Periodic Approximants to Aperiodic Hamiltonians

Jean BELLISSARD

Westfälische Wilhelms-Universität, Münster
Department of Mathematics

Georgia Institute of Technology, Atlanta
School of Mathematics & School of Physics
e-mail: jeanbel@math.gatech.edu

Sponsoring

CRC 701, Bielefeld, Germany

SFB 878, Münster, Germany

Contributors

G. De Nittis, *Facultad de Matemáticas*, Pontifica Universidad Católica de Chile, Santiago, Chile

S. Beckus, *Mathematisches Institut*, Friedrich-Schiller-Universität Jena, Germany
Department of Mathematics, Technion, Haifa, Israel

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U.C. Irvine, May 15-19, 2013
WCOAS, UC Davis, October 26, 2013
online at `http://people.math.gatech.edu/~jeanbel/talksjbE.html`

Content

Warning *This talk is reporting on a work in progress.*

1. The Bloch-Floquet Theory
2. Aperiodicity
3. Continuous Fields
4. Dynamical Systems
5. Periodic Approximations for Subshifts

I - The Bloch-Floquet Theory

The Goal

- Compute the spectrum of the *Schrödinger operator* describing the electron motion in a solid

$$H = -\frac{\hbar^2}{2m}\Delta + \sum_a \sum_{x \in \mathcal{L}_a} v_a(\cdot - x) \qquad \text{acting on} \qquad \mathcal{H} = L^2(\mathbb{R}^d)$$

  - a labels the *atomic species*
  - $\mathcal{L}_a$ denotes the sets of *positions* of atoms of type a
  - v_a is the *atomic potential* around an atom of type a

The Goal

- **Tight-binding representation:** if $\psi \in \mathcal{H} = \bigoplus_a \ell^2(\mathcal{L}_a)$

$$(H\psi)_a(x) = \sum_b \sum_{y \in \mathcal{L}_b} t_{ab}(x,y)\, \psi_b(y)$$

The wave function representing the electron is *peaked at each atom* with amplitude $\psi_a(x)$ if $x \in \mathcal{L}_a$.

Periodic Materials: Crystals

- There is a *co-compact discrete* subgroup $G \subset \mathbb{R}^d$ such that translations by elements of G leave the sets $\mathcal{L}_a$ *invariant* for all a's.
- G is *unitarily* represented in $\mathcal{H}$ and $U(g)HU(g)^{-1} = H$
- *Diagonalizing simultaneously* U and H leads to

$$\mathcal{H} = \int_{\mathbb{B}}^{\oplus} \mathcal{H}_k \, dk \qquad\qquad H = \int_{\mathbb{B}}^{\oplus} H_k \, dk$$

  - $\mathbb{B}$ is the Pontryagin dual of G, called *Brillouin zone*,
  - $\mathcal{H}_k = L^2(\mathbb{R}^d/G)$ or $\mathcal{H}_k = \bigoplus_a \ell^2(\mathcal{L}_a/G)$,
  - H_k is the restriction of H to $\mathcal{H}_k$ with k-dependent boundary conditions (*Bloch boundary conditions)*.

Periodic Materials: Crystals

- In general, H_k has a *discrete* spectrum depending smoothly on k.
- The maps $k \in \mathbb{B} \to E(k) \in \mathbb{R}$ representing the eigenvalues are called *bands*.
- The spectrum of H is the union of the image $E(\mathbb{B})$ over all bands. It is a union of intervals possibly separated by *gaps*.

II - Aperiodicity

Aperiodic Media

- Crystals in a magnetic field *(Peirls, 1933; Harper, 1955; Hofstadter, 1976)*.

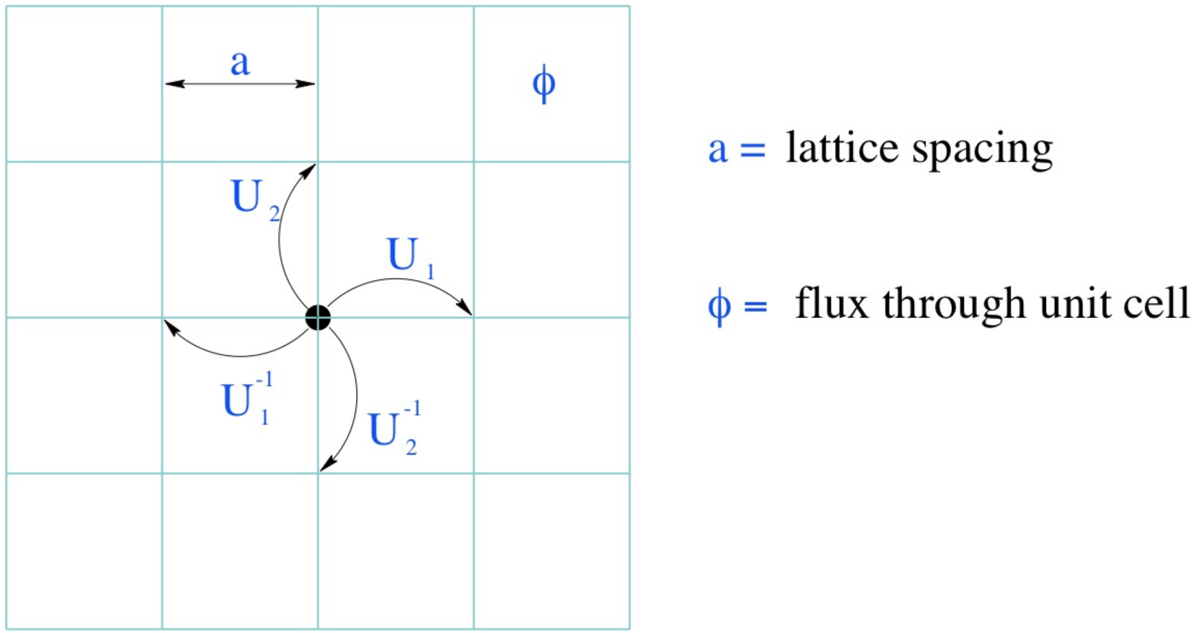
- Amorphous materials, silicon, metallic glasses, even liquids.

- Disordered systems: semiconductors at very low temperature. Anderson weak and strong localization *(Anderson, 1958)*.

- Quasicrystal *(Shechtman et al., 1984)*.

The Harper Model

- Perfect *square lattice*, nearest neighbor hoping terms, *uniform magnetic field* B perpendicular to the plane of the lattice
- Translation operators U_1, U_2



The Harper Model

- Commutation rules *(Rotation Algebra)*

$$U_1\, U_2 = e^{2\imath\pi\alpha}\, U_2\, U_1 \qquad \alpha = \frac{\phi}{\phi_0} \qquad \phi = Ba^2 \quad \phi_0 = \frac{h}{e}$$

- Kinetic Energy *(Hamiltonian)*

$$H = t\left(U_1 + U_2 + U_1^{-1} + U_2^{-1}\right)$$

- Landau gauge $\psi(m,n) = e^{2\imath\pi mk}\varphi(n)$.
  Hence $H\psi = E\psi$ means

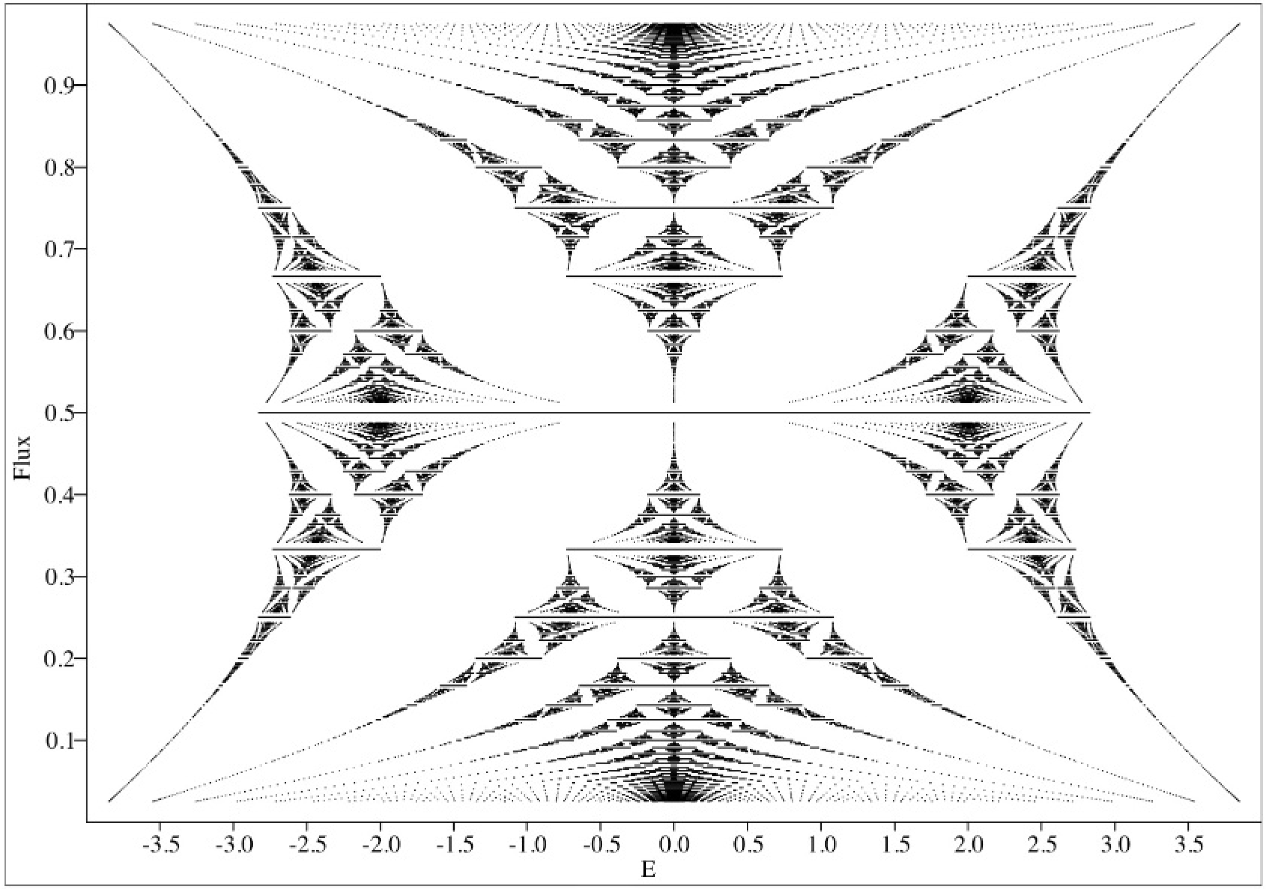
$$\varphi(n+1) + \varphi(n-1) + 2\cos 2\pi(n\alpha - k)\varphi(n) = \frac{E}{t}\,\varphi(n)$$

The Harper Model

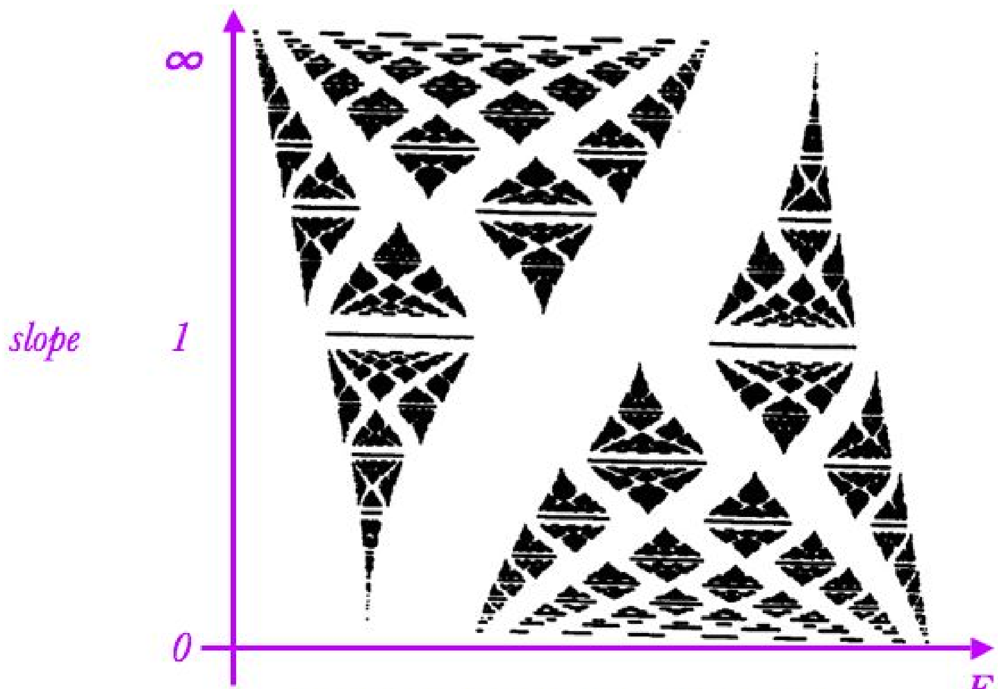
PHYSICAL REVIEW B VOLUME 14, NUMBER 6 15 SEPTEMBER 1976

Energy levels and wave functions of Bloch electrons in rational and irrational magnetic fields*

Douglas R. Hofstadter†
Physics Department, University of Oregon, Eugene, Oregon 97403
(Received 9 February 1976)



1D-Quasicrystals



Energy spectrum for particle in a 1D-quasicrystal as a function of the slope in a cut-and-project scheme

Physica Scripta. Vol. T9, 193–198, 1985

Renormalization of Quasiperiodic Mappings

Stellan Ostlund and Seung-hwan Kim

Spectrum of the Kohmoto model
(Fibonacci Hamiltonian)

$$(H\psi)(n) = \psi(n+1) + \psi(n-1) + \lambda\, \chi_{(0,\alpha]}(x - n\alpha)\, \psi(n)$$

as a function of α.

Method:
transfer matrix calculation

2D-Quasicrystals

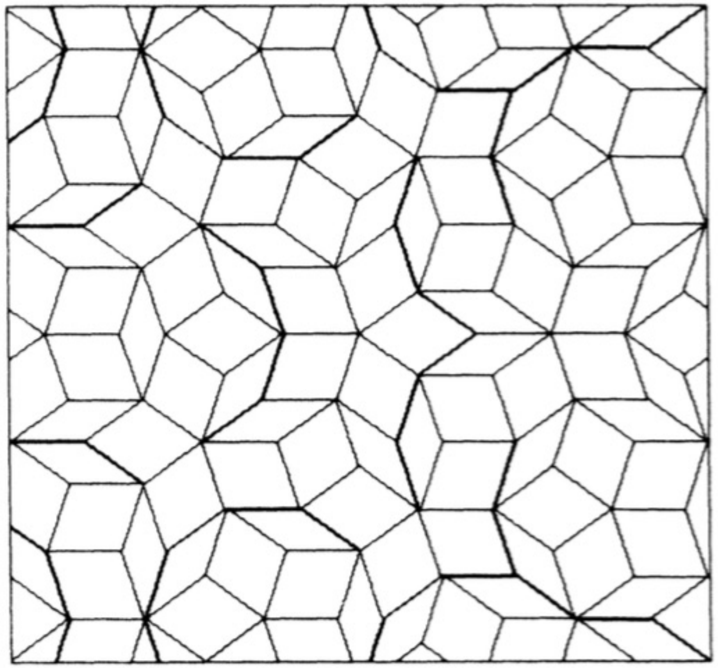


FIG. 1. A section of a Penrose lattice. The center of the pattern is the center of the figure, and the ten tiles at the center are the seed from which the pattern was grown.

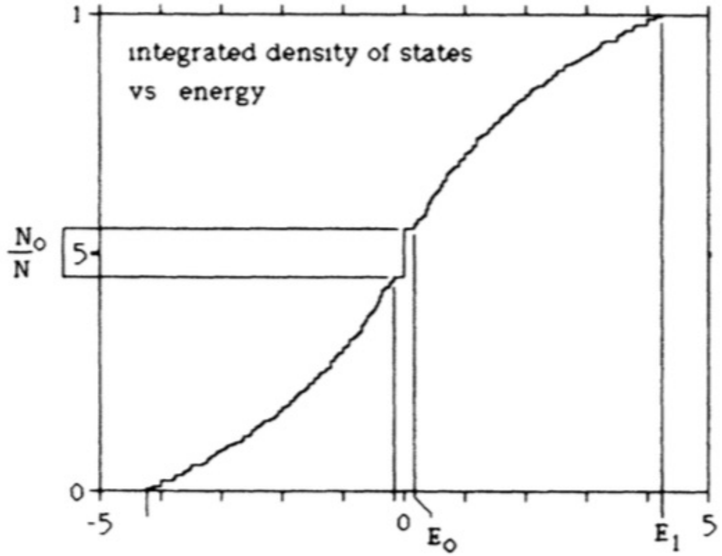


FIG. 2. The integrated density of states, normalized to unity, as a function of energy. This is for the lattice inflated five times, with 1211 lattice sites. The quantities N_0/N, E_0, and E_1 are shown here.

VOLUME 56, NUMBER 25 PHYSICAL REVIEW LETTERS 23 JUNE 1986

Electronic States on a Penrose Lattice

Mahito Kohmoto and Bill Sutherland
Deparment of Physics, University of Utah, Salt Lake City, Utah 84112
(Received 13 January 1986)

2D-Quasicrystals

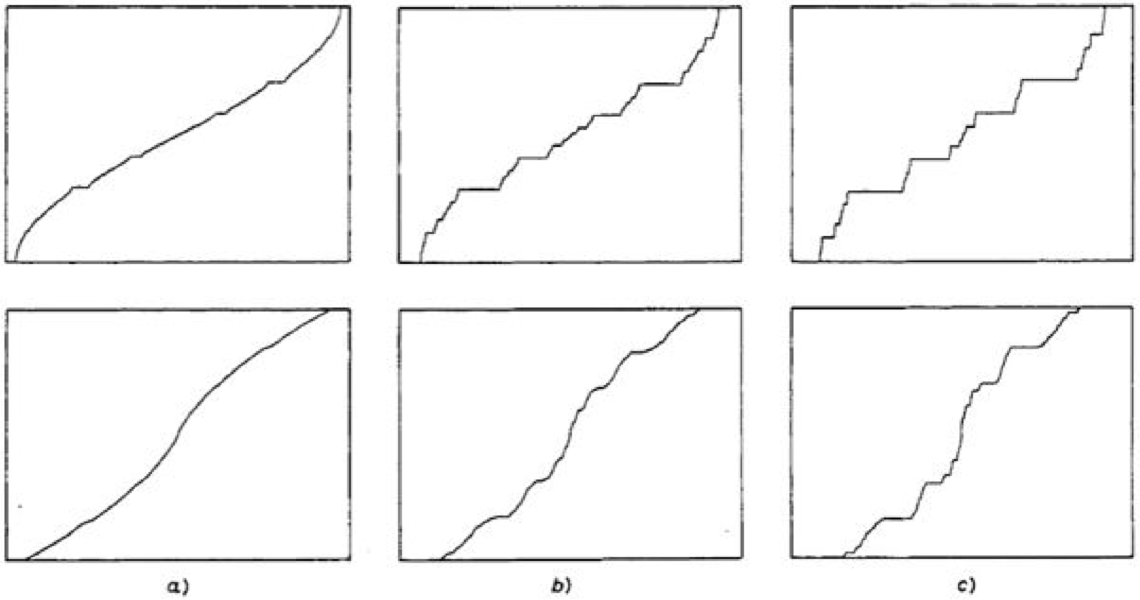


Fig. 3. – We show, respectively, the IDOS of the Octonacci chain (up) and the IDOS of the labyrinth, for *a*) $r = 0.8$ (no gap, finite measure), *b*) $r = 0.6$ (some gaps and finite measure) and *c*) $r = 0.3$ (infinity of gaps and zero measure). The energy varies between -2 and 2, since $r < 1$.

C. Sire

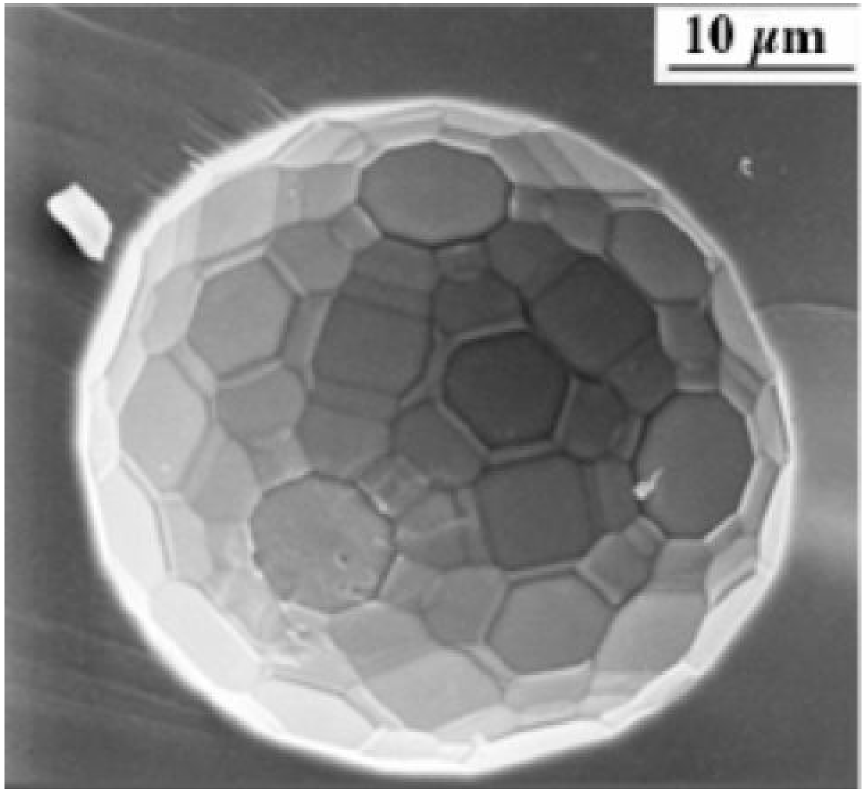
Electronic Spectrum of a 2D Quasi-Crystal Related to the Octagonal Quasi-Periodic Tiling.

EUROPHYSICS LETTERS

Europhys. Lett., **10** (5), pp. 483-488 (1989)

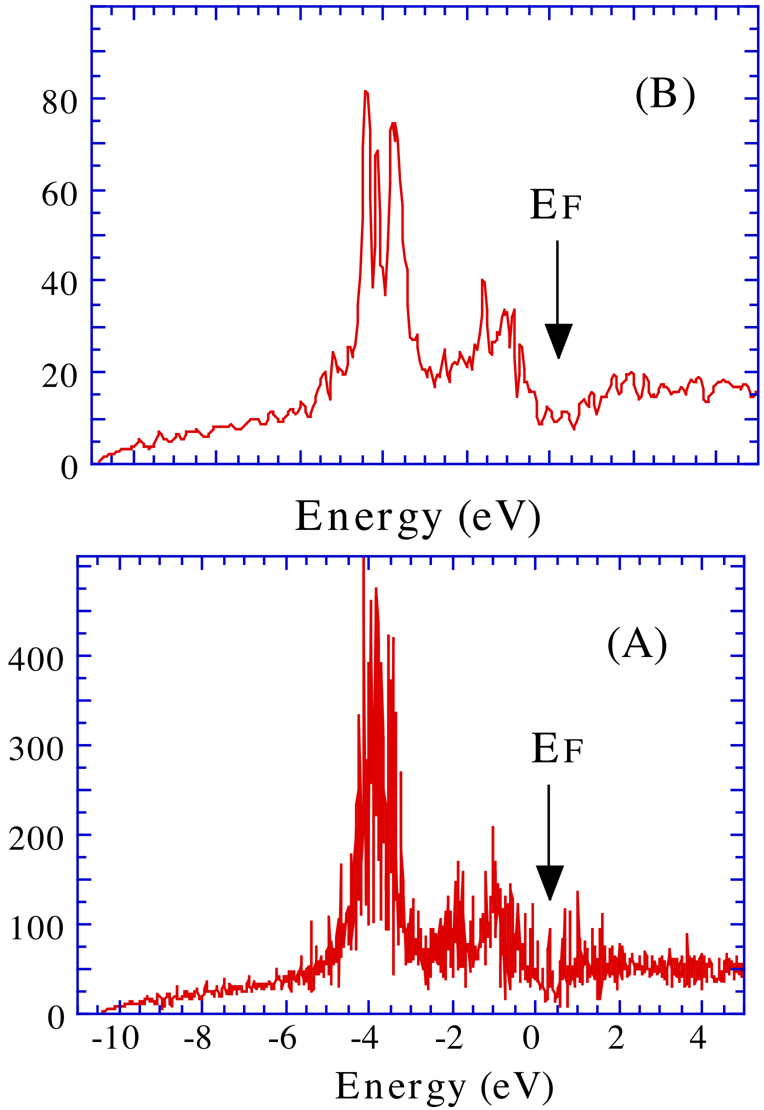
Solvable 2D-model, reducible to 1D-calculations

3D-Quasicrystals



A sample of the icosahedral quasicrystal AlPdMn

3D-Quasicrystals



The Density of States for
(A) a periodic approximant of the icosahedral quasicrystal $Al_{62.5}Cu_{25}Fe_{12.5}$ (28 atoms/unit cell)
(B) the crystal Al_7Cu_2Fe (40 atoms/unit cell).

S. Roche, G. Trambly de Laissardière, D. Mayou, *Electronic transport properties of quasicrystals*, J. Math. Phys., **38**, 1794-1822, (1997).

Methodologies

- For *one dimensional Schrödinger* equation of the form

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

  a *transfer matrix* approach has been used for a long time to analyze the spectral properties *(Bogoliubov '36)*.

- A *KAM-type* perturbation theory has been used successfully *(Dinaburg, Sinai '76, JB '80's)*.

Methodologies

- For *discrete* one-dimensional models of the form

$$H\psi(n) = t_{n+1}\psi(n+1) + t_n\psi(n-1) + V_n\psi(n)$$

a *transfer matrix approach* is the most efficient method, both for numerical calculation and for mathematical approach:

  - the *KAM-type* perturbation theory also applies *(JB '80's)*.
  - models defined by substitutions using the *trace map*

    (Khomoto et al., Ostlundt et al. '83, JB '89, JB, Bovier, Ghez, Damanik... in the nineties)
  - theory of cocycle *(Avila, Jitomirskaya, Damanik, Krikorian, Gorodestsky...)*.

Methodologies

- In higher dimension almost no rigorous results are available
- Exceptions are for models that are Cartesian products of $1D$ models *(Sire '89, Damanik, Gorodestky,Solomyak '14)*
- Numerical calculations performed on quasi-crystals have shown that
  - Finite cluster calculation lead to a large number of *spurious edge states*.
  - *Periodic approximations* are much more efficient
  - Some periodic approximations exhibit *defects* with *contribution* to the energy spectrum.

III - Continuous Fields

Warm Up: the Hausdorff Topology

- If (X, d) is a *compact metric* space, the space $\mathcal{K}(X)$ of compact subsets of X becomes a compact metric space when endowed with the *Hausdorff metric*

$$d_H(F, G) = \max\{\delta(F, G), \delta(G, F)\}$$

$$\delta(F, G) = \sup_{x \in F} \operatorname{dist}(x, G)$$

- If X is only compact and metrizable, a *Haudorff topology* on $\mathcal{K}(X)$ can similarly be defined, which makes $\mathcal{K}(X)$ compact and metrizable as well. *(Hausdorff 1914, Vietoris 1922, Fell 1961)*

Warm Up: C*-algebras

A *C^*-algebra* is a complex Banach algebra $\mathcal{A}$ such that

- there is an antilinear involution $a \in \mathcal{A} \mapsto a^* \in \mathcal{A}$ such that,

$$(ab)^* = b^* a^* \qquad\qquad ||a^* a|| = ||a||^2$$

  for any $a, b \in \mathcal{A}$.

Remark: Such a norm comes only from the *algebraic structure*

- *if $\mathcal{A}, \mathcal{B}$ are two C^*-algebras, then any injective $*$-homomorphism is isometric*
- *the norm is the square root of the spectral radius of $a^* a$.*

Continuous Fields of Hamiltonians

$A = (A_t)_{t \in T}$ is a *field of self-adjoint operators* whenever

1. T is a topological space,
2. for each $t \in T$, $\mathcal{H}_t$ is a Hilbert space,
3. for each $t \in T$, A_t is a self-adjoint operator acting on $\mathcal{H}_t$.

The field $A = (A_t)_{t \in T}$ is called *p2-continuous* whenever, for every polynomial $p \in \mathbb{R}(X)$ with degree at most 2, the following norm map is *continuous*

$$\Phi_p : t \in T \mapsto \|p(A_t)\| \in [0, +\infty)$$

Continuous Fields of Hamiltonians

Theorem: *(S. Beckus, J. Bellissard '16)*

1. *A field $A = (A_t)_{t \in T}$ of self-adjoint bounded operators is p2-continuous if and only if the spectrum of A_t, seen as a compact subset of $\mathbb{R}$, is a continuous function of t with respect to the Hausdorff metric.*

2. *Equivalently $A = (A_t)_{t \in T}$ is p2-continuous if and only if the spectral gap edges of A_t are continuous functions of t.*

Continuous Fields of Hamiltonians

The field $A = (A_t)_{t \in T}$ is called *p2-α-Hölder continuous* whenever, for every polynomial $p \in \mathbb{R}(X)$ with degree at most 2, the following norm map is *α-Hölder continuous*

$$\Phi_p : t \in T \mapsto \|p(A_t)\| \in [0, +\infty)$$

uniformly *w.r.t.* $p(X) = p_0 + p_1 X + p_2 X^2 \in \mathbb{R}(X)$ such that $|p_0| + |p_1| + |p_2| \leq M$, for some $M > 0$.

Continuous Fields of Hamiltonians

Theorem: *(S. Beckus, J. Bellissard '16)*

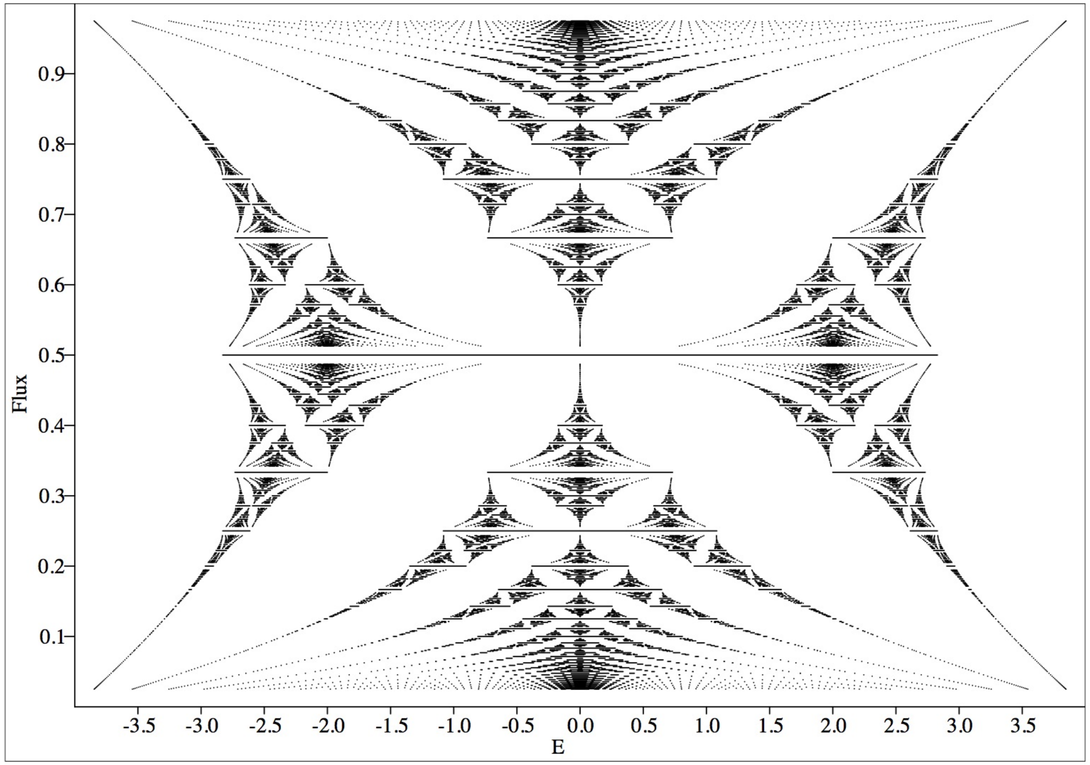
1. *A field $A = (A_t)_{t \in T}$ of self-adjoint bounded operators is p2-α-Hölder continuous then the spectrum of A_t, seen as a compact subset of $\mathbb{R}$, is an $\alpha/2$-Hölder continuous function of t with respect to the Hausdorff metric.*

2. *In such a case, the edges of a spectral gap of A_t are α-Hölder continuous functions of t at each point t where the gap is open.*

3. *At any point t_0 for which a spectral gap of A_t is closing, if the tip of the gap is isolated from other gaps, then its edges are $\alpha/2$-Hölder continuous functions of t at t_0.*

4. *Conversely if the gap edges are α-Hölder continuous, then the field A is p2-α-Hölder continuous.*

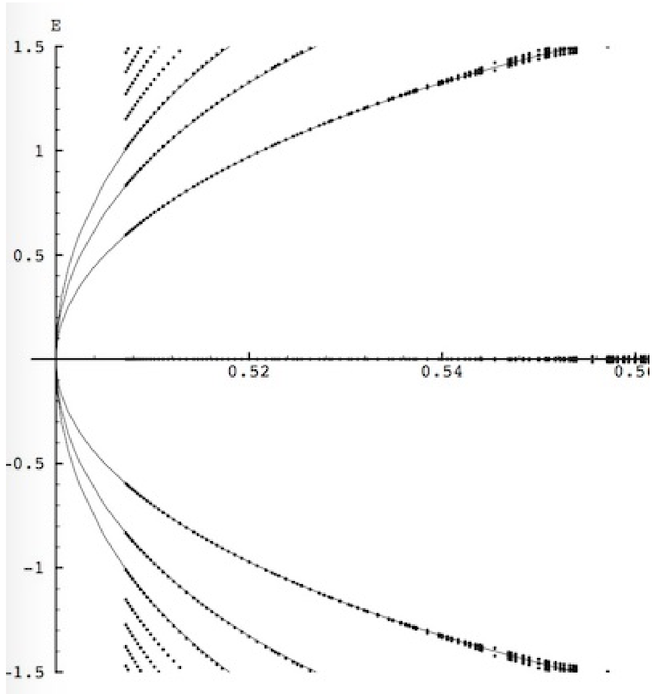
Continuous Fields of Hamiltonians



The spectrum of the Harper model

the Hamiltonina is p2-Lipshitz continuous

(JB, '94)



A gap closing (enlargement)

Continuous Fields on C*-algebras

(Tomyama 1958, Dixmier-Douady 1962)

Given a topological space T, let $\mathcal{A} = (\mathcal{A}_t)_{t\in T}$ be a family of *C^*-algebras*.

A *vector field* is a family $a = (a_t)_{t\in T}$ with $a_t \in \mathcal{A}_t$ for all $t \in T$.

$\mathcal{A}$ is called *continuous* whenever there is a family Υ of vector fields such that,

- for all $t \in T$, the set Υ_t of elements a_t with $a \in \Upsilon$ is a *dense $*$-subalgebra* of $\mathcal{A}_t$
- for all $a \in \Upsilon$ the map $t \in T \mapsto \|a_t\| \in [0, +\infty)$ is *continuous*
- a vector field $b = (b_t)_{t\in T}$ belongs to Υ if and only if, for any $t_0 \in T$ and any $\epsilon > 0$, there is U an open neighborhood of t_0 and $a \in \Upsilon$, with $\|a_t - b_t\| < \epsilon$ whenever $t \in U$.

Continuous Fields on C*-algebras

Theorem *If $\mathcal{A}$ is a continuous field of C*-algebras and if $a \in \Upsilon$ is a continuous self-adjoint vector field, then, for any continuous function $f \in C_0(\mathbb{R})$, the maps $t \in T \mapsto \|f(a_t)\| \in [0, +\infty)$ are continuous*

In particular, such a vector field is p2-continuous

Continuous Fields on C*-algebras

How does one construct a continuous field of C-algebras ?*

IV - Dynamical Systems

Hull

- The set $\mathcal{L}$ of atomic position is *Delone*:
  - There is a minimum distance $2a$ between two distinct atoms
  - The diameter $2b$ of the largest hole is finite.
- There is a topology on the set $\mathfrak{D}_{a,b}$ of Delone sets with given a, b making it a *compact second countable space*.
- The *Hull* Ω of $\mathcal{L}$ is the closure of its orbit under $\mathbb{R}^d$ inside the space of Delone sets. Hence Ω is a *compact second countable space*.
- The translation group $\mathbb{R}^d$ acts on $\mathfrak{D}_{a,b}$ and on Ω by *homeomorphisms*.
- Hence $(\mathfrak{D}_{a,b}, \mathbb{R}^d)$ and $(\Omega, \mathbb{R}^d)$ are *topological dynamical systems*.

Transversal

- The set $\mathfrak{D}^0_{a,b} \subset \mathfrak{D}_{a,b}$ is defined as the set of Delone sets containing the *origin* of $\mathbb{R}^d$.

- Given $\mathcal{L} \in \mathfrak{D}_{a,b}$ its *transversal* is defined as $\Xi = \Omega \cap \mathfrak{D}^0_{a,b}$.

- **Assumption:** *to avoid technicalities, it will be assumed that there is a co-compact discrete subgroup $G \subset \mathbb{R}^d$, acting on Ξ, with at least one dense orbit.*

C*-algebras

Given a topological dynamical system (X, G), where X is a compact space and G a unimodular locally compact group, the *reduced crossed product* C*-algebra $C(X) \rtimes_{red} G$ is built as follows:

- if $A, B \in C_c(X \times G)$ of continuous functions with compact support, the *product* is defined by

$$AB(x,g) = \int_G A(x,h)B(h^{-1}x, h^{-1}g)\, dg$$

- The *adjoint* is defined by

$$A^*(x,g) = \overline{A(g^{-1}x, g^{-1})}$$

C*-algebras

- Given $x \in X$ let π_x be the *representation* of $C_c(X \times G)$ on $L^2(G)$ defined by

$$\pi_x(A)\psi(g) = \int_G A(g^{-1}x, g^{-1}h)\psi(h)\, dh$$

- Then a C^**-norm* is defined by

$$||A|| = sup_{x \in X} ||\pi_x(A)||$$

- By completing the space $C_c(X \times G)$ *w.r.t.* this norm leads to the C*-algebra $C(X) \rtimes_{red} G$.

Invariant Subsets

- A subset $F \subset X$ is *G-invariant* whenever $x \in F$, $g \in G$ implies $gx \in F$.

- Let $\mathcal{J}_G(X)$ be the set of *closed G-invariant subsets* of X.

- Endowed with the *Hausdorff topology*, it is a *compact Hausdorff* space.

- For $F \in \mathcal{J}_G(X)$ let $\mathcal{A}_F = C(F) \rtimes_{red} G$. This gives a *field* $\mathcal{A} = (\mathcal{A}_F)_{F \in \mathcal{J}_G(X)}$ of C*-algebras.

Invariant Subsets

Theorem: *If G is discrete and amenable, and if X is second countable, then the field $\mathcal{A} = (\mathcal{A}_F)_{F \in \mathfrak{I}_G(X)}$ is continuous.*

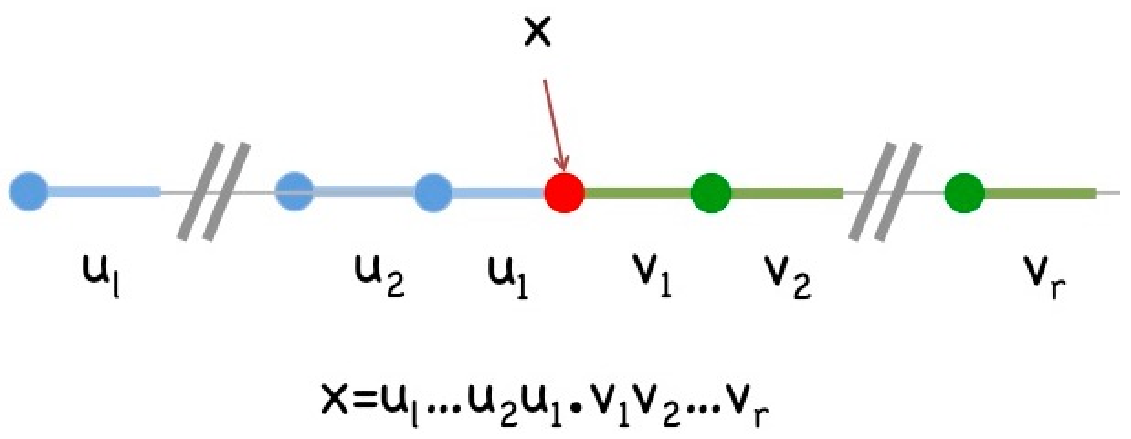
- If $G = \mathbb{Z}^d$ a point $x \in X$ is *periodic* whenever there is a subgroup $H \subset G$ of *finite index*, such that $hx = x$ for $h \in H$.
- *x is periodic if and only if its orbit $O_x = Gx$ is finite and minimal*.
- If $F \in \mathfrak{I}_G(X)$ is the limit (in the Hausdorff topology) of a sequence $(F_n)_{n \in \mathbb{N}}$ of minimal finite invariant sets, then $\mathcal{A}_F$ *is the limit* of $\mathcal{A}_{F_n}$ in the sense of continuous fields of C*-algebras.

V - Periodic Approximations for Subshifts

Subshifts: de Bruijn Graphs

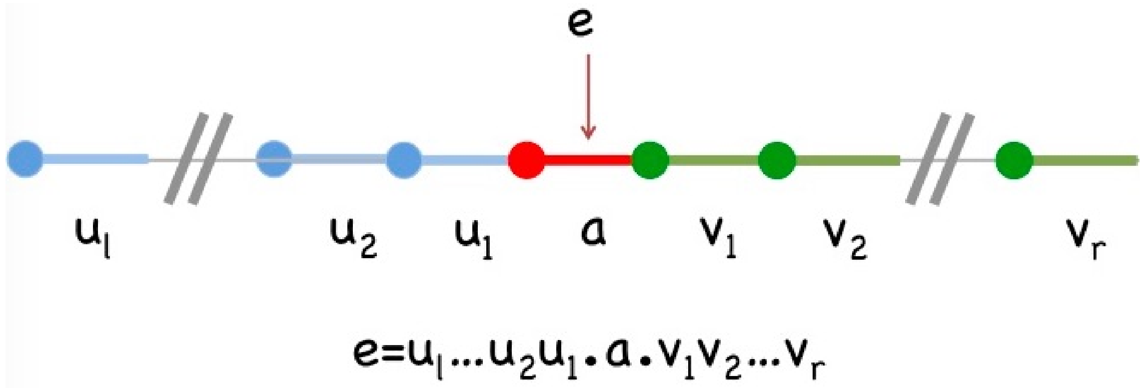
Let $\mathcal{A}$ be a finite *alphabet*, let $\Xi = \mathcal{A}^{\mathbb{Z}}$ be equipped with the shift S. Let $\Sigma \in \mathfrak{I}(\Xi)$ be a subshift. Then

- given $l, r \in \mathbb{N}$ an *(l, r)-collared dot* is a dotted word of the form $u \cdot v$ with u, v being words of length $|u| = l, |v| = r$ such that uv is a *sub-word* of at least one element of Σ



Subshifts: de Bruijn Graphs

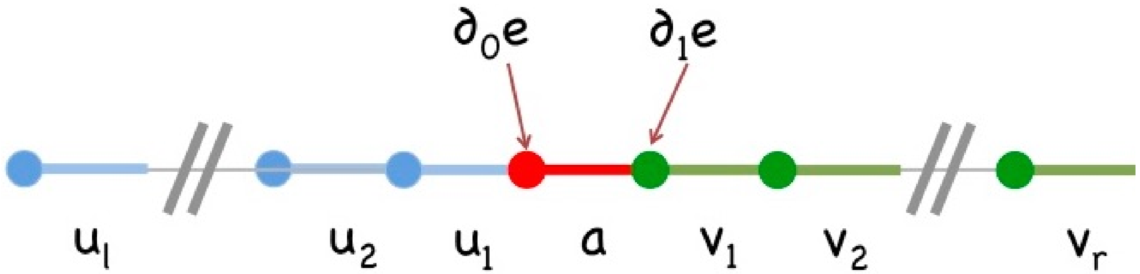
- an *(l, r)-collared letter* is a dotted word of the form $u \cdot a \cdot v$ with $a \in \mathcal{A}$, u, v being words of length $|u| = l, |v| = r$ such that uav is a sub-word of at least one element of Σ: *a collared letter links two collared dots*



Subshifts: de Bruijn Graphs

- let $\mathcal{V}_{l,r}$ be the set of (l,r)-collared dots, let $\mathcal{E}_{l,r}$ be the set of (l,r)-collared letters: then the pair $\mathcal{G}_{l,r} = (\mathcal{V}_{l,r}, \mathcal{E}_{l,r})$ gives a finite *directed graph*. *(de Bruijn, '46, Anderson-Putnam '98, Gähler, '01)*

- The origin $\partial_0 e$ and the end $\partial_1 e$ are the collared dots to the left and the right of the collared letter e

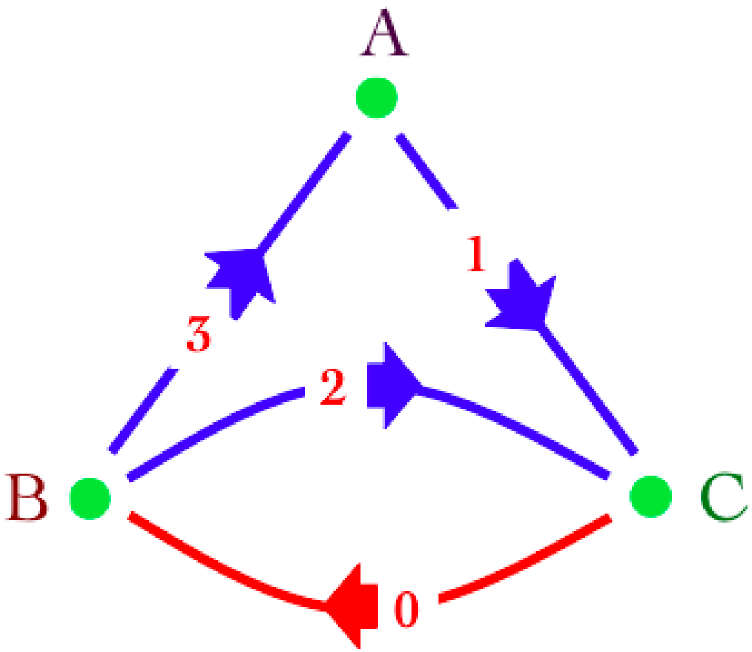


$\partial_0 e = u_l \ldots u_2 u_1 \cdot a v_1 v_2 \ldots v_{r-1}$

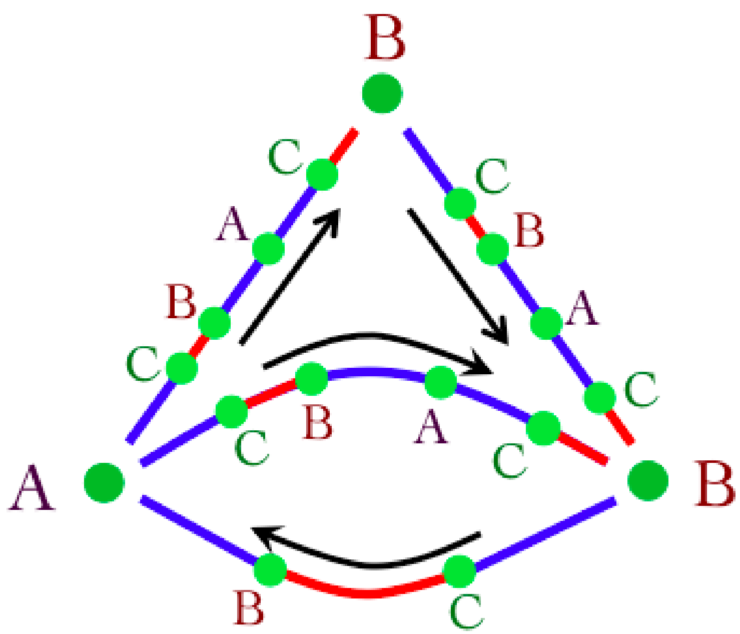
$\partial_1 e = u_{l-1} \ldots u_2 u_1 a \cdot v_1 v_2 \ldots v_r$

The Fibonacci Tiling

- **Alphabet:** $\mathcal{A} = \{a, b\}$
- **Fibonacci sequence:** generated by the *substitution* $a \to ab$, $b \to a$ starting from either $a \cdot a$ or $b \cdot a$



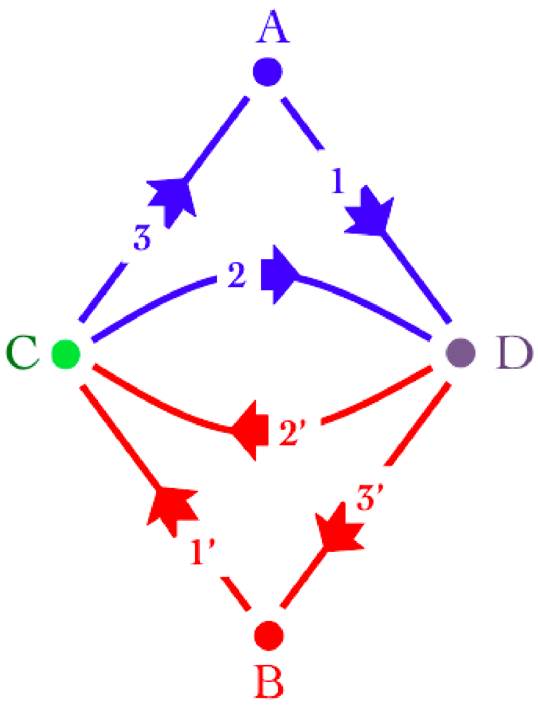
Left: $\mathcal{G}_{1,1}$



Right: $\mathcal{G}_{8,8}$

The Thue-Morse Tiling

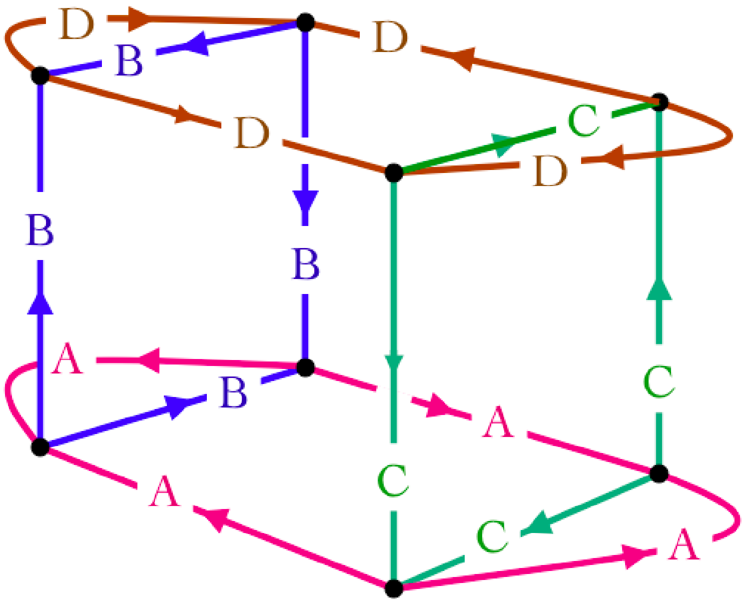
- **Alphabet:** $\mathcal{A} = \{a, b\}$
- **Thue-Morse sequences:** generated by the *substitution* $a \to ab$, $b \to ba$ starting from either $a \cdot a$ or $b \cdot a$



Thue-Morse $\mathcal{G}_{1,1}$

The Rudin-Shapiro Tiling

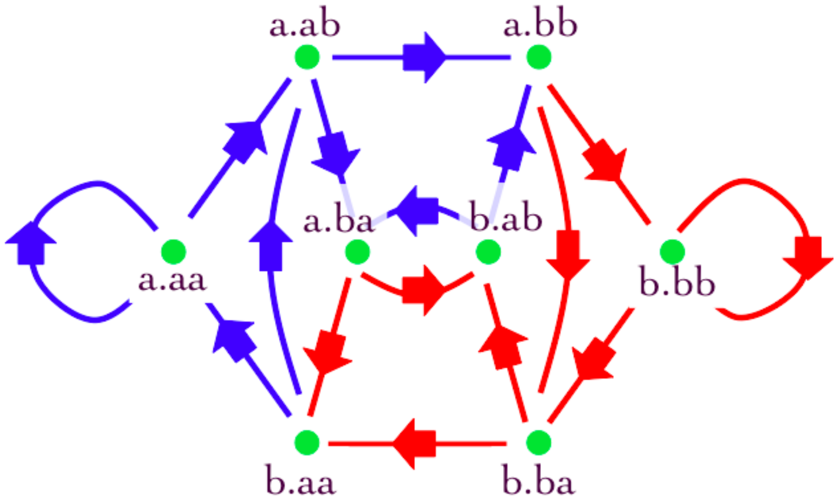
- **Alphabet:** $\mathcal{A} = \{a, b, c, d\}$
- **Rudin-Shapiro sequences:** generated by the *substitution* $a \to ab\,,\ b \to ac\,,\ c \to db\,,\ d \to dc$ starting from either $b \cdot a\,,\ c \cdot a$ or $b \cdot d\,,\ c \cdot d$



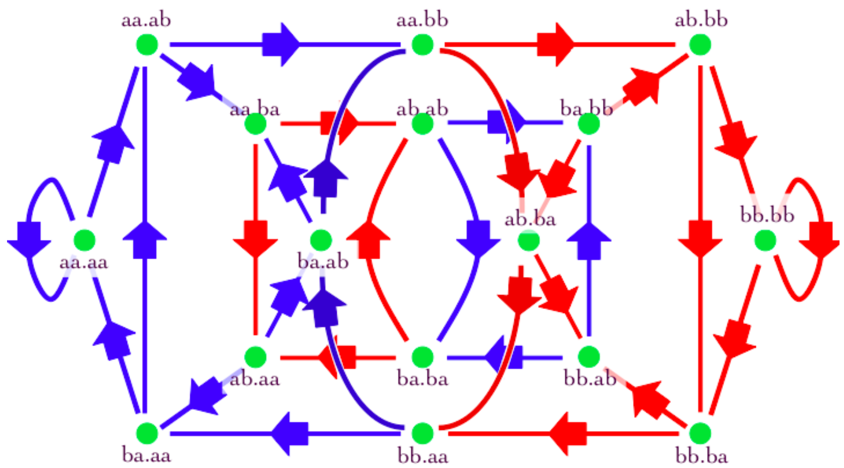
Rudin-Shapiro $\mathcal{G}_{1,1}$

The Full Shift on Two Letters

- **Alphabet:** $\mathcal{A} = \{a, b\}$ all possible word allowed.



$\mathcal{G}_{1,2}$



$\mathcal{G}_{2,2}$

Strongly Connected Graphs

The de Bruijn graphs are

- *simple:* between two vertices there is at most one edge,
- *connected:* if the sub-shift is *topologically transitive*, (*i.e.* one orbit is dense), then between any two vertices, there is at least one path connected them,
- has *no dandling vertex:* each vertex admits at least one ingoing and one outgoing vertex,
- if $n = l + r = l' + r'$ then the graphs $\mathcal{G}_{l,r}$ and $\mathcal{G}_{l',r'}$ are *isomorphic* and denoted by $\mathcal{G}_n$.

Strongly Connected Graphs

(S. Beckus, PhD Thesis, 2016)

A directed graph is called *strongly connected* if any pair x, y of vertices there is an *oriented path* from x to y and another one from y to x.

Proposition: *If the sub-shift Σ is minimal* (i.e. *every orbit is dense), then each of the de Bruijn graph is stongly connected.*

Strongly Connected Graphs

(S. Beckus, PhD Thesis, 2016)

Main result:

Theorem: *A subshift $\Sigma \subset \mathcal{A}^{\mathbb{Z}}$ can be Hausdorff approximated by a sequence of periodic orbits if and only if it admits is a sequence of strongly connected de Bruijn graphs.*

Construction: Periodic approximations can be obtained from *simple closed paths* in the sequence of strongly connected de Bruijn graphs.

Open Problem

Question:

Is there a similar criterion for the space of Delone sets in $\mathbb{R}^d$ or for some remarkable subclasses of it ?

Some *sufficient conditions* have been found for $\Omega = \mathcal{A}^G$, where G is a discrete, countable and *amenable group*, in particular when $G = \mathbb{Z}^d$.

(S. Beckus, PhD Thesis, 2016)

Thanks for listening !