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Happy 60th Birthday Jean-Marc!!

Periodic Approximants to Aperiodic Hamiltonians

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Groups, Geometry & Actions

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Content

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I - 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.*

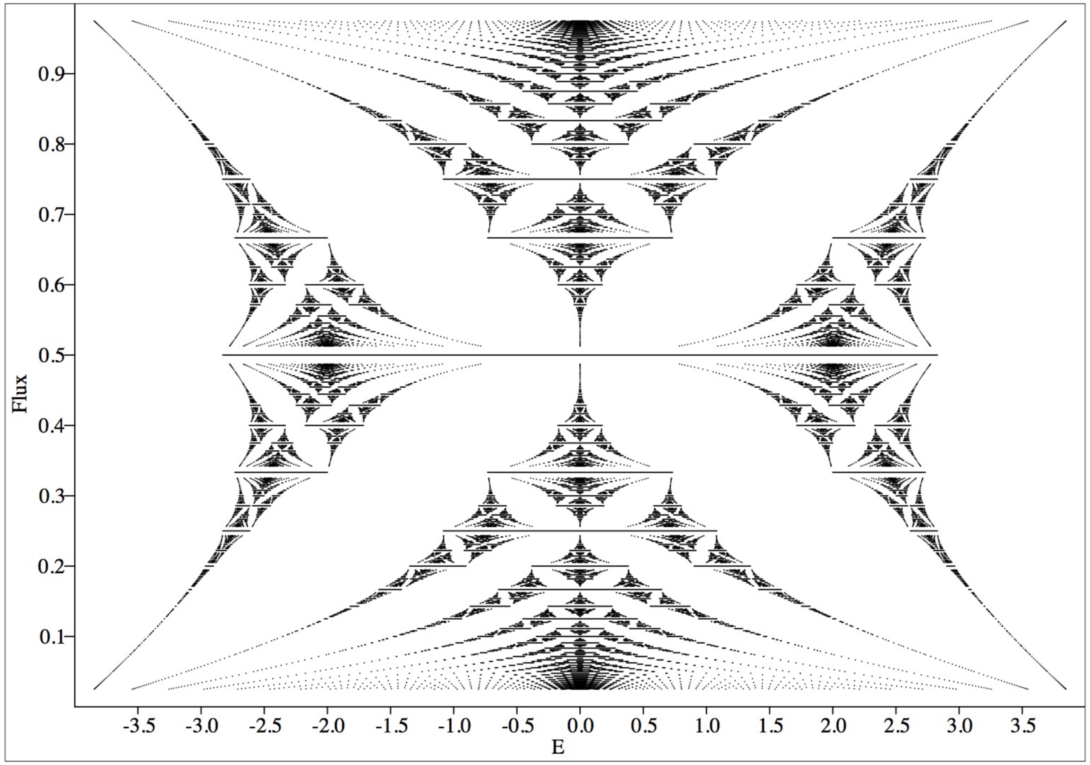
2. *In such a case, the edges of a spectral gap of A_t are α-Hölder continuous functions of t at each point t where the gap is open.*

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

(J. B. 1994)

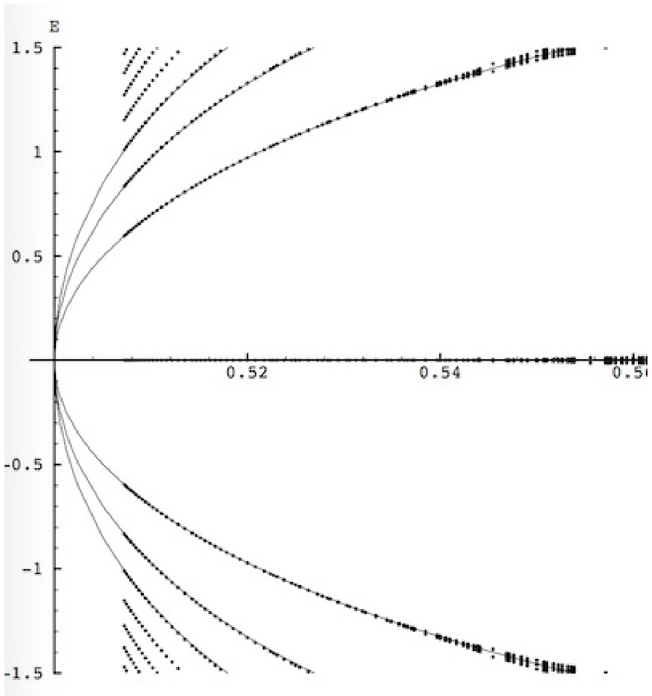


The spectrum of the Harper model

the Hamiltonian is p2-Lipshitz continuous

(JB, '94)

$$H = U + U^{-1} + V + V^{-1}$$



A gap closing (enlargement)

Proving Continuity

- Prove that the field $A = (A_t)_{t \in T}$ is a continuous section of a continuous field $\mathcal{A} = (\mathcal{A}_t)_{t \in T}$ of *C^*-algebras*
  ((Kaplansky '51, Tomyama '58, Dixmier-Douady '62).
- Use *groupoid C^*-algebras* *(Renault '80)*.
- Use a *continuous field* of groupoids *(Landsman, Ramazan '01)*.
- Due to possible presence of a *magnetic field*, use also a continuous field of 2-cycles *(Rieffel '89)*.
- Build the *tautological groupoid* *(Beckus, JB, De Nittis '17)* through the set of closed invariant subsets and the *Hausdorff topology*
  (Hausdorff '14, Vietoris '22, Chabauty '50, Fell '62).

Continuity

(Landsman, Ramazan '01, Rieffel '89, Beckus, JB, De Nittis '17)

Theorem *Let Γ be a locally compact, Hausdorff, amenable groupoid, with a Haar system and compact set of unit. Let $\mathfrak{J}(\Gamma)$ denote its set of invariant subspaces equipped with the Hausdorff topology. Let θ denote a continuous field of 2-cocycles of Γ, continuous over $\mathfrak{J}(\Gamma)$.*

If $f \in C^*(\Gamma, \theta)$, and if F is a closed invariant subset of the unit space of Γ, let f_F denotes the restriction of f on the sub-groupoid restricted to F. Let $\sigma(f)$ denotes the spectrum of f.

Then, if f is self-adjoint, the map $F \in \mathfrak{J}(\Gamma) \mapsto \sigma(f_F) \in \mathcal{K}(\mathbb{R})$ is continuous

In particular, such a vector field is p2-continuous

II - Approximations

Finite Clusters

- The earliest numerical calculation on quasicrystals were made on *finite clusters*, reducing the Hamiltonian to a finite dimensional matrix *(see for instance Kohmoto, Sutherland, PRL* **56***, 2740, 1986)*
- Boundary effects can be huge, representing *up to* 20% of the *Density of States (DOS)* in some cases. Using symmetries and inflation rules, algebraic arguments, it is possible to reduce the computational time and to increase tremendously the accuracy of numerical results *(Kohmoto, Sutherland, loc. cit.)*
- It is how *molecular states* were discovered: these are eigenstates localized on a finite cluster. Such eigenstates have a nonzero DOS and lead to a *discontinuity* in the *Integrated DOS*. It was proved later *(Lenz, Stollmann '03)*, that such discontinuity can only come from molecular state.

Periodic Approximations

- Periodic approximations were used for quasicrystal as those materials admits periodic phases *(Mackay phases)* close to the aperiodic one in the phase diagram.
- For the 2*D-octagonal tiling* such approximations where theoretically calculated in *(Dumeau, Mossery, Oguey '89)*
- The numerical calculation of periodic approximation benefits from software using the Bloch theory to calculate the band structure. The 2*D-octagonal tiling* was resolved in this way *(Benza, Sire '91)*
- It was later proved that errors are *exponentially small in the period* of the approximation *(see for instance Prodan '12)*, which gives a computational advantage over other methods

Building a Groupoid: methodology

- Let Γ_∞ denote the groupoid associated with the aperiodic system under study.
- Let Γ_n denote an approximate groupoid used in the approximation scheme.
- Take the disjoint union of all of them $\Gamma = \coprod_{n\in\mathbb{N}\cup\{\infty\}} \Gamma_n$
- Define a *topology* on Γ making it a *continuous field* over $\mathbb{N} \cup \{\infty\}$, namely a *convergent sequence*.

III - One-Dimensional FLC Tilings

GAP-graphs

(also called de Bruijn graphs, Rauzy graphs, Anderson-Putnam complex)

Let $\mathcal{A}$ be a finite *alphabet*, let $\Omega = \mathcal{A}^{\mathbb{Z}}$ be equipped with the shift S. Let $\Sigma \in \mathfrak{I}(\Omega)$ 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* *(Flye 1894, de Bruijn '46, Good '46, Rauzy '83, Anderson-Putnam '98, Gähler, '01)*

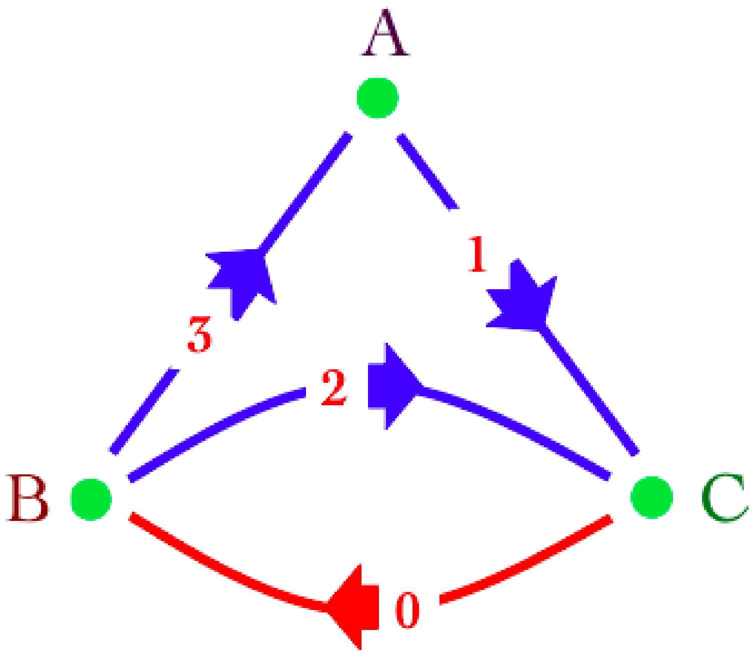
GAP-graphs

(also called de Bruijn graphs, Rauzy graphs, Anderson-Putnam complex)

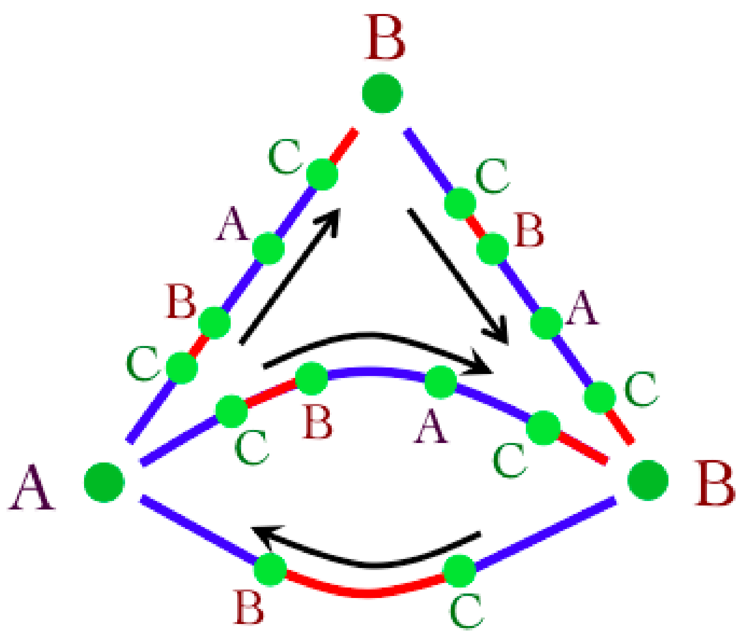
These graphs will be called **GAP**, in reference to the *Gähler* version of the *Anderson-Putnam complexes* for tilings with *Finite Local Complexity (FLC)* in any dimensions

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 $b \cdot a$



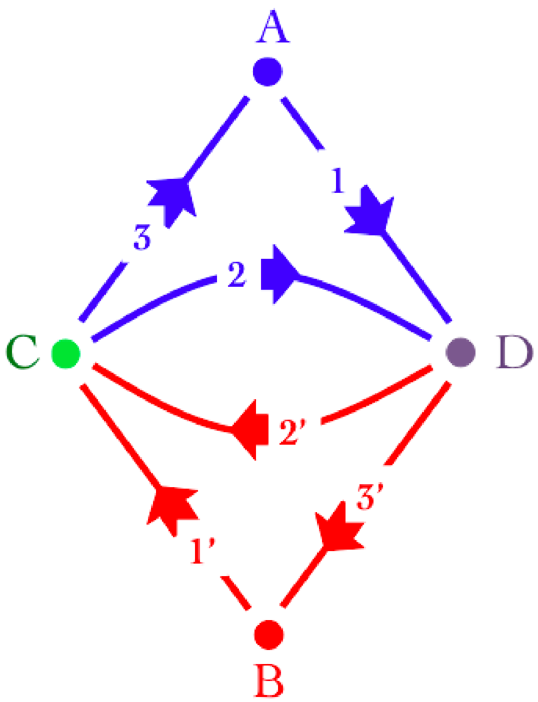
Left: $\mathcal{G}_{1,1}$



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

The Thue-Morse Tiling

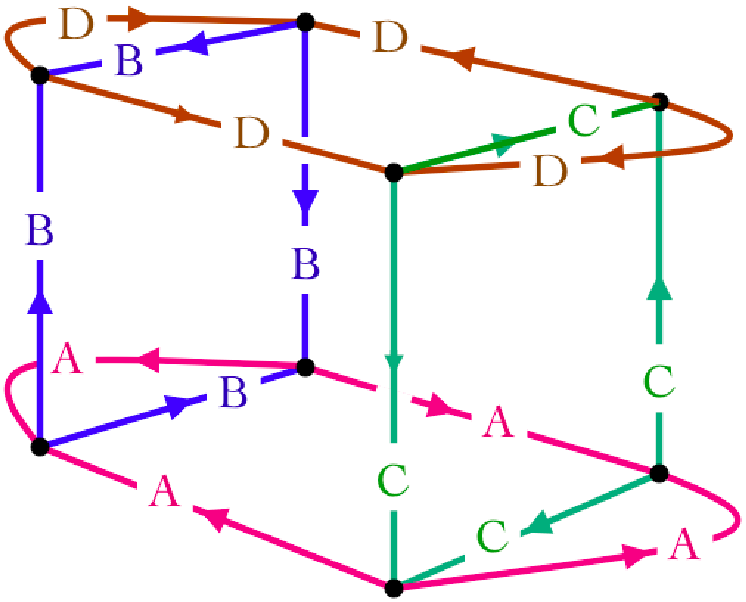
- **Alphabet:** $\mathcal{A} = \{a, b\}$
- **Thue-Morse sequences:** generated by the *substitution* $a \to ab$, $b \to ba$ starting from either $a \cdot a$ or $b \cdot a$



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

The Rudin-Shapiro Tiling

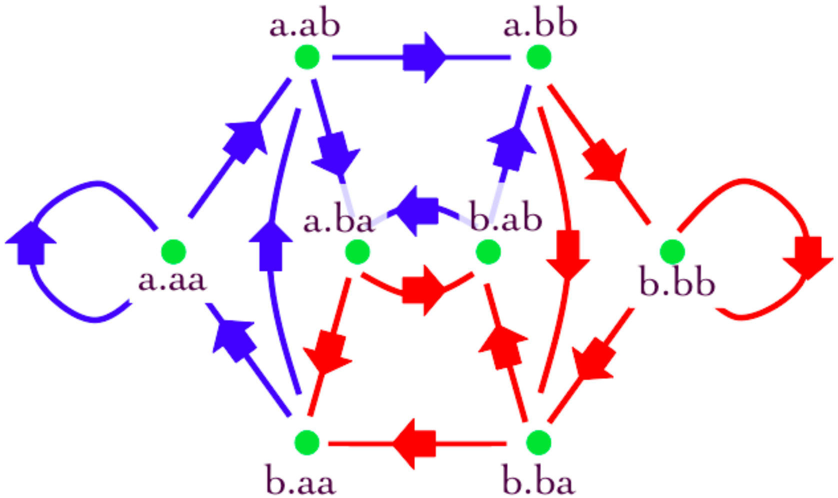
- **Alphabet:** $\mathcal{A} = \{a, b, c, d\}$
- **Rudin-Shapiro sequences:** generated by the *substitution* $a \to ab\,,\ b \to ac\,,\ c \to db\,,\ d \to dc$ starting from either $b \cdot a\,,\ c \cdot a$ or $b \cdot d\,,\ c \cdot d$



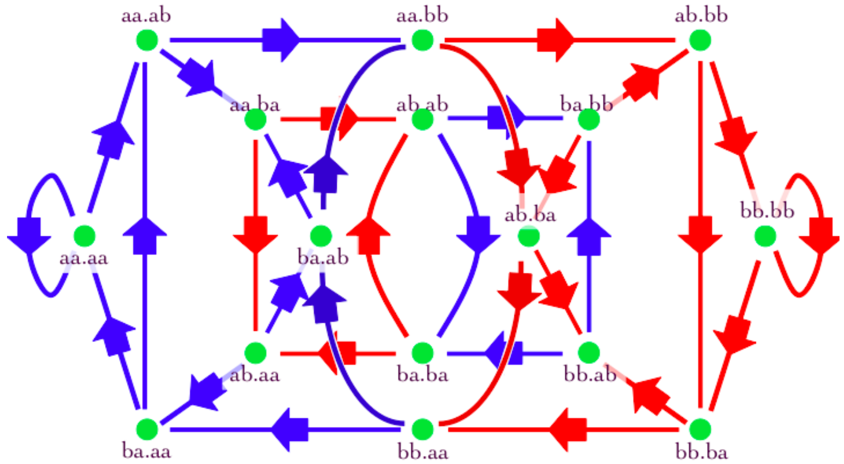
Rudin-Shapiro $\mathcal{G}_{1,1}$

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 GAP 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; Beckus, JB, De Nittis '18)

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 GAP graph is stongly connected.*

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 GAP graphs.*

VI - To Conclude

Lipshitz Continuity

1. **Theorem:** *An aperiodic system with disorder described by a subshift of finite type (finite alphabet) on the lattice $\mathbb{Z}^d$ and a Hamiltonian with finite range has a spectrum Lipshitz continuous with respect to the subshift expressed as a closed invariant subset of the full shift.*

   (Beckus, JB, Cornean, 2018, in preparation)

2. **Theorem:** *An aperiodic system describing a 1D-quasicrystal, described by cut-and-projection from $\mathbb{Z}^2$ onto $\mathbb{R}$, described by a line of slope α, by a Hamiltonian with finite range and pattern equivariant coefficients, has a spectrum Lipshitz continuous with respect to α once the real line is equipped with a suitable ultrametric inducing a Cantor set topology.*

   (Beckus, JB, 2018, in preparation)

Lipshitz Continuity

- **Open Problems:** extend the two results on either *FLC tilings* in any dimension or on quasicrystals in any *cut-and-project* situation.

  (Beckus, JB, De Nittis, in project)

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