Periodic Approximants to 1D Aperiodic Hamiltonians

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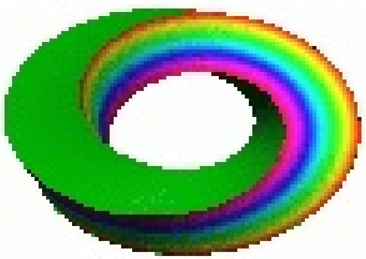

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Main References

J. E. Anderson, I. Putnam,
Topological invariants for substitution tilings and their associated C^*-algebras,
Ergodic Theory Dynam. Systems, **18**, (1998), 509-537.

F. Gähler, Talk given at *Aperiodic Order, Dynamical Systems, Operator Algebra and Topology*
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J. Bellissard, R. Benedetti, J. M. Gambaudo,
Spaces of Tilings, Finite Telescopic Approximations,
Comm. Math. Phys., **261**, (2006), 1-41.

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EPFL, Lausanne, June 3rd, 2010
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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.*

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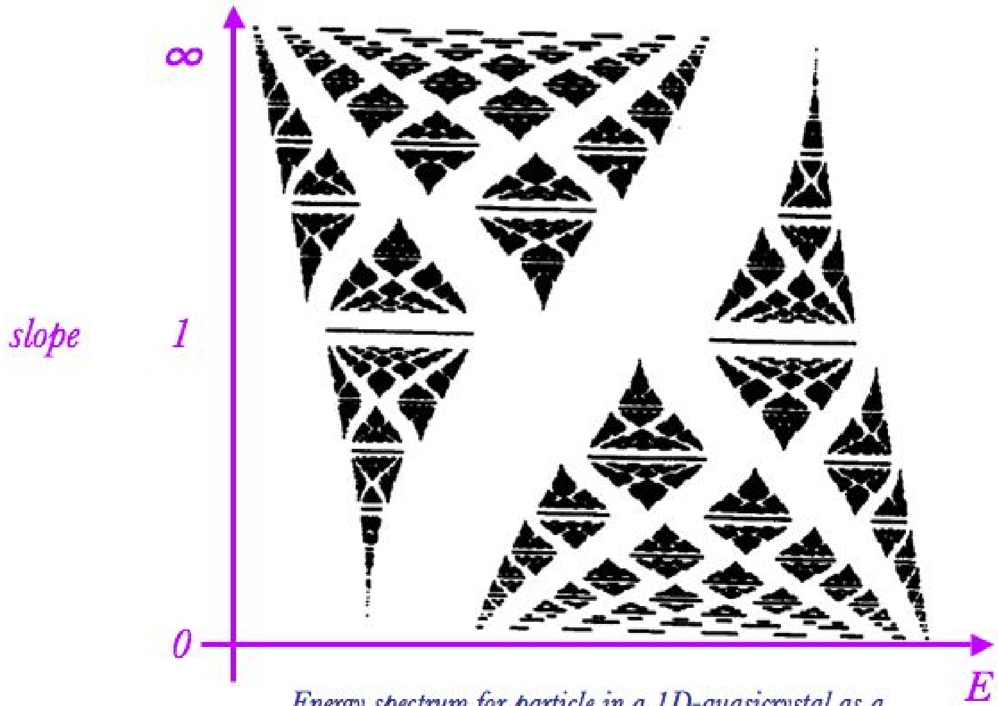
I - Motivations

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

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

as a function of α.

Method:
transfer matrix calculation

Motivation

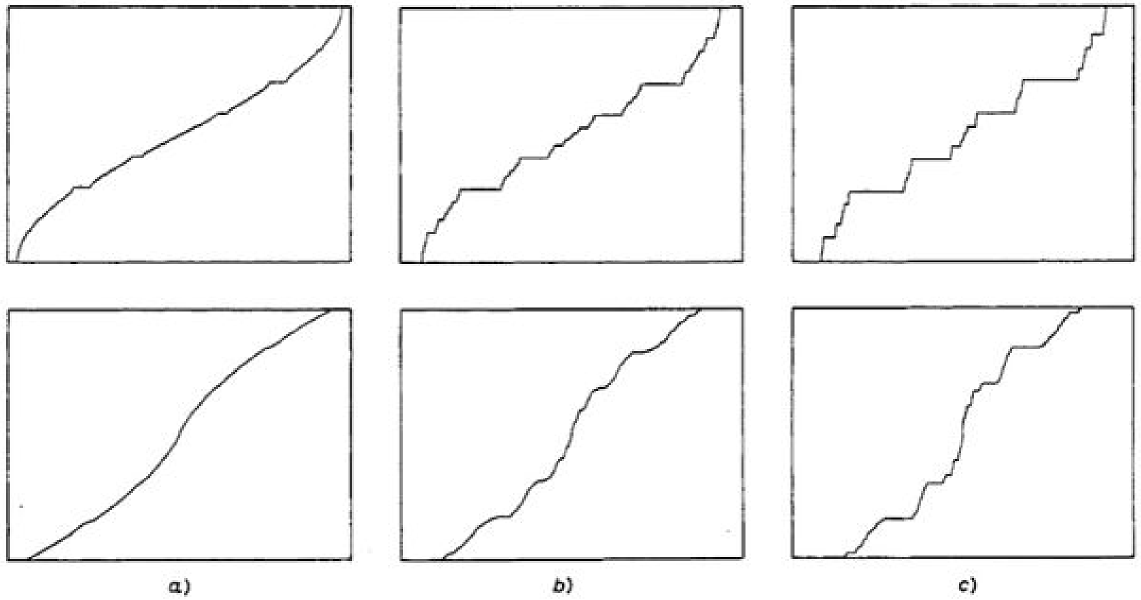


Fig. 3. – We show, respectively, the IDOS of the Octonacci chain (up) and the IDOS of the labyrinth, for *a*) $r = 0.8$ (no gap, finite measure), *b*) $r = 0.6$ (some gaps and finite measure) and *c*) $r = 0.3$ (infinity of gaps and zero measure). The energy varies between -2 and 2, since $r < 1$.

C. SIRE

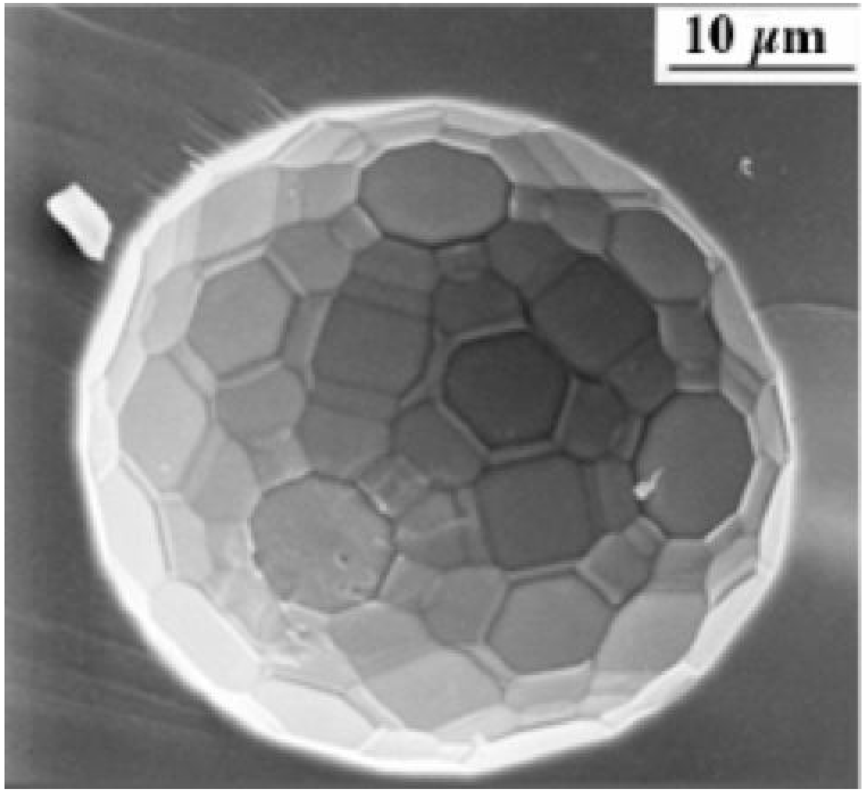
Electronic Spectrum of a 2D Quasi-Crystal Related to the Octagonal Quasi-Periodic Tiling.

EUROPHYSICS LETTERS

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

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

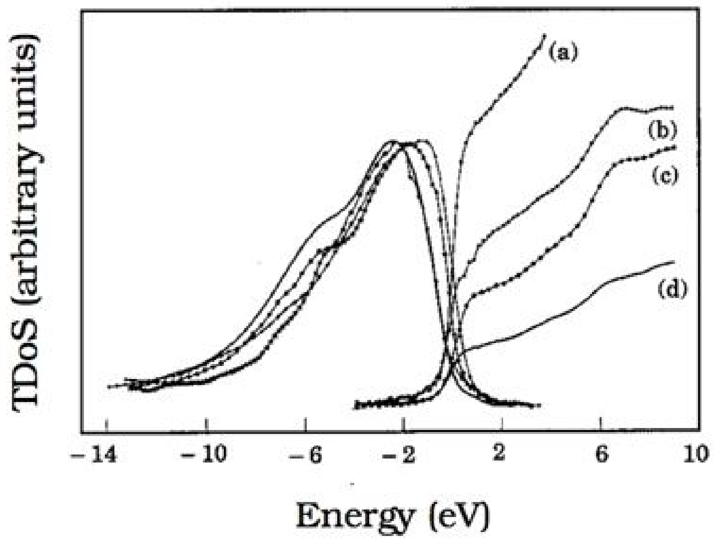
Motivation



A sample of the icosahedral quasicrystal AlPdMn

Motivation

† = *Density of States*



Partial DoS† measured by SXES* or SXAS*

(a) Pure Al
(b) ω-Al_7Cu_2Fe
(c) Rhombohedral approximant $Al_{62.5}Cu_{26.5}Fe_{11}$
(d) Icosahedral phase $Al_{62}Cu_{25.5}Fe_{12.5}$

* = *Soft X-ray Emission or Absorption Spectroscopy*

E. Belin, Z. Dankhazi, A. Sadoc, Y. Calvayrac, T. Klein, J.-M. Dubois, *J. Phys.:Condens. Matter*, **4**, (1992), 4459

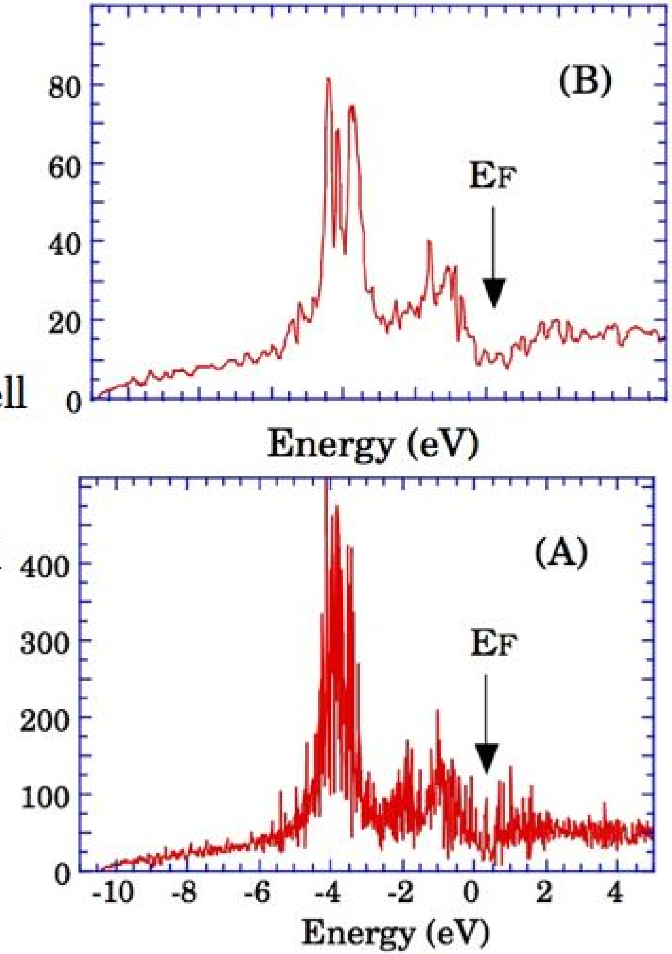
Motivation

DoS† for alloys with close composition

(A) Approximant 1/1
$Al_{62.5}Cu_{25}Fe_{12.5}$, 128 atom/cell

(B) Non approximant
ω-Al_7Cu_2Fe 40 atom/cell

† = Density of States



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

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 - One Dimensional Models

The Fibonacci Sequence

The *Fibonacci sequence* is an infinite word generated by the substitution

$$\hat{\sigma} : \qquad a \longrightarrow ab\,, \qquad\qquad b \longrightarrow a$$

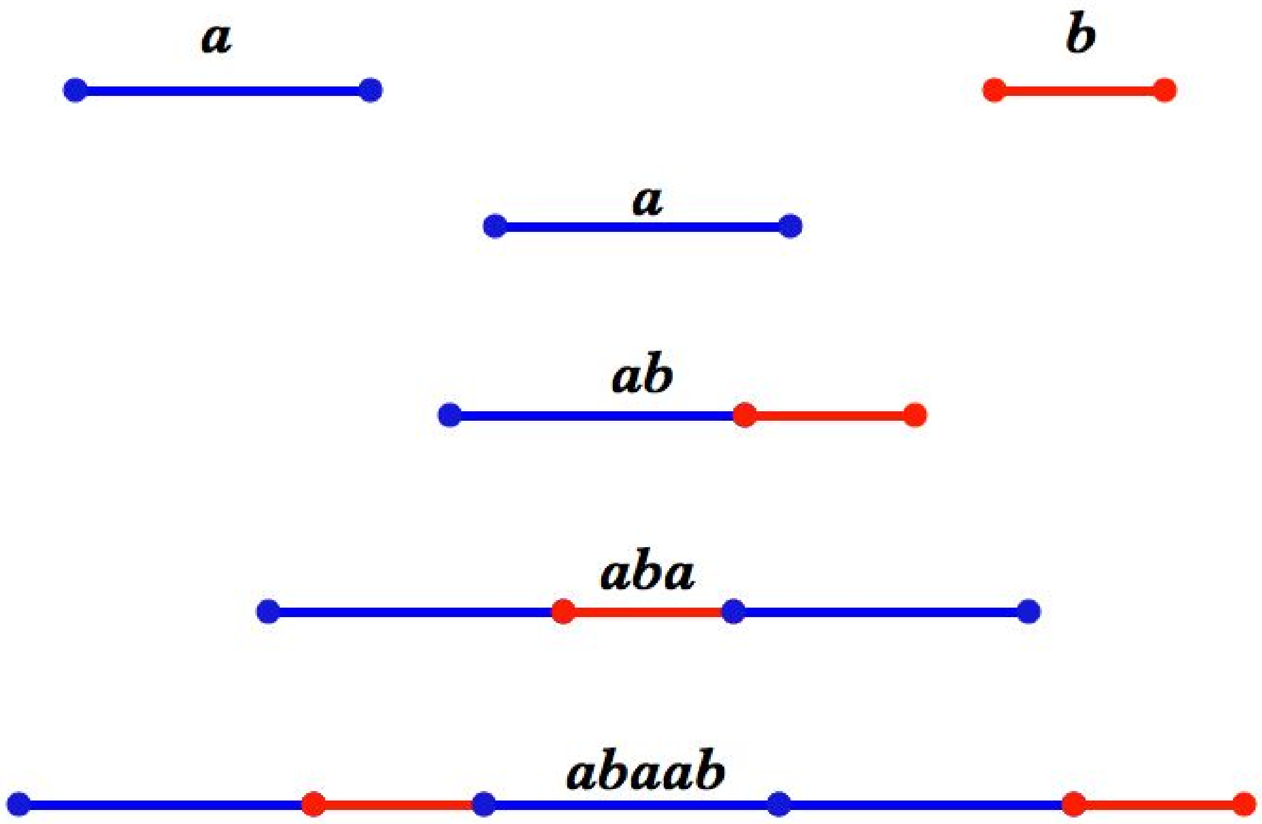
Iterating gives

$$\underbrace{a}_{a_0} \to \underbrace{ab}_{a_1} \to \underbrace{ab|a}_{a_2=a_1a_0} \to \underbrace{aba|ab}_{a_3=a_2a_1} \to \underbrace{abaab|aba}_{a_4=a_3a_2} \to \underbrace{abaababa|abaab}_{a_5=a_4a_3}$$

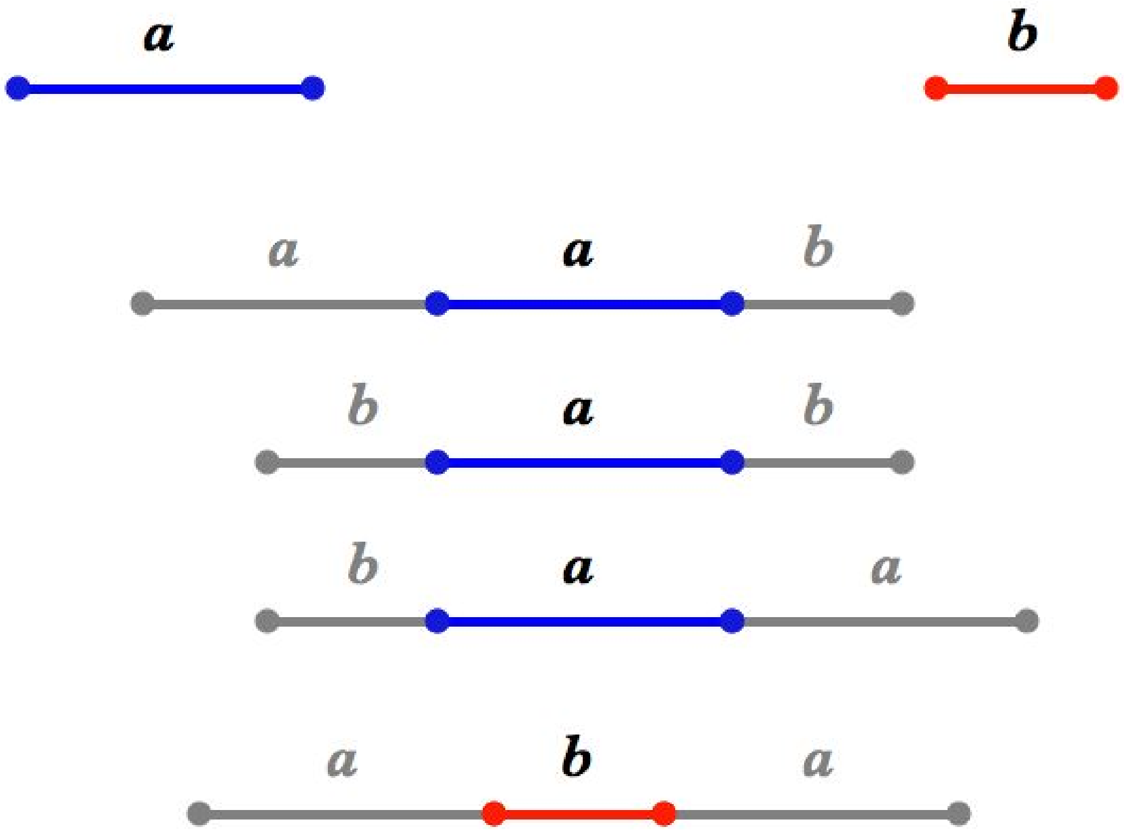
It can be represented by a *1D-tiling* if

$$a \to [0,1] \qquad b \to [0,\sigma] \qquad \sigma = \frac{\sqrt{5}-1}{2} \sim .618$$

The Fibonacci Sequence

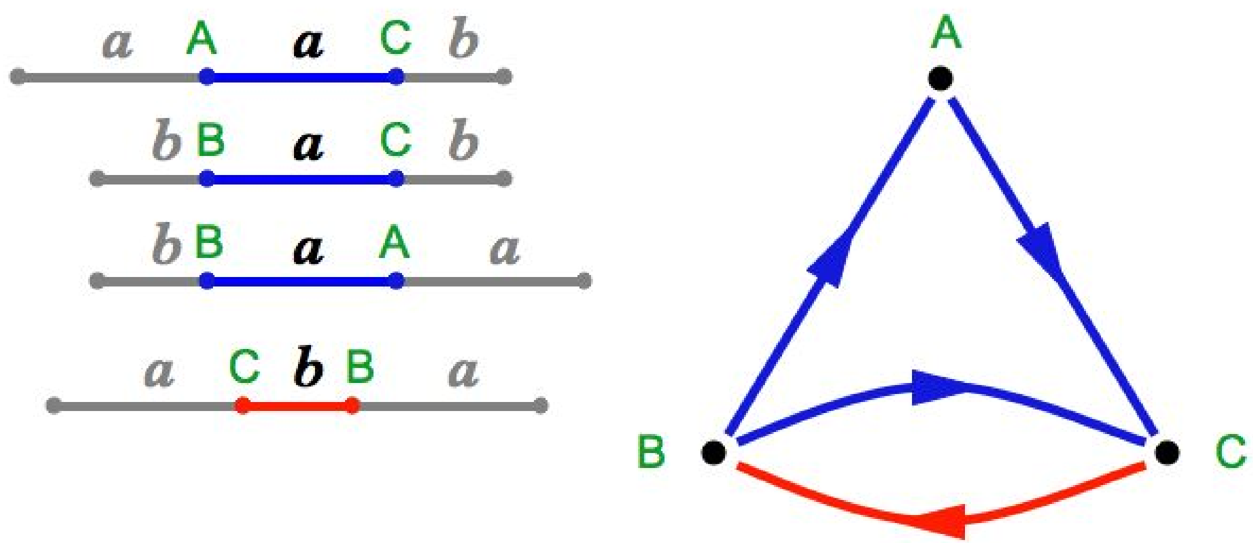


The Fibonacci Sequence



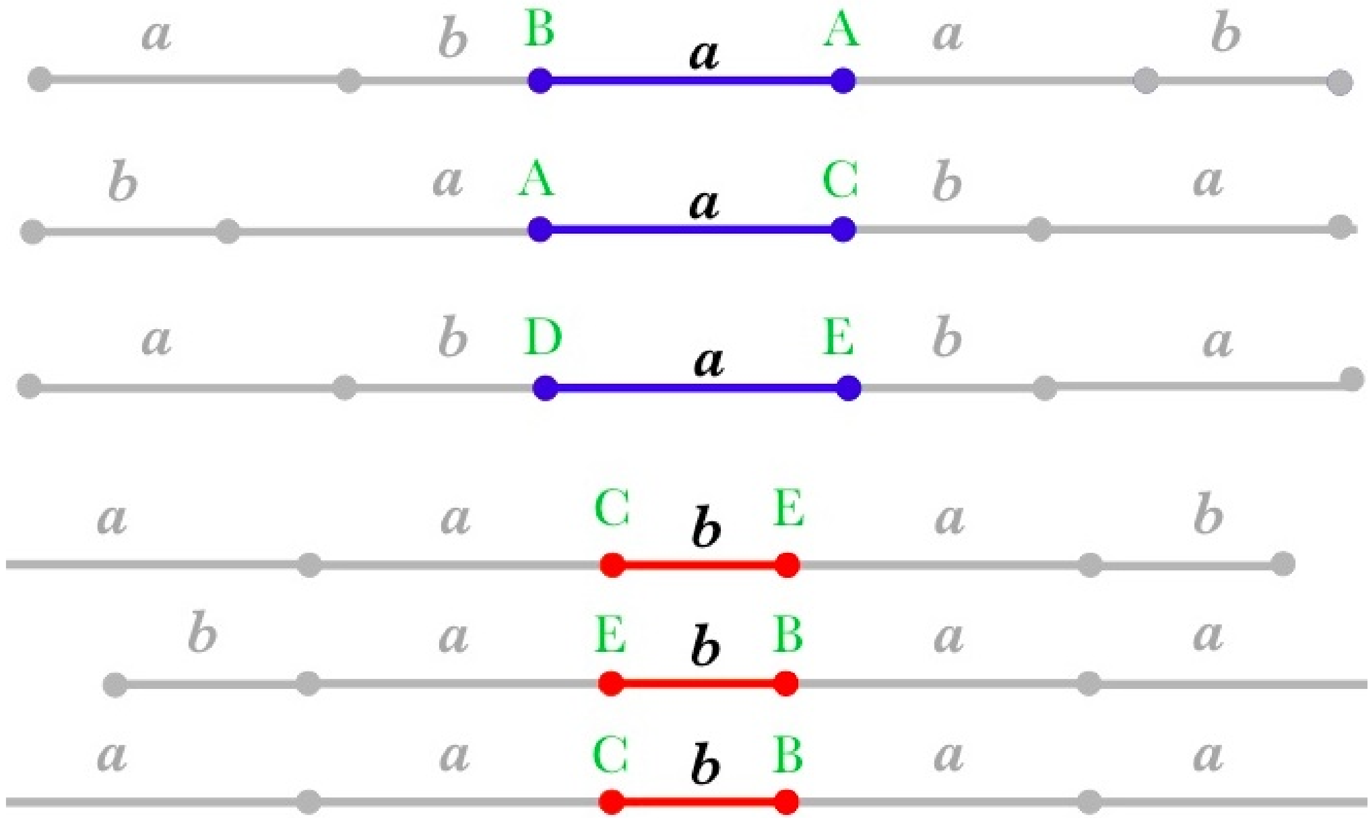
- Collared tiles in the Fibonacci tiling -

The Fibonacci Sequence



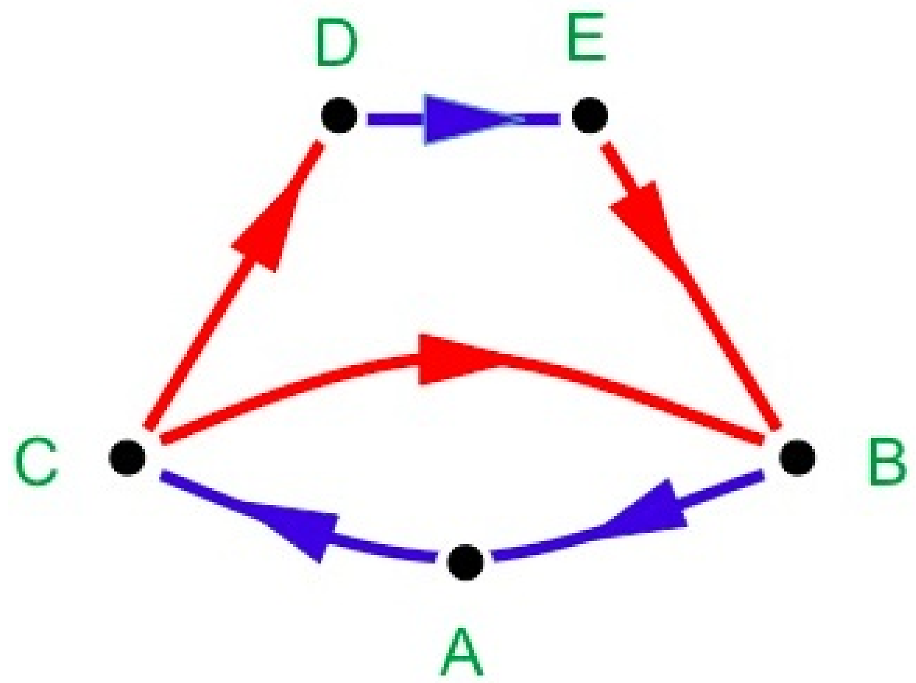
- Gähler-Anderson-Putnam graph for 1.1-collared tiles -

The Fibonacci Sequence



- Gähler's collaring of order 2 -

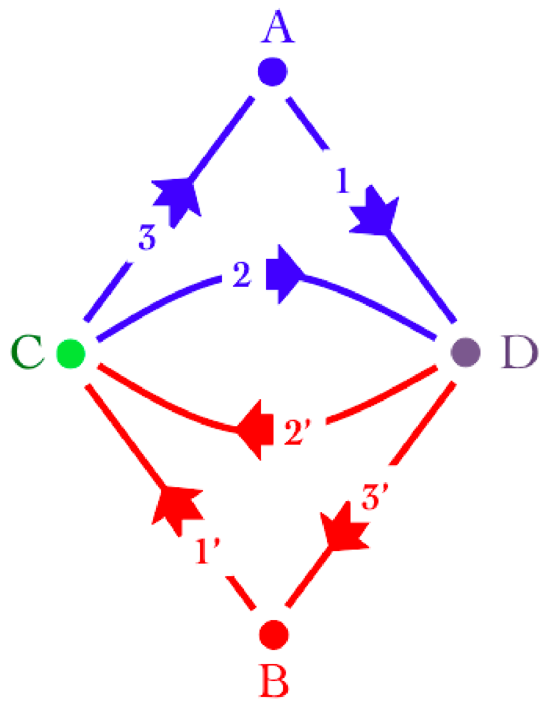
The Fibonacci Sequence



- Gähler-Anderson-Putnam graph for 2.2-collared tiles -

The Thue-Morse Tiling

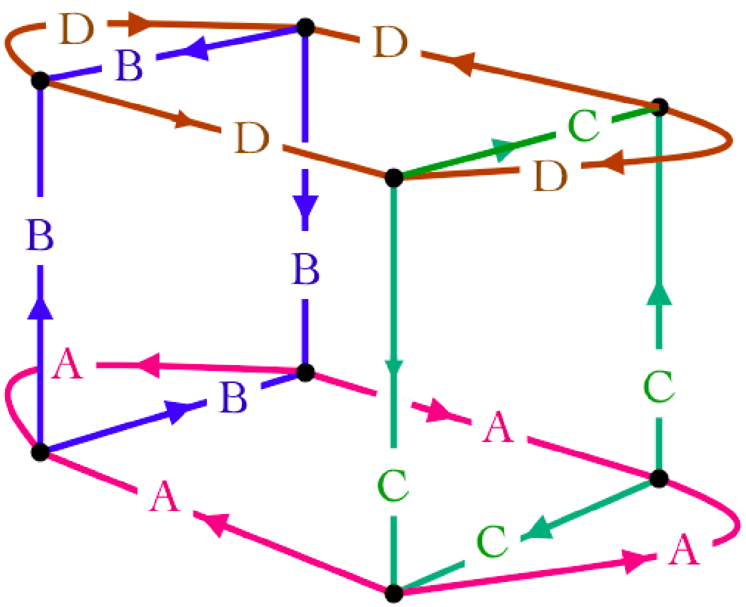
- **Alphabet:** $\mathcal{A} = \{a, b\}$
- **Thue-Morse sequences:** generated by the *substitution* $a \to ab$, $b \to ba$ starting from either $a \cdot a$ or $b \cdot a$



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

The Rudin-Shapiro Tiling

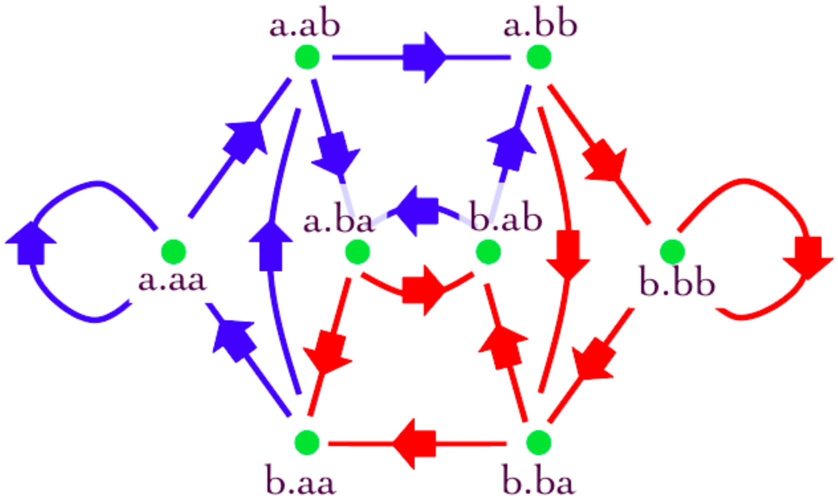
- **Alphabet:** $\mathcal{A} = \{a, b, c, d\}$
- **Rudin-Shapiro sequences:** generated by the *substitution* $a \to ab\,,\ b \to ac\,,\ c \to db\,,\ d \to dc$ starting from either $b \cdot a\,,\ c \cdot a$ or $b \cdot d\,,\ c \cdot d$



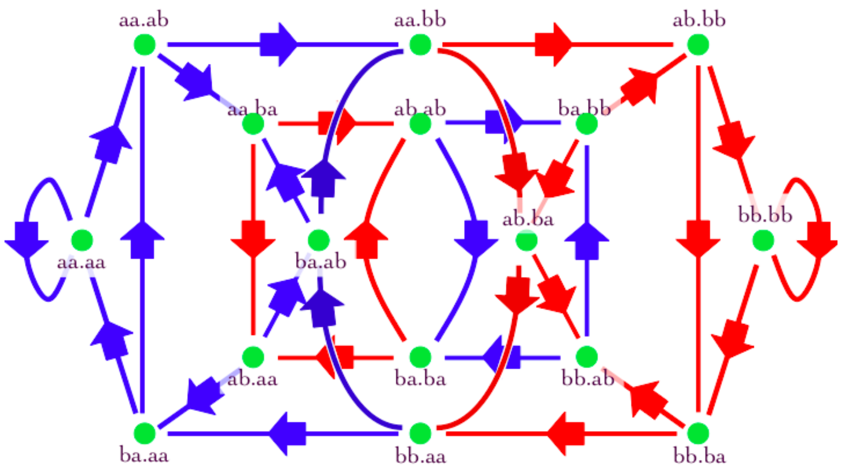
Rudin-Shapiro $\mathcal{G}_{1,1}$

The Full Shift on Two Letters

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



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



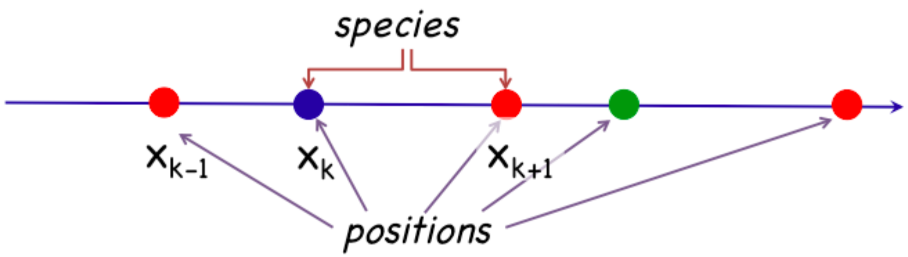
$\mathcal{G}_{2,2}$

III - GAP-graphs

J. E. Anderson, I. Putnam,
Topological invariants for substitution tilings and their associated C^*-algebras,
Ergodic Theory Dynam. Systems, **18**, (1998), 509-537.

F. Gähler, Talk given at *Aperiodic Order, Dynamical Systems, Operator Algebra and Topology*
Victoria, BC, August 4-8, 2002, *unpublished*.

One-Dimensional FLC Atomic Sets



- Atoms are labelled by their *species* (color c_k) and by their *position* x_k with $x_0 = 0$
- The *colored proto-tile* is the pair $([0, x_{k+1} - x_k], c_k)$
- **Finite Local Complexity:** *(FLC)*
  the set $\mathcal{A}$ of colored proto-tiles is *finite*,
  it plays the role of an *alphabet*.
- The atomic *configuration* $\mathcal{L}$ is represented by a *dotted infinite word*

$$\cdots\ a_{-3}\ a_{-2}\ a_{-1} \bullet a_0\ a_1\ a_2\ \cdots \qquad\qquad \bullet\ =\ \textbf{origin}$$

Collared Proto-points and Proto-tiles

- The set of *finite sub-words* in the atomic configuration $\mathcal{L}$ is denoted by $\mathcal{W}$ and called the *dictionary* of $\mathcal{L}$
- If $u \in \mathcal{W}$ is a finite word, $|u|$ denotes its *length*.
- $\mathcal{V}_{l,r}$ is the set of (l, r)-*collared proto-point*, namely, a dotted word $u \cdot v$ with

$$uv \in \mathcal{W} \qquad |u| = l \qquad |v| = r$$

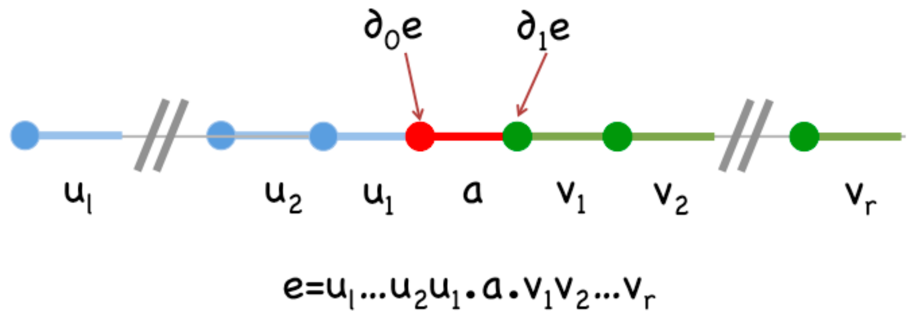
- $\mathcal{E}_{l,r}$ is the set of (l, r)-*collared proto-tiles*, namely, a dotted word $u \cdot a \cdot v$ with

$$a \in \mathcal{A} \qquad uav \in \mathcal{W} \qquad |u| = l \qquad |v| = r$$

Restriction and Boundary Maps

- If $l' \geq l$ and $r' \geq r$ then $\pi^{v}_{(l,r)\leftarrow(l',r')} : \mathcal{V}_{l',r'} \to \mathcal{V}_{l,r}$ is the natural *restriction map* pruning the $l' - l$ leftmost letter and the $r' - r$ rightmost letters $\Rightarrow$ compatibility.
- Similarly $\pi^{e}_{(l,r)\leftarrow(l',r')} : \mathcal{E}_{l',r'} \to \mathcal{E}_{l,r}$, $\Rightarrow$ compatibility.
- **Boundary Maps:** if $e = u \cdot a \cdot v \in \mathcal{E}_{l,r}$ then

$$\partial_0 e = \pi^{v}_{(l,r)\leftarrow(l,r+1)}(u \cdot av) \qquad \partial_1 e = \pi^{v}_{(l,r)\leftarrow(l+1,r)}(ua \cdot v)$$



GAP-graphs

- **GAP:** stands for Gähler-Anderson-Putnam
- **GAP-graph:** $\mathcal{G}_{l,r} = (\mathcal{V}_{l,r}, \mathcal{E}_{l,r}, \partial_0, \partial_1)$ is an oriented graph.
- The restriction map $\pi_{(l,r)\leftarrow(l',r')} = (\pi^v_{(l,r)\leftarrow(l',r')}, \pi^e_{(l,r)\leftarrow(l',r')})$ is a *graph map (compatible with the boundary maps)*

$$\pi_{(l,r)\leftarrow(l',r')} : \mathcal{G}_{l',r'} \to \mathcal{G}_{l,r}$$

$$\pi_{(l,r)\leftarrow(l',r')} \circ \pi_{(l',r')\leftarrow(l'',r'')} = \pi_{(l,r)\leftarrow(l'',r'')}$$ **(compatibility)**

$$(l,r) \leq (l',r') \leq (l'',r'')$$ (**with** $(l,r) \leq (l'r') \Leftrightarrow l \leq l'\,,\; r \leq r'$)

GAP-graphs Properties

- **Theorem** *If* $n = l + r = l' + r'$ *then* $\mathcal{G}_{l,r}$ *and* $\mathcal{G}_{l',r'}$ *are isomorphic graphs. They all might be denoted by* $\mathcal{G}_n$

- *Any GAP-graph is connected without dandling vertex*

- **Loops are Growing:** *if* $\mathcal{L}$ *is aperiodic the minimum size of a loop in* $\mathcal{G}_n$ *grows to infinity as* $n \to \infty$

Complexity Function

- The *complexity function* of $\mathcal{L}$ is $p = (p(n))_{n\in\mathbb{N}}$ where $p(n)$ is the number of words of length n.
- $\mathcal{L}$ is *Sturmian* if $p(n) = n + 1$
- $\mathcal{L}$ is *amenable* if

$$\lim_{n\to\infty} \frac{p(n+1)}{p(n)} = 1$$

- The *configurational entropy* of a sequence is defined as

$$h = \limsup_{n\to\infty} \frac{\ln(p(n))}{n}$$

- *Amenable sequence have zero configurational entropy*

Branching Points of a GAP-graph

- *Branching points* play the role of a *boundary*.
- A vertex v of $\mathcal{G}_{l,r}$ is a *forward branching point* if there is more then one edge starting at v. It is a *backward branching point* if there is more then one edge ending at v.
- The number of *forward (backward)* branching points is bounded by $p(n+1) - p(n)$

Branching Points of a GAP-graph

- *Any GAP-graph of a Sturmian sequence has at most one forward and one backward branching points.*

- *$\mathcal{L}$ is amenable if and only if the number of branching points in $\mathcal{G}_n$ becomes eventually negligible as $n \to \infty$*

- *If the configurational entropy h is positive the ratio of the number of branching points in $\mathcal{G}_n$ to the number of vertices is bounded below by $e^h - 1$ in the limit $n \to \infty$*

Tiling Space

- The *tiling space* Ξ of $\mathcal{L}$ is the set of all tilings having the same *dictionary* as $\mathcal{L}$.
- For any *FLC* tiling, the tiling space is *completely disconnected*.
  (Kellendonk '96)
- If Ξ has *no periodic point* under the translation group it is a *Cantor set*.

Periodic Approximations

- **Result 1:** *The family of simple non self-intersecting loops in one of the GAP-graphs leads to periodic approximations without defects in the infinite period limit.*

- **Result 2:** *The family of all simple non self-intersecting loops in all GAP-graphs can be glued to the tiling space* Ξ *to make up a compact metric space* X.

IV - Spectral Properties

Pattern Equivariance

- Hamiltonian considered are *one dimension lattice models* of the form

$$(H\psi)(n) = \sum_{m\in\mathbb{Z}} h_m(n)\psi(n-m)$$

- H is pattern-equivariant *(Kellendonk)* whenever
  - **Finite Range:** there is $M > 0$ such that the coefficients $h_m(n)$ vanish for $m > M$,
  - **Local Pattern** there is $N > 0$ such that each coefficient $h_m(n)$ is defined only by the local environment of the site n at distance N.

Main Result

Theorem

Let H be a pattern equivariant self-adjoint operator defined on a one-dimensional aperiodic FLC lattice.

Then there is a sequence of periodic approximants, the spectrum of which converges in the Hausdorff metric as the period goes to infinity.

In addition the spectral measures of the approximants converges weakly to the spectral measure of the limit

Expectation: The convergence of the spectrum is *exponentially fast* *w.r.t.* the period.

Convergence Techniques

- Each triple $(r, \wp, u)$ where $r \in \mathbb{N}$ and $\wp$ is a simple non self-intersecting loop in the GAP-graph $\mathcal{G}_{r,r}$ and $u \in \wp$ defines a *periodic approximation* $H_{r,\wp,u}$ of H.

- Each point $\xi \in \Xi$ defines an *atomic configuration* $\mathcal{L}_\xi$ and thus an *Hamiltonian* H_ξ defined like H on $\mathcal{L}$.

- If $(r, \wp, u)$ *converges* in X to a point $\xi \in \Xi$, then the family $H_{r,\wp,u}$ converges to H_ξ, in the sense of *continuous family* of operators.

Convergence Techniques

- **Corollary** *The spectrum edges and the gap edges of the field* $\left(H_{n,\wp}\right)_{n,\wp}$ *converges to the spectrum edges and the corresponding gap edges of* H_ξ *as* $n \to \infty$.

- **Proposition** *The spectral measures of the field* $\left(H_{n,\wp}\right)_{n,\wp}$ *converges weakly to the corresponding spectral measures of* H_ξ *as* $n \to \infty$.

Lipshitz Constant

- Let (T, d) be a complete metric space. A function $f : T \to \mathbb{C}$ is called *Lipshitz continuous* on T if there is a constant $K > 0$ such that

$$|f(s) - f(t)| \leq K\, d(s,t)\,, \qquad\qquad s,t \in T$$

- If $f : T \to \mathbb{C}$ is Lipshitz continuous it *Lipshitz constant* is defined by

$$\|f\|_{Lip} = \sup_{s \neq t} \frac{|f(s) - f(t)|}{d(s,t)}$$

Gap Edges Continuity

- **Definition** *Let* (T, d) *be a complete metric space. A family* $(A_t)_{t\in T}$ *of self-adjoint operators on a Hilbert space* $\mathcal{H}$ *is called Lipshitz continuous if the maps* $t \in T \mapsto \|A_t^2 + aA_t + b\|$ *are uniformly Lipshitz for* a, b *in a compact subset of* $\mathbb{R}$.

- **Theorem** *If* $(A_t)_{t\in T}$ *is a Lipshitz continuous family of self-adjoint operators on the Hilbert space* $\mathcal{H}$*, such that* $\sup_t \|A_t\| < \infty$*, then the spectrum edges and the gap edges of the spectrum of* A_t *are Lipshitz continuous* w.r.t. $t \in T$ *as long as the corresponding gap is open, and Hölder continuous of exponent* $1/2$ *otherwise.*

Noncommutative Geometry Tools

- *C^*-algebras* of operator with unit are used as the *noncommutative* analog of *compact space*.
- *Spectral triples* (Connes, '94) are used as the noncommutative analog of *compact metric space*.
- This *may allow* to prove that the family $H_{r,\wp,u}$ together with its limit points H_ξ is *Lipshitz continuous*.

Conclusion

Interpretation

- **Noncommutative Geometry versus Analysis:** The previous formalism puts together both the knowledge about the tiling space developed during the last fifteen years and the C^*-algebraic approach proposed since the early 80's to treat the electronic properties of aperiodic solids.

- **Finite Volume Approximation:** the Anderson-Putnam complex, presented here in the version proposed by Franz Gähler, provides a way to express the finite volume approximation without creating spurious boundary states.

Defects

- **Defects and Branching Points:** The main new feature is the appearance of defects expressed combinatorially in terms of the branching points.

- **Branching:** Since branching comes from an ambiguity in growing clusters, it is likely that such defects be systematic in any material which can be described through an FLC tiling.

- **Amenability:** If the tiling is *not amenable*, the accumulation of defects makes the present approach inefficient. The use of techniques developed for disordered systems might be more appropriate.

Prospect

- **Continuous case:** This formalism can be extended to the case of the continuous Schrödinger equation with similar consequences.
- **Higher Dimension:** It also extends to higher dimensional colored tilings. However, the geometry is much more demanding.
- **A Conjecture:** The most expected result is the following conjecture
  in dimension $d \geq 3$ in the perturbative regime, namely if the potential part is small compared to the kinetic part, the Schrödinger operator for an electron in the field of an FLC configuration of atoms should have a purely absolutely continuous simple spectrum
- **Level Repulsion:** It is expected also that this *a.c. spectrum* corresponds to a *Wigner-Dyson statistics of level repulsion*.