Periodic Approximants to Aperiodic Hamiltonians

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Groups, Geometry & Actions

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online at `http://people.math.gatech.edu/~jeanbel/talksjbE.html`

Content

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

1. Motivation
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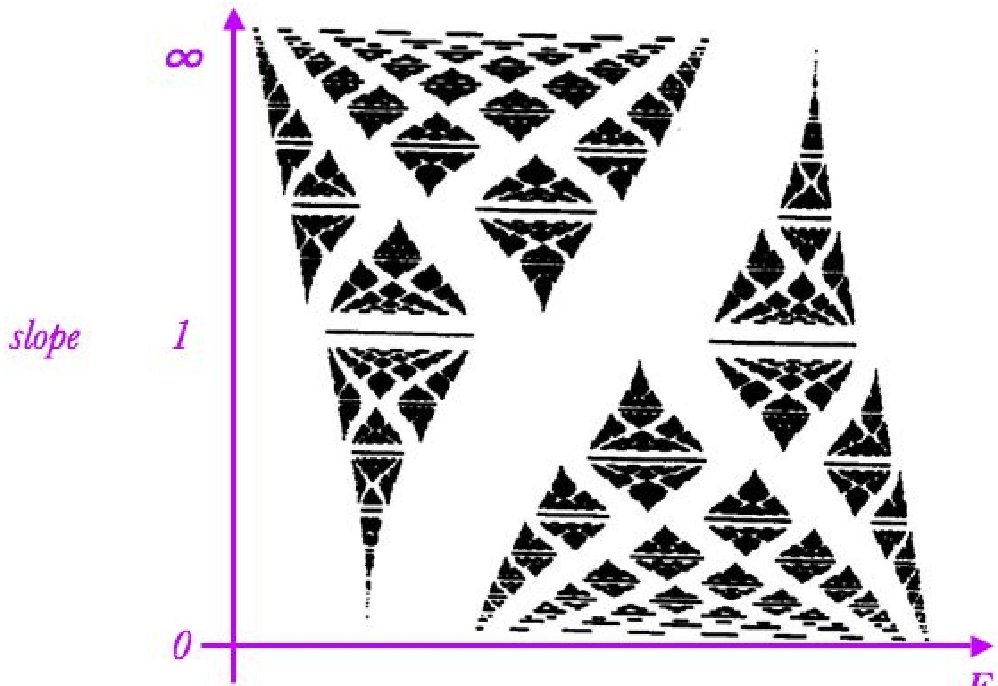
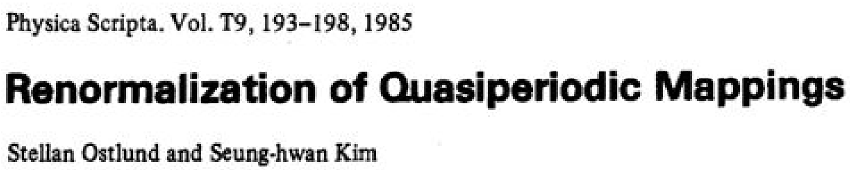
I - Motivations

Motivation



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

Motivation

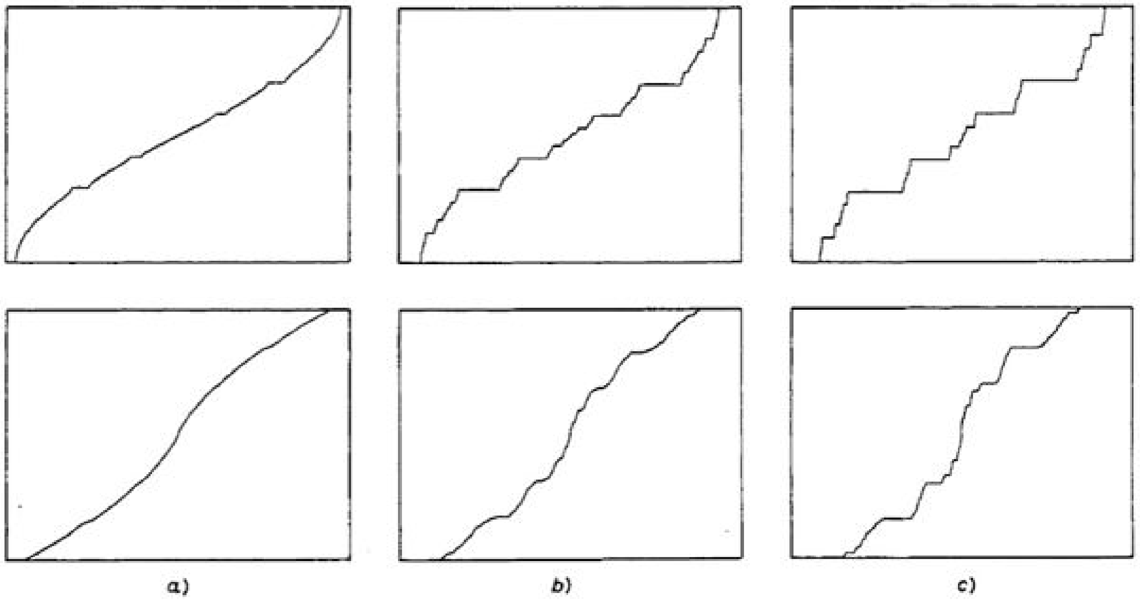


Fig. 3. – We show, respectively, the IDOS of the Octonacci chain (up) and the IDOS of the labyrinth, for *a*) $r = 0.8$ (no gap, finite measure), *b*) $r = 0.6$ (some gaps and finite measure) and *c*) $r = 0.3$ (infinity of gaps and zero measure). The energy varies between -2 and 2, since $r < 1$.

C. Sire

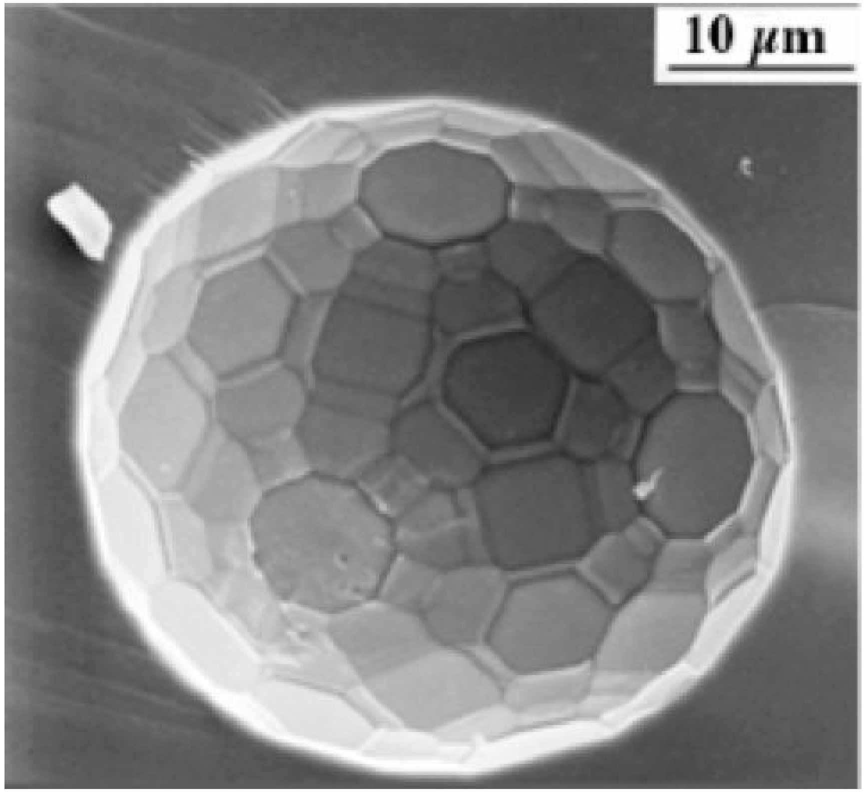
Electronic Spectrum of a 2D Quasi-Crystal Related to the Octagonal Quasi-Periodic Tiling.

EUROPHYSICS LETTERS

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

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

Motivation



A sample of the icosahedral quasicrystal AlPdMn

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* giving *contributions* in the energy spectrum.

II - Continuous Fields

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)*

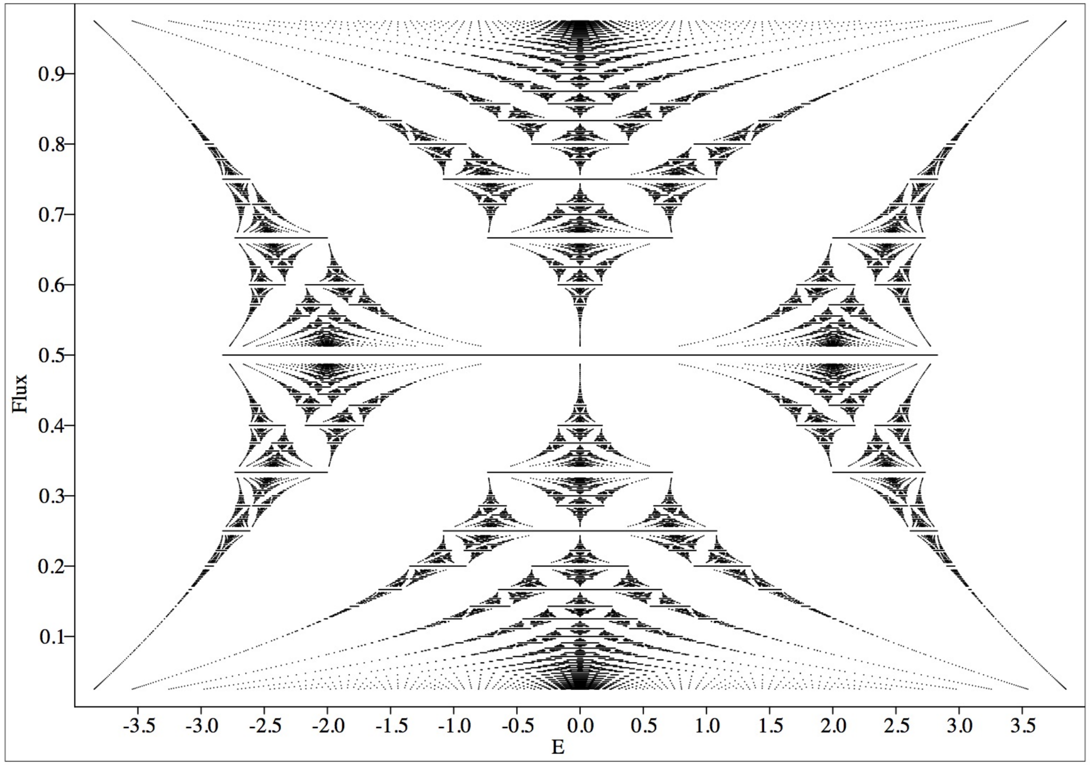
1. *A field $A = (A_t)_{t \in T}$ of self-adjoint bounded operators is p2-α-Hölder continuous then the spectrum of A_t, seen as a compact subset of $\mathbb{R}$, is an $\alpha/2$-Hölder continuous function of t with respect to the Hausdorff metric.*

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.*

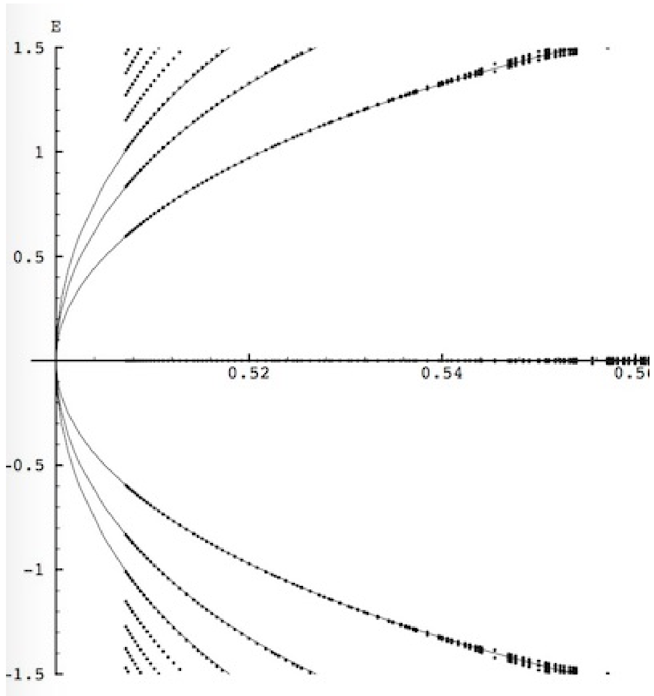
Continuous Fields of Hamiltonians



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

Groupoids

(Ramsay '76, Connes, 79, Renault '80)

A *groupoid* G is a category the object of which G_0 and the morphism of which G make up two sets. More precisely

- there are two maps $r, s : G \to G_0$ (*range* and *source*)
- $(\gamma, \gamma') \in G_2$ are *compatible* whenever $s(\gamma) = r(\gamma')$
- there is an associative *composition law* $(\gamma, \gamma') \in G_2 \mapsto \gamma \circ \gamma' \in G$, such that $r(\gamma \circ \gamma') = r(\gamma)$ and $s(\gamma \circ \gamma') = s(\gamma')$
- a *unit* e is an element of G such that $e \circ \gamma = \gamma$ and $\gamma' \circ e = \gamma'$ whenever compatibility holds; then $r(e) = s(e)$ and the map $e \to x = r(e) = s(e) \in G_0$ is a *bijection* between units and objects;
- each $\gamma \in G$ admits an *inverse* such that $\gamma \circ \gamma^{-1} = r(\gamma) = s(\gamma^{-1})$ and $\gamma^{-1} \circ \gamma = s(\gamma) = r(\gamma^{-1})$

Locally Compact Groupoids

- A groupoid G is *locally compact* whenever
  - G is endowed with a locally compact Hausdorff topology
  - the maps r, s, the *composition* and the *inverse* are *continuous* functions.

  Then the set of units is a closed subset of G.

- A *Haar system* is a family $\lambda = (\lambda^x)_{x\in G_0}$ of positive Borel measures on the fibers $G^x = r^{-1}(x)$, such that
  - if $\gamma : x \to y$, then $\gamma^*\lambda^x = \lambda^y$
  - if $f \in C_c(G)$ is continuous with compact support, then the map $x \in G_0 \mapsto \lambda^x(f)$ is *continuous*.

Locally Compact Groupoids

Example:

Let Ω be a *compact Hausdorff* space, let G be a *locally compact group* acting on Ω by homeomorphisms. Then $\Gamma = \Omega \times G$ becomes a locally compact groupoid as follows

- $\Gamma_0 = \Omega$, is the set of *units*,
- $r(\omega, g) = \omega$ and $s(\omega, g) = g^{-1}\omega$
- $(\omega, g) \circ (g^{-1}\omega, h) = (\omega, gh)$
- Each fiber $\Gamma^\omega \simeq G$, so that if μ is the *Haar measure* on G, it gives a Haar system λ with $\lambda^\omega = \mu$ for all $\omega \in \Omega$.

This groupoid is called the *crossed-product* and is denoted $\Omega \rtimes G$

Groupoid C*-algebra

Let G be a locally compact groupoid with a Haar system λ. Then the complex vector space space $C_c(G)$ of complex valued continuous functions with compact support on G becomes a $*$-algebra as follows

- **Product (convolution):**

$$ab(\gamma) = \int_{G^x} a(\gamma')\, b(\gamma'^{-1} \circ \gamma)\, d\lambda^x(\gamma') \qquad\qquad x = r(\gamma)$$

- **Adjoint:**

$$a^*(\gamma) = \overline{a(\gamma^{-1})}$$

Groupoid C*-algebra

The following construction gives a *C^*-norm*

- for each $x \in G_0$, let $\mathcal{H}_x = L^2(G^x, \lambda^x)$
- for $a \in C_c(G)$, let $\pi_x(a)$ be the operator on $\mathcal{H}_x$ defined by

$$\pi_x(a)\psi(\gamma) = \int_{G^x} a(\gamma^{-1} \circ \gamma')\, \psi(\gamma') d\lambda^x(\gamma')$$

- $(\pi_x)_{x \in G_0}$ gives a faithful covariant family of *$*$-representations* of $C_c(G)$, namely if $\gamma : x \to y$ then $\pi_x \sim \pi_y$.
- then $\|a\| = \sup_{x \in G_0} \|\pi_x(a)\|$ is a C*-norm; the completion of $C_c(G)$ with respect to this norm is called the *reduced C^*-algebra* of G and is denoted by $C^*_{red}(G)$.

Continuous Fields of Groupoids

(N. P. Landsman, B. Ramazan, 2001)

- A *field of groupoid* is a triple (G, T, p), where G is a groupoid, T a set and $p : G \to T$ a map, such that,
  if $p_0 = p \restriction_{G_0}$, then $p = p_0 \circ r = p_0 \circ s$

- Then the subset $G_t = p^{-1}\{t\}$ is a groupoid depending on t.

- If G is *locally compact*, T a *Hausdorff* topological space and *p continuous* and *open*, then $(G, T, P) = (G_t)_{t \in T}$ is called a *continuous field of groupoids*.

Continuous Fields of Groupoids

Theorem: *(N. P. Landsman, B. Ramazan, 2001)*

Let (G, T, p) be a continuous field of locally compact groupoids with Haar systems. If G_t is amenable for all $t \in T$, then the field $\mathcal{A} = (\mathcal{A}_t)_{t \in T}$ of C^*-algebras defined by $\mathcal{A}_t = C^*(G_t)$ is continuous.

III - Tautological Groupoid

Periodic Approximations

Approximating an aperiodic system by a periodic one makes sense within the following framework

- Ω is a *compact* Hausdorff metrizable space,
- a locally compact *group* G acts on Ω by homeomorphisms,
- $\mathcal{J}(\Omega)$ is the set of *closed G-invariant* subsets of Ω:
  - a subset $M \in \mathcal{J}(\Omega)$ is *minimal* if all its G-orbits are dense.
  - a point $\omega \in \Omega$ is called *periodic* if there is a *uniform lattice* $\Lambda \subset G$ such that $g\omega = \omega$ for $g \in \Lambda$. In such a case $\mathrm{Orb}(\omega)$ is a quotient of G/Λ, and is thus is compact.
  - if G is *discrete*, any periodic orbit is a *finite set*.

Periodic Approximations

Example 1)- Subshifts

Let $\mathcal{A}$ be a finite set (alphabet). Let $\Omega = \mathcal{A}^{\mathbb{Z}}$: it is compact for the product topology. The shift operator S defines a *$\mathbb{Z}$-action*.

1. A sequence $\xi = (x_n)_{n\in\mathbb{Z}}$ is *periodic* if and only if ξ can be written as an infinite repetition of a finite word. The S-orbit of ξ is then *finite*.

2. The set of periodic points of Ω is *dense*.

3. A *subshift* is provided by a closed S-invariant subset, namely a point in $\mathfrak{J}(\Omega)$.

Periodic Approximations

Example 2)- Delone Sets A *Delone* set $\mathcal{L} \subset \mathbb{R}^d$ is

- a discrete closed subset,
- there is $0 < r$ such that each ball of radius r intersects $\mathcal{L}$ at one point *at most*,
- here is $0 < R$ such that each ball of radius R intersects $\mathcal{L}$ at one point *at least*.

Then

1. the set $\Omega = \mathrm{Del}_{r,R}$ of such Delone sets in $\mathbb{R}^d$ can be endowed with a topology that makes it *compact*,
2. the group $\mathbb{R}^d$ *acts* on Ω by homeomorphisms,
3. the periodic Delone sets make up a *dense subset* in Ω.

Periodic Approximations

Question: *in which sense can one approximate a minimal infinite G-invariant subset by a sequence of periodic orbits ?*

The Fell and Vietoris Topologies

(Vietoris 1922, Fell 1962)

Given a *topological space* X, let $\mathcal{C}(X)$ be the set of *closed subsets* of X.

Let $F \subset X$ be closed and let $\mathcal{F}$ be a finite family of open sets. Then

$$\mathcal{U}(F, \mathcal{F}) = \{G \in \mathcal{C}(X)\,;\, G \cap F = \emptyset\,,\, G \cap O \neq \emptyset\,,\, \forall O \in \mathcal{F}\}$$

Then the family of $\mathcal{U}(F, \mathcal{F})$'s is a basis for a topology called the *Vietoris topology*.

Replacing F by a compact set K, the same definition leads to the *Fell topology*.

The Fell and Vietoris Topologies

- $\mathcal{C}(X)$ is *Fell-compact*,
- if X is locally compact and Hausdorff, $\mathcal{C}(X)$ is *Hausdorff* for both Fell and Vietoris,
- if (X, d) is a *complete metric* space, the Vietoris topology coincides with the topology defined by the *Hausdorff metric*.
- If X is *compact* both topologies *coincide*.

Theorem *If (Ω, G) is a topological dynamical system, the set $\mathcal{J}(\Omega)$ is compact for both the Fell and the Vietoris topologies.*

The Fell and Vietoris Topologies

Example:

If $(\Omega = \mathcal{A}^{\mathbb{Z}}, S)$, periodic orbits *ARE NOT* Vietoris-dense in $\mathfrak{J}(\Omega)$

For instance, if $\mathcal{A} = \{0, 1\}$ let $\xi_0 \in \Omega$ be the sequence defined by

$$\xi_0 = (x_n)_{n\in\mathbb{Z}} \qquad\qquad x_n = \begin{cases} 0 \text{ if } & n < 0 \\ 1 \text{ if } & n \geq 0 \end{cases}$$

Then $\mathrm{Orb}(\xi)$ is *isolated* in $\mathfrak{J}(\Omega)$ for the Vietoris topology.

The Tautological Groupoid

- Let $\mathfrak{T}(\Omega) \subset \mathfrak{J}(\Omega) \times \Omega$ be the set of pairs (M, ω) such that $\omega \in M$. Endowed with the product topology it is *compact Hausdorff*.
- G *acts* on it by homeomorphisms through $g(M, \omega) = (M, g\omega)$.
- Let $\Gamma = \mathfrak{T}(\Omega) \rtimes G$, let $T = \mathfrak{J}(\Omega)$ and let $p : \Gamma \to T$ defined by

$$p(M, \omega, g) = M$$

  Then (G, T, p) is a *continuous field* of locally compact groupoids.
- If G is *amenable*, then the family $\mathcal{A} = (\mathcal{A}_M)_{M \in \mathfrak{J}(\Omega)}$ where $\mathcal{A}_M = C^*(\Gamma_M)$ gives a continuous field of C*-algebras.

The Tautological Groupoid

Hence

If M is a closed invariant subset of Ω that is a Vietoris-limit point of the set of periodic orbit, then any continuous field of Hamiltonian in $\mathcal{A}$ has a spectrum that can be approximated by the spectrum of a suitable sequence of periodic approximations.

Question: *Which invariant subsets of Ω are Vietoris limit points of periodic orbits ?*

IV - Periodic Approximations for Subshifts

Subshifts

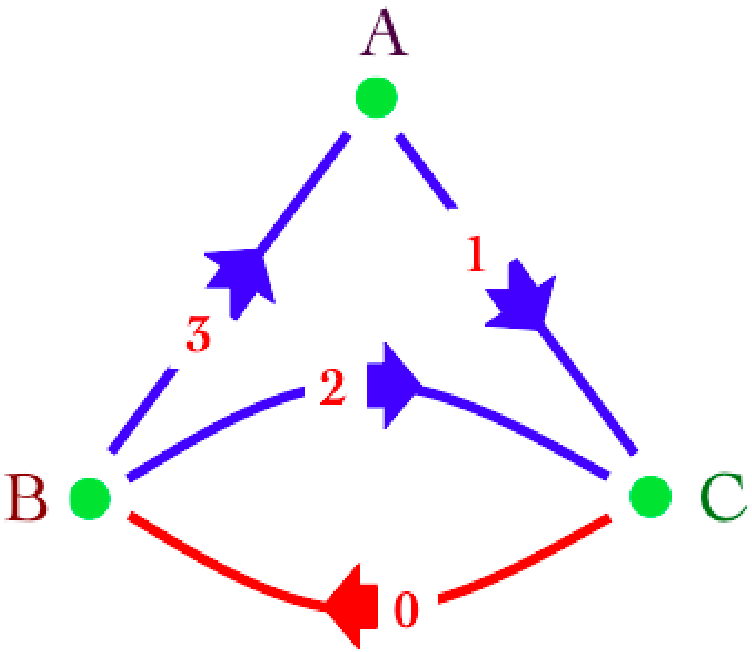
Let $\mathcal{A}$ be a finite *alphabet*, let $\Omega = \mathcal{A}^{\mathbb{Z}}$ be equipped with the shift S. Let $\Sigma \in \mathfrak{J}(\Omega)$ be a subshift. Then

- 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
- 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*
- 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*

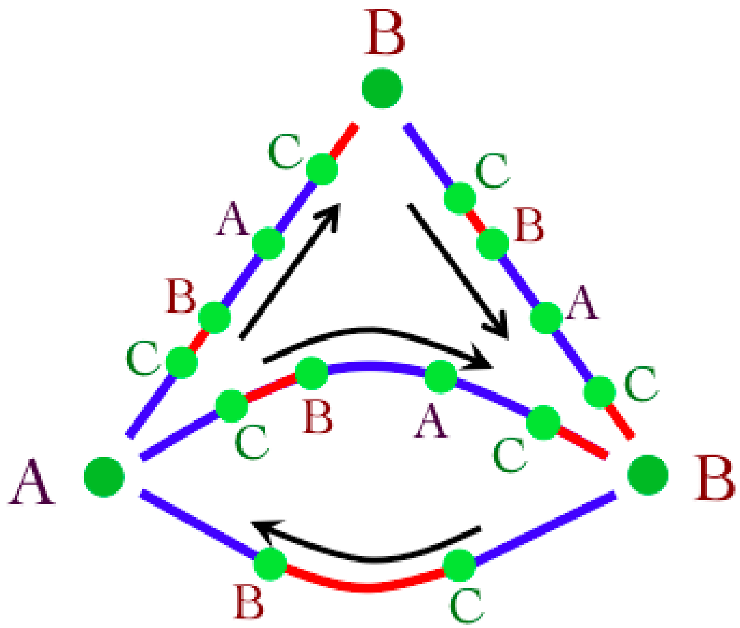
(de Bruijn, '46, Anderson-Putnam '98, Gähler, '01)

The 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 $b \cdot a$



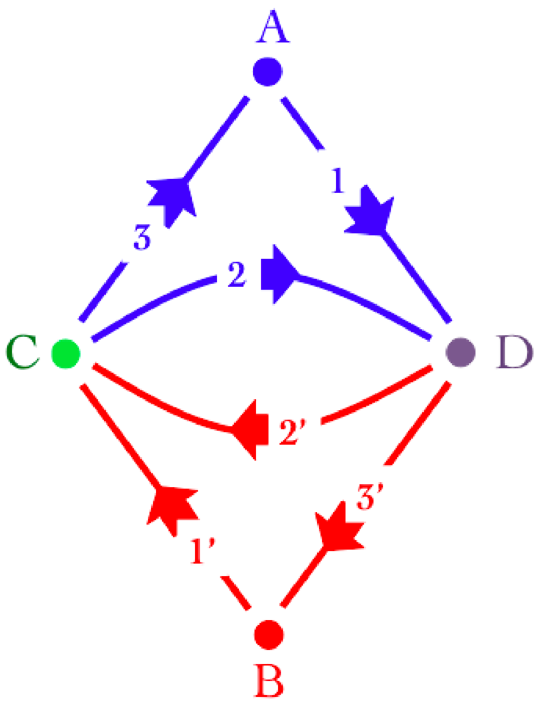
Left: $\mathcal{G}_{1,1}$



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

The Thue-Morse Tiling

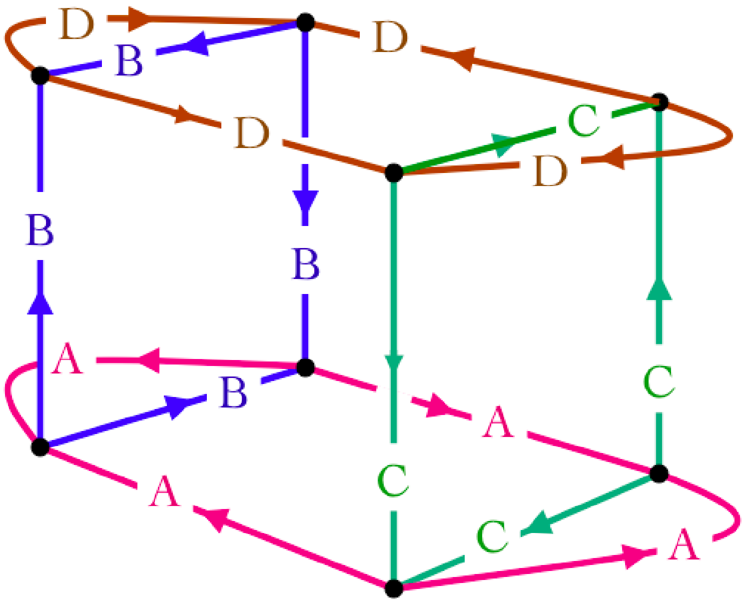
- **Alphabet:** $\mathcal{A} = \{a, b\}$
- **Thue-Morse sequences:** generated by the *substitution* $a \rightarrow ab$, $b \rightarrow ba$ starting from either $a \cdot a$ or $b \cdot a$



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

The Rudin-Shapiro Tiling

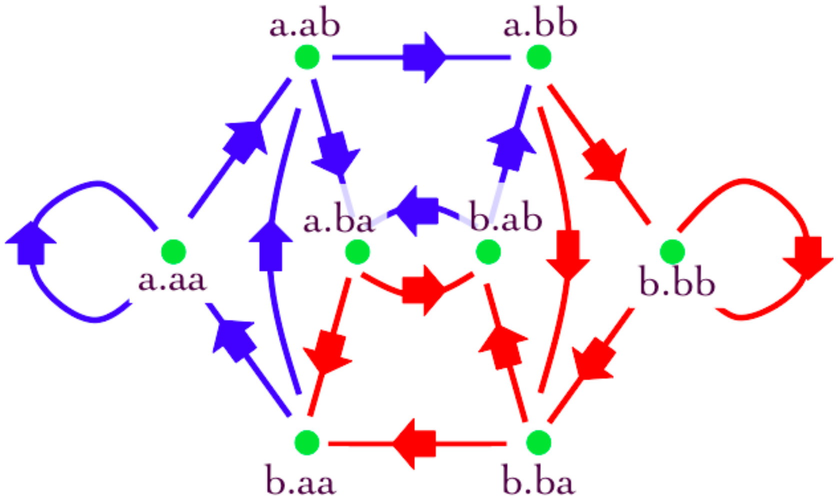
- **Alphabet:** $\mathcal{A} = \{a, b, c, d\}$
- **Rudin-Shapiro sequences:** generated by the *substitution* $a \to ab$, $b \to ac$, $c \to db$, $d \to dc$ starting from either $b \cdot a$, $c \cdot a$ or $b \cdot d$, $c \cdot d$



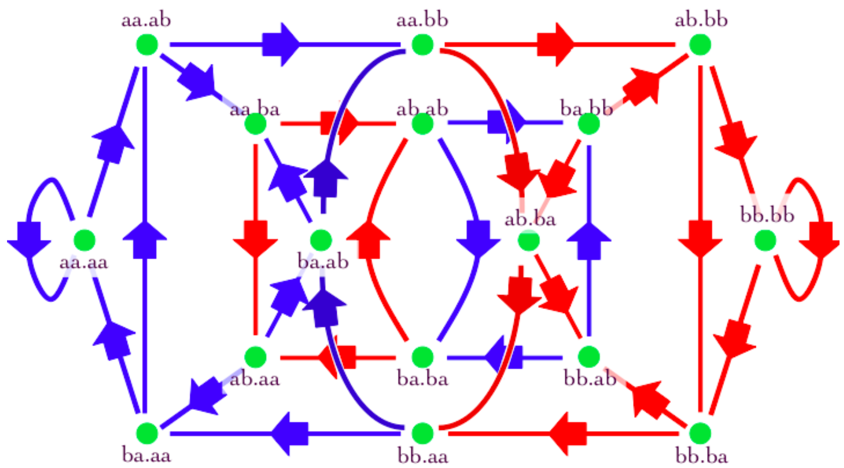
Rudin-Shapiro $\mathcal{G}_{1,1}$

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.*

Main result:

Theorem: *A subshift $\Sigma \subset \mathcal{A}^{\mathbb{Z}}$ can be Vietoris approximated by a sequence of periodic orbits if and only if it admits is a 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 !

Now it's time for tea !

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