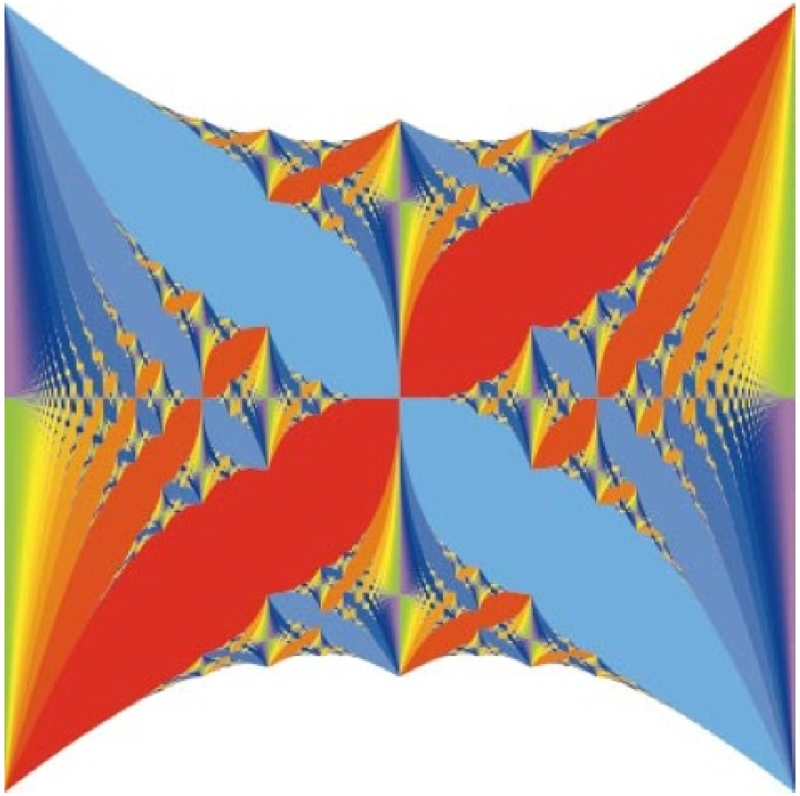
  (numerical calculation Hofstadter '76)



0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
Flux
-3.5 -3.0 -2.5 -2.0 -1.5 -1.0 -0.5 0.0 0.5 1.0 1.5 2.0 2.5 3.0 3.5
E

- 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

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

$$(H\psi)(n) = \psi(n+1) + \psi(n-1) + V_n\psi(n) \qquad \text{on } \ell^2(\mathbb{Z})$$

Tight Binding Representation

J. Bellissard, Lecture Notes in Physics, **257**, 99-156, (1986)

- 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

J. BELLISSARD, Lecture Notes in Physics, **257**, 99-156, (1986)

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

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

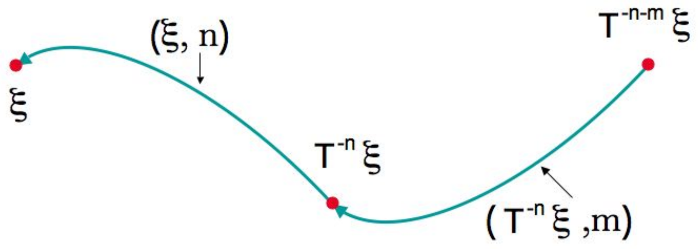
- There is a *continuous* function $v : \Xi \to \mathbb{R}$ such that $V_n = v(\mathrm{T}^{-n}\xi_0)$.

- Any point in the Hull $\xi \in \Xi$ defines a potential $V_\xi(n) = v(\mathrm{T}^{-n}\xi)$, which satisfies $T^n V_\xi T^{-n} = V_{\mathrm{T}^n\xi}$, *($T$ 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:** $r(\xi, n) = \xi, \;\; s(\xi, n) = \mathrm{T}^{-n}\xi$
- **Product:** $(\xi, m) \circ (\mathrm{T}^{-m}\xi, n) = (\xi, m + n)$
- **Inverse:** $(\xi, n)^{-1} = (\mathrm{T}^{-n}\xi, -n)$



C^*-algebra

The *convolution algebra* on the space $C_c(\Xi \times \mathbb{Z})$ of continuous functions with compact support is defined as follows

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

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

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

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

- **Hamiltonian:** $h(\xi, n) = \delta_{n,1} + \delta_{n,-1} + \delta_{n,0}\, v(\xi)$

$$\pi_\xi(h) = H_\xi \quad \Rightarrow \quad \big(H_\xi \psi\big)(n) = \psi(n+1) + \psi(n-1) + V_\xi(n)\psi(n)$$

- **Trace:** if $\mathbb{P}$ is a $\mathbb{Z}$-invariant *ergodic* probability on Ξ, then

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

- **Shubin's formula:** The integrated density of state is given by

$$\mathcal{N}(E) = \mathcal{T}_{\mathbb{P}}\left(\chi(h \leq E)\right)$$

Gap labeling Theorem

J. Bellissard, Lecture Notes in Physics, **153**, 356-359, (1982).

- 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 $\tau : K_0(\mathcal{A}) \to \mathbb{R}$. The image $\tau(K_0(\mathcal{A}))$ is the set of *gap labels*.
- **Algebraic spectrum:** $\mathrm{Sp}_{\mathcal{A}}(h) = \bigcup_{\xi\in\Xi} \mathrm{Sp}(H_\xi) = \mathrm{Sp}(H_{\xi_0})$
- **Spectral gaps:** If S is a clopen subset in $\mathrm{Sp}(h)$ 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 $[P_S] = [P_{S_1}] + [P_{S_2}]$.

Rotation Number

R. Johnson, J. Moser, Comm. Math. Phys., **84**, (1982), 403-438.

- The number $\Phi_\xi(n) = \psi(n) + \imath\psi(n-1)$ 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 $\Phi_{\xi,\pm}(n)$

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

- No analog of this formula is available in higher dimension.

III - Cantor Spectra

Moser's Result

J. Moser, Comment. Math. Helv., **56**, (1981), 198-224.
A.Ya. Gordon, Usp. Ma. Nauk., **31**, (1976), 257-258.

- **Cantor spectrum:** A limit periodic potential of the form

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

  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

J. Bellissard, B. Simon, J. Funct. Ana., **48**, (1982), 408-419.

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A. Avila, S. Jitomirskaya, Ann. of Math., **170**, (2009), 303-342.

- 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 Lipshitz continuous in α 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 α and the two derivatives are distinct and computable explicitly.

1D-quasicrystals

M. Kohmoto, L.P. Kadanoff, C. Tang, Phys. Rev. Lett., **50**, (1983), 1870-1872.
S. Ostlund, R. Pandit, D. Rand, H.J. Schellnhuber, E.D Siggia, Phys. Rev. Lett., **50**, (1983), 1873-1877.
S. Ostlund, S. Kim, Physica Scripta, **9**, (1985), 193-198.
M. Casdagli, Commun. Math. Phys., **107**, (1986), 295-318.
A. Sütò, Commun. Math. Phys., **111**, (1987), 409-415.
J. Bellissard, B. Iochum, E. Scoppola, D. Testard, Commun. Math. Phys., **125**, (1989), 527-543.

- $V(n) = \lambda$ 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 $A \to BA\,,\; B \to A$.
- Note that $\det(A) = \det(B) = 1$.

- The three variables $x = \mathrm{Tr}\,(A), y = \mathrm{Tr}\,(B), z = \mathrm{Tr}\,(AB)$ are sufficient to compute the spectrum. Under the substitution, it becomes *(trace map)*

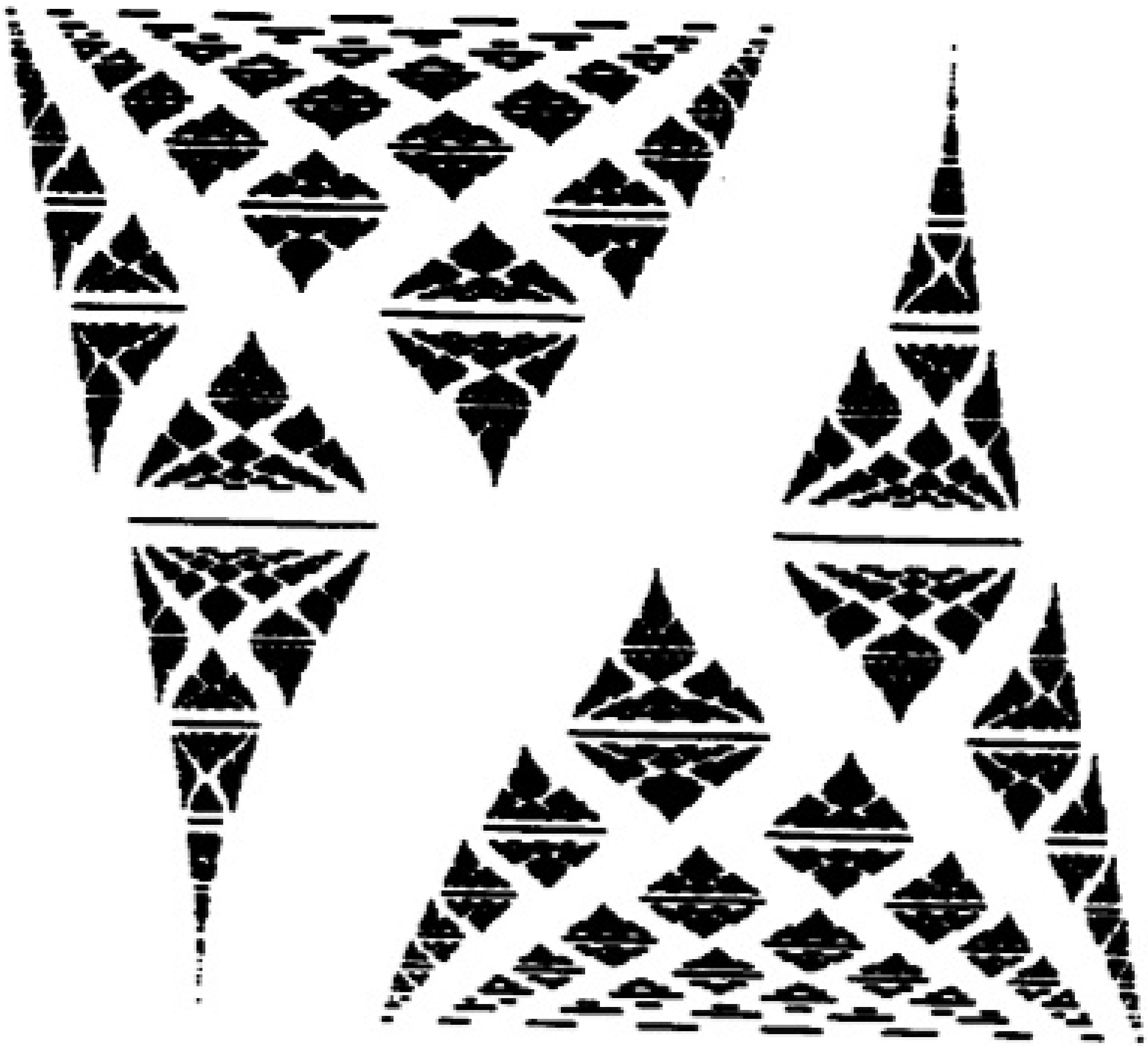
$$x_{n+1} = z_n\,, \quad y_{n+1} = x_n\,, \quad z_{n+1} = x_n z_n - y_n$$

- $I(x, y, z) = x^2 + y^2 + z^2 - xyz$ 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.* In *Number theory and physics*, (J.M. Luck, P. Moussa, M. Waldschmidt, eds.) Springer Proc. in Phys. **47** (1990).

- The Thue-Morse sequence is obtained from the substitution $A \to BA\,,\ B \to AB$ 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 $l = 0 \bmod 3$ 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* $\mathscr{A}$, the set $\mathscr{W}_k$ of words of length k, $\mathscr{W}$, set of finite words, $\mathscr{W}_*$ the set of infinite sequences of letters.
- **Potential:** if $\mathrm{ev} : \mathscr{A} \to \mathbb{R}$, any sequence $(V_n)_{n\in\mathbb{Z}}$ with $V_n \in \mathrm{ev}(\mathscr{A})$.

- 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:** $\sigma : \mathscr{A} \to \mathscr{W}$ extended as a map $\sigma : \mathscr{W}_* \to \mathscr{W}_*$ by *concatenation*.
- **Extension:** σ_k is the substitution induced by σ on the set of words of length k.

- **Regularity:** σ is *regular* if (i) the substitution is primitive, (ii) the length of $\sigma^n(a)$ diverges as $n \uparrow \infty$, (iii) there is a letter $0 \in \mathscr{A}$ such that $\sigma(0) = w0w'$ with w, w' non empty words.

  If σ 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 $a, b \in \mathscr{W}_k$ let $M^{(k)}_{ba}$ be the number of occurrences of b in $\sigma_k(a)$. The Perron-Frobenius eigenvalue θ 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

$$\left(H_\xi \psi\right)(n) = \psi(n+1) + \psi(n-1) + \lambda V_\xi(n)\psi(n)\,,$$

$$\lambda \geq 0$$

Gap Opening

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

$$\mathcal{N}_0(E) = \frac{1}{\pi}\ \text{arccos}\left(\frac{E}{2}\right) \quad \Leftrightarrow \quad E = 2\cos\pi\mathcal{N}_0(E)$$

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 (Ξ, τ) 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)*

Spectrum and Transport Exponents

B. MALGRANGE, Ann. scient. Éc. Norm. Sup., **7**, (1974), 405-430.

For $\lambda = 0$ an expression of the form

$$C(t) = \langle \psi | e^{\imath t H} \psi \rangle = \int_{\mathbb{T}} |\psi(k)|^2 \, e^{\imath t h(k)} \, dk$$

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 ?