

Periodic Approximant to Aperiodic Hamiltonians

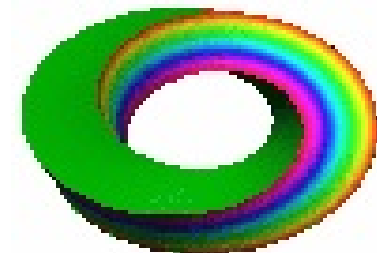
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Main Result

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 exponentially fast w.r.t. the period, in the *Hausdorff metric*.

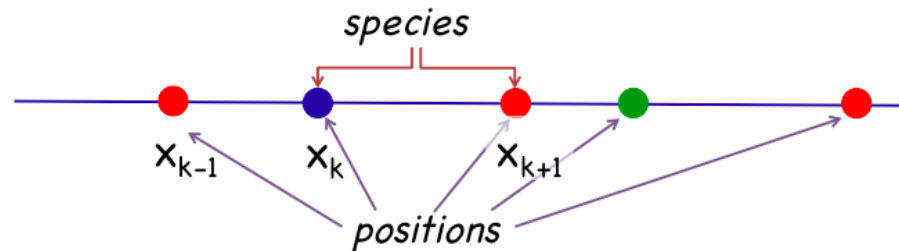
In addition the spectral measures of the approximants converges weakly to the spectral measure of the limit

I - GAP-graphs

J. E. ANDERSON, I. PUTNAM,
Topological invariants for substitution tilings and their associated C^ -algebras,*
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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*

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

Collared Proto-points and Proto-tiles

- The set of *finite sub-words* in the atomic configuration \mathcal{L} is denoted by \mathcal{W}
- 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

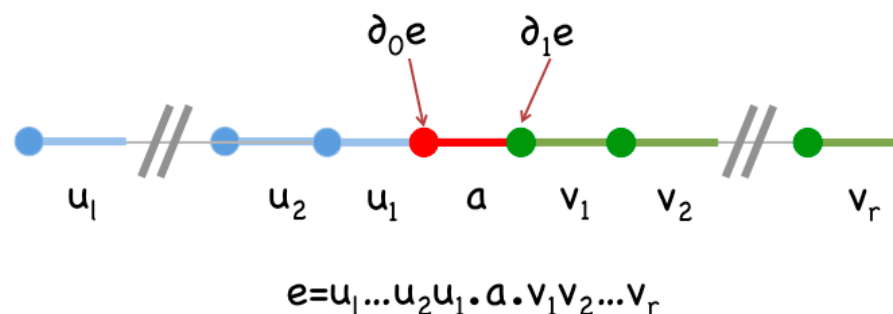
$$a \in A \qquad uav \in \mathcal{W} \qquad |u| = l \qquad |v| = r$$

Restriction and Boundary Maps

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

$$\partial_0 e = \pi_{(l,r) \leftarrow (l,r+1)}^v (u \cdot av)$$

$$\partial_1 e = \pi_{(l,r) \leftarrow (l+1,r)}^v (ua \cdot v)$$



GAP-graphs

- **GAP:** stands for **GÄHLER-ANDERSON-PUTNAM**
- **GAP-graph:** $\mathcal{G}_{l,r} = (\mathcal{V}_{l,r}, \mathcal{E}_{l,r}, \partial)$ is an oriented graph.
- The restriction map $\pi_{(l,r) \leftarrow (l',r')} = (\pi_{(l,r) \leftarrow (l',r')}^v, \pi_{(l,r) \leftarrow (l',r')}^e)$ is a *graph map* (compatible with the boundary maps)

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

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

$$(l,r) \leq (l',r') \leq (l'',r'') \quad \text{(with } (l,r) \leq (l',r') \Leftrightarrow l \leq l', r \leq r')$$

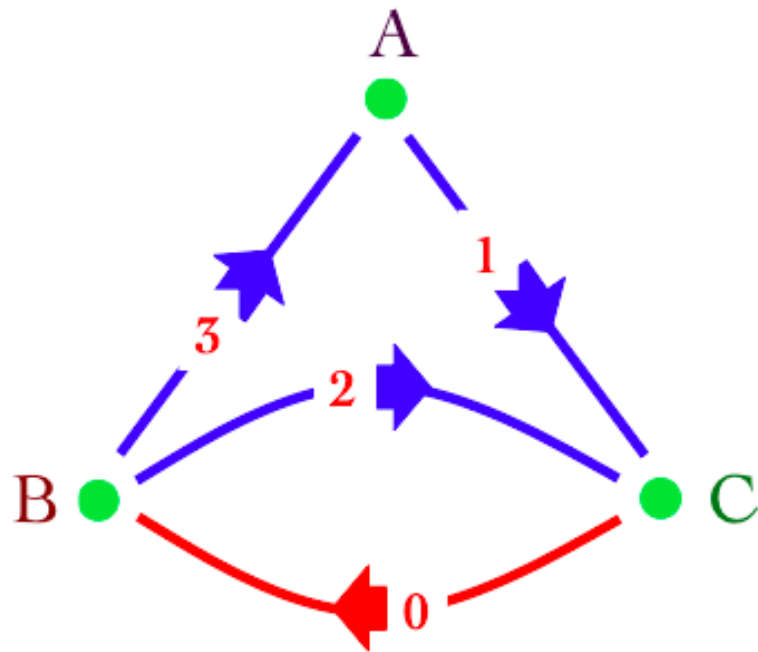
GAP-graphs Properties

- **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 as $n \rightarrow \infty$*

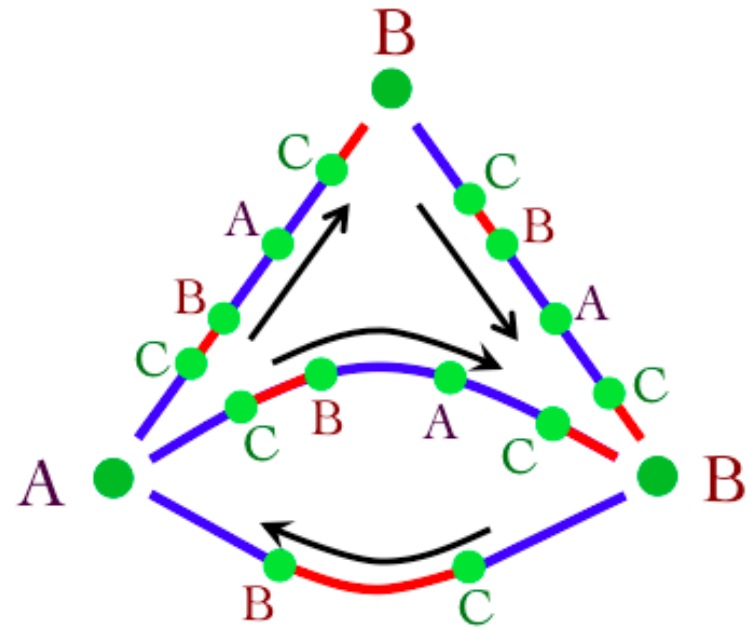
II - Examples of GAP-graphs

The Fibonacci Tiling

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



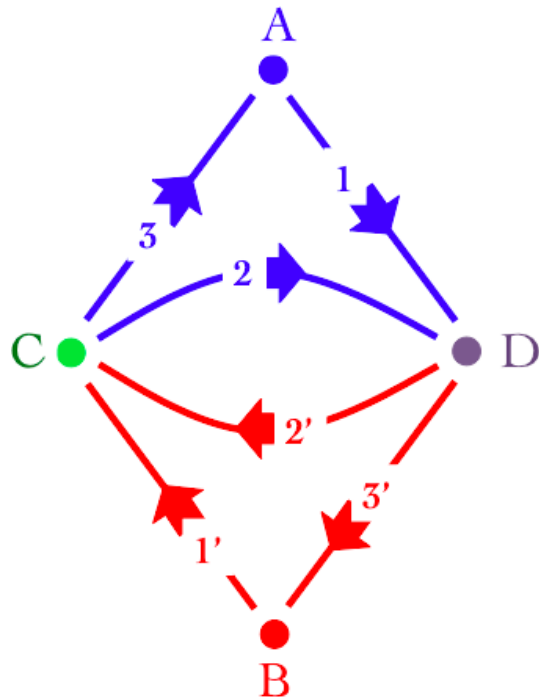
Left: $\mathcal{G}_{1,1}$



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

The Thue-Morse Tiling

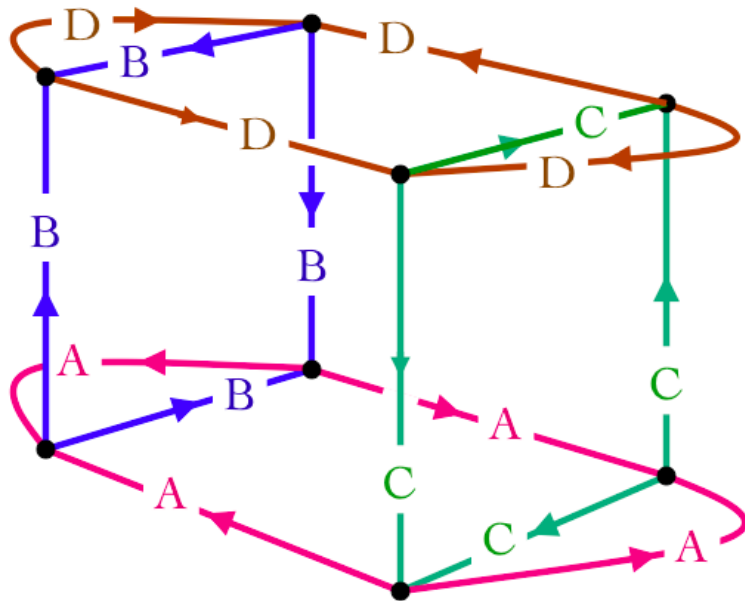
- **Alphabet:** $\mathcal{A} = \{a, b\}$
- **Thue-Morse sequences:** generated by the *substitution* $a \rightarrow ab, b \rightarrow ba$ starting from either $a \cdot a$ or $b \cdot a$



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

The Rudin-Shapiro Tiling

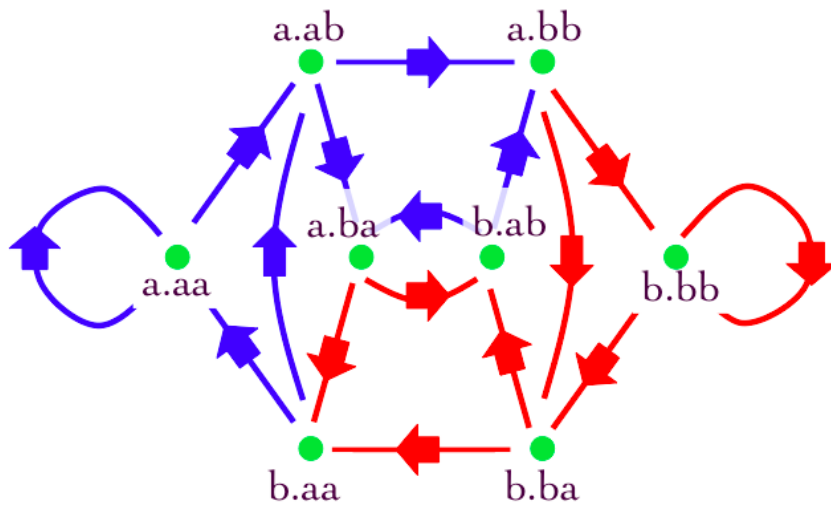
- **Alphabet:** $\mathcal{A} = \{a, b, c, d\}$
- **Rudin-Shapiro sequences:** generated by the *substitution* $a \rightarrow ab, b \rightarrow ac, c \rightarrow db, d \rightarrow dc$ starting from either $b \cdot a, c \cdot a$ or $b \cdot d, c \cdot d$



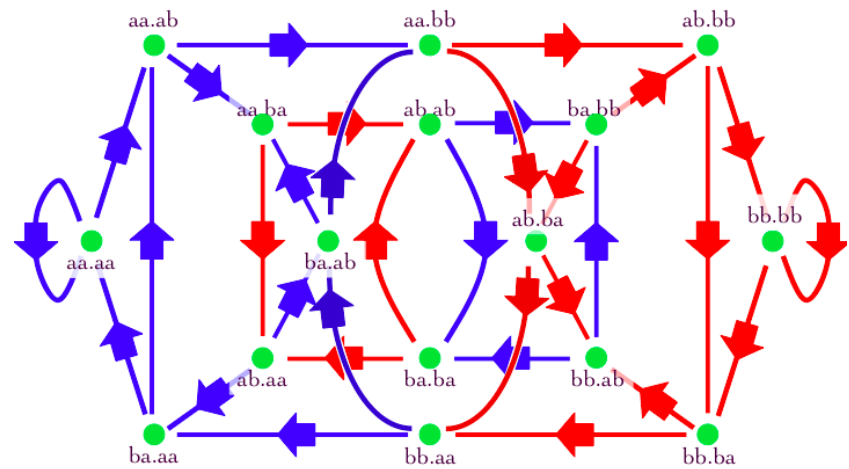
Rudin-Shapiro $\mathcal{G}_{1,1}$

The Full Shift on Two Letters

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



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



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

III - Graph Complexity

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

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

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

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

- *Amenable sequence have zero configurational entropy*

Branching Points of a GAP-graph

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

IV - Global Properties

The Tiling Space

- The ordered set $\{(l, r) \in \mathbb{N}^2; \leq\}$ is a *net* and the restriction maps are *compatible*.
- The *tiling space* of \mathcal{L} is the inverse limit

$$\Xi = \varprojlim \left(\mathcal{V}_{l,r}, \pi_{(l,r) \leftarrow (l',r')}^v \right)$$

- *The Tiling Space of \mathcal{L} is compact and completely disconnected. If no element of Ξ is periodic then Ξ is a Cantor set.*
- *The Tiling Space of \mathcal{L} can be identified with the subset of the orbit of \mathcal{L} by translation, made of configurations with one atom at the origin.*

The Groupoid of the Transversal

- Given a letter $a \in \mathcal{A}$, let $\Xi(\cdot a)$ (resp. $\Xi(a\cdot)$) be the set of points in Ξ made of sequences of the form $u \cdot av$ (resp. $ua \cdot v$) with u, v one-sided infinite words. Then there is a canonical homeomorphism $s_a : \Xi(\cdot a) \rightarrow \Xi(a\cdot)$ obtained from the inverse limit of the GAP-graphs as moving the dot by one edge.
- The family of partial maps $\{s_a ; a \in \mathcal{A}\}$ generates a *locally compact étale groupoid* Γ_{Ξ} with unit space Ξ .

The Lagarias group

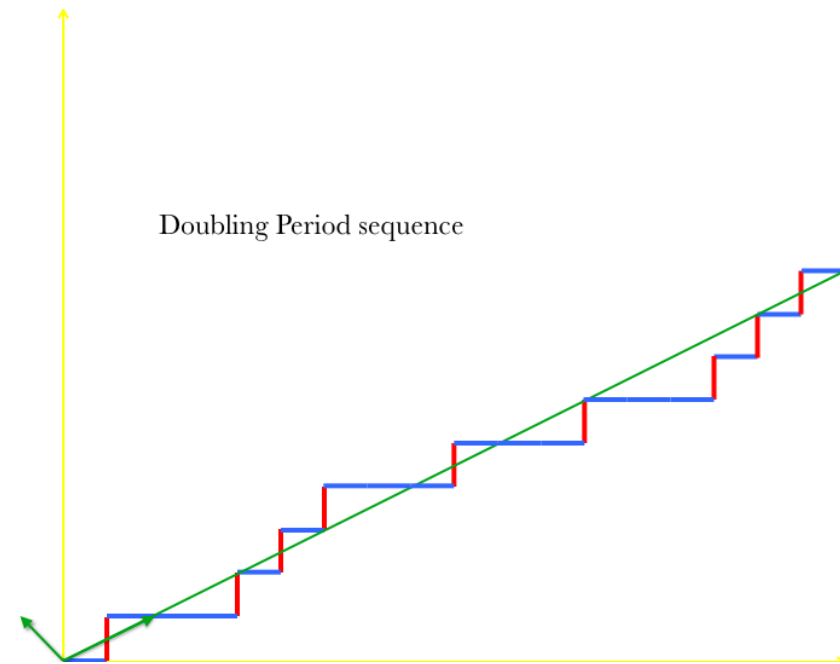
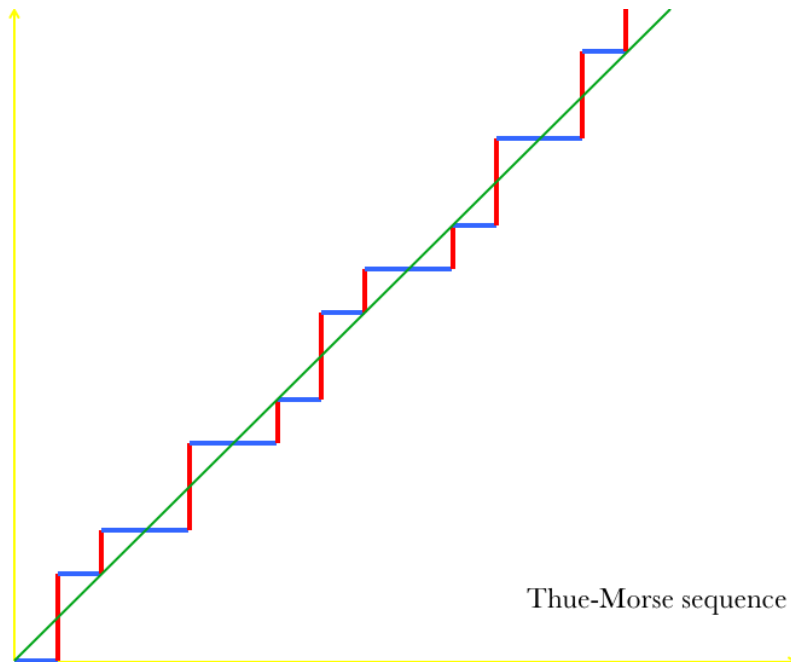
- The *Lagarias group* \mathbb{L} is the free abelian group generated by the alphabet \mathcal{A} . *By FLC, \mathbb{L} has finite rank.*
- Given a GAP-graph \mathcal{G}_n , $\mathbb{L}_n \subset \mathbb{L}$ is the subgroup generated by the words representing the union of edges separating two branching points. *\mathbb{L}_n has finite index.*
- The *Lagarias-Brillouin (LB)-zones* are the dual groups

$$\mathbb{B}_n = \text{Hom}\{\mathbb{L}_n, \mathbb{T}\}$$

- **Reminder:** *If $B \subset A$ are abelian groups with dual A^* , B^* , then B^* is isomorphic to A^*/B^\perp and B^\perp is isomorphic to the dual of A/B*

Address Map

- Since one atom is at the origin, \mathcal{L} can be mapped into the Lagarias group: this is the *address map*.



V - Bloch Theory

Labeling atomic sites

- For $\xi \in \mathbb{E}$ let \mathcal{L}_ξ denotes the atomic configuration associated with ξ , which can be seen as a *doubly infinite dotted word*, the dot representing the position of the origin.
- Letters in \mathcal{A} are the *generators* of \mathbb{L} .
Through the address map, $\mathcal{L}_\xi \subset \mathbb{L}$.
- For a proto-point of the form $v = a_{-l} \cdots a_{-1} \bullet a_1 \cdots a_r$ let $\mathcal{L}_\xi(v)$ denote the set of elements $x \in \mathcal{L}_\xi$ such that

$$x - a_{-1} + \cdots - a_{-i} \in \mathcal{L}_\xi \quad 1 \leq i \leq l$$

$$x + a_1 + \cdots + a_j \in \mathcal{L}_\xi \quad 1 \leq j \leq r$$

Remark: v is a vertex in the GAP-graph $\mathcal{G}_{l,r}$.

Hilbert Spaces

- Through *Fourier transform* $\mathcal{K} = \ell^2(\mathbb{I}) \simeq L^2(\mathbb{B})$.
- Let $\mathcal{H}_\xi = \ell^2(\mathcal{L}_\xi) \subset \mathcal{K}$ with *orthogonal projection* Π_ξ .
- $\mathcal{H}_\xi(v) = \ell^2(\mathcal{L}_\xi(v)) \subset \mathcal{H}_\xi$ with projection $P_\xi(v)$. Then

$$\mathcal{V}_{l,r} \ni v \neq w \Rightarrow P_\xi(v) \perp P_\xi(w)$$

$$\sum_{v \in \mathcal{V}_{l,r}} P_\xi(v) = \Pi_\xi$$

Wannier Transform

- **Wannier transform:** if $f \in \mathcal{H}_\xi$, $v \in \mathcal{V}_{l,r}$, $\kappa \in \mathbb{B}$

$$(\mathcal{W}_\xi f)(v; \kappa) = \sum_{x \in \mathcal{L}_\xi(v)} f(x) e^{i\kappa \cdot x}$$

- **Parseval Formula:**

$$\sum_{v \in \mathcal{V}_{l,r}} \int_{\mathbb{B}} d\kappa |(\mathcal{W}_\xi f)(v; \kappa)|^2 = \sum_{x \in \mathcal{L}_\xi(v)} |f(x)|^2$$

- In particular $\mathcal{W}_\xi f \in \ell^2(\mathcal{V}_{l,r}) \otimes \Pi_\xi L^2(\mathbb{B})$

Shift Representation

- Given a letter $a \in \mathcal{A}$, two vertices $v, w \in \mathcal{V}_{l,r}$ are *a-related*, denoted by $v \xrightarrow{a} w$, if there is an edge $e \in \mathcal{E}_{l,r}$ of the form $u \cdot a \cdot u'$ with $\partial_0 e = v$, $\partial_1 e = w$
- Then

$$\mathcal{W}_\xi P_\xi(w) S_\xi(a) P_\xi(v) \mathcal{W}_\xi^{-1} = \begin{cases} e^{\iota \kappa \cdot a} & \text{if } v \xrightarrow{a} w \\ 0 & \text{otherwise} \end{cases}$$

- Hence $S_\xi(a)$ is associated with the *κ -dependent matrix* indexed by the vertices $\mathcal{V}_{l,r}$

$$S_{v,w}(a; \kappa) = \begin{cases} e^{\iota \kappa \cdot a} & \text{if } v \xrightarrow{a} w \\ 0 & \text{otherwise} \end{cases}$$

A Strategy For Spectral Theory

- Let $H = H^*$ be a *polynomial* w.r.t the shift operators $\{S(a); a \in \mathcal{A}\}$ then:

H is called pattern-equivariant

- Let H_ξ be its representative in \mathcal{H}_ξ :

How can one get its spectral properties ?

- **The Main Idea:**

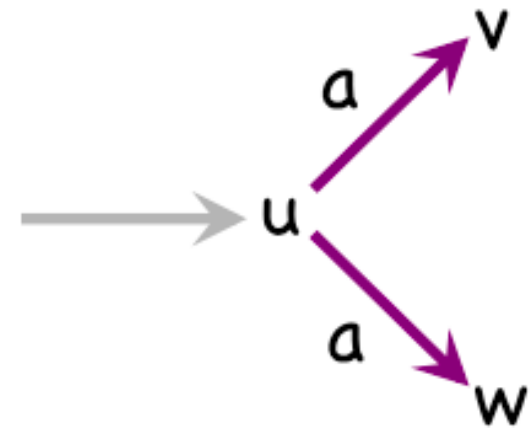
- *Replace H by the corresponding polynomial in the matrices $S_{v,w}(a; \kappa)$,*
- *Compute the spectrum (band spectrum)*
- *Let $(l, r) \rightarrow \infty$*

Hopefully the spectrum of H is recovered in the limit.

The Branching Points Problem

- If u is a branching point *a-related* to both v, w , the matrix $S_{v,w}(a; \kappa)$ admits the following submatrix

$$T = e^{i\kappa \cdot a} \begin{array}{l} u \rightarrow \\ v \rightarrow \\ w \rightarrow \end{array} \overbrace{\begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}}^{u \ v \ w} \Rightarrow \|T^*T\| = 2$$



- Hence $S_{v,w}(a; \kappa)$ cannot be a partial isometry, while $S_{\xi}(a)$ is.

The Branching Points Problem

- The following rules provides a solution: *change* the matrix elements corresponding to the edge $e = v \xrightarrow{a} w$ into χ_e so that

$$T = e^{i\kappa \cdot a} \begin{bmatrix} 0 & 0 & 0 \\ \chi_{uv} & 0 & 0 \\ \chi_{uw} & 0 & 0 \end{bmatrix} \Rightarrow \|T^*T\| = 1$$

- This requires the *formal elements* χ_e 's to commute and satisfy

$$\chi_e^2 = \chi_e = \chi_e^* \quad \sum_{e; \partial_0 e = u} \chi_e = 1 \quad \sum_{e; \partial_1 e = u} \chi_e = 1$$

- This *defect algebra* is commutative and finite dimensional with spectrum given by the set of *branching points* $\mathcal{B}_{l,r}$.

The Branching Points Problem

- Choosing a point in the spectrum of the edge algebra leading to defining *paths* in the GAP-graph.
- In such a case either none of these paths are closed or at least one is closed: a *loop* will design a closed path.
- Loops provide *periodic approximants* for the initial lattice.
- Unclosed paths represents approximants with *defects*

VI - Periodic Approximants

The Augmented Tiling Space

- For each n , the set of *loops* in \mathcal{G}_n is called \mathcal{O}_n
- The idea is to *glue together* the *vertices* of each such loops with the transversal and to define a topology of this set implying that as $n \rightarrow \infty$ the loops are getting closer to \mathbb{E} .
- This can be done using an *ultrametric* d .
- Note: if the initial Delone set is *aperiodic*, the size of the loops goes to *infinity* as $n \rightarrow \infty$.
- The result is the *augmented tiling space* $(\widehat{\mathbb{E}}, d)$

The Augmented Groupoid

- Each loop $\gamma \in \mathcal{O}_n$ admits a (*periodic*) \mathbb{Z} -action by *translation* along the loop. Hence it define a groupoid $\Gamma_{n,\gamma}$.
- The *augmented groupoid* $\widehat{\Gamma}$ is obtained by gluing together all the $\Gamma_{n,\gamma}$'s with the groupoid $\Gamma_{\mathbb{E}}$ of the transversal. This can be done by using a topology implying that given any neighborhood \mathcal{U} of $\Gamma_{\mathbb{E}}$, there is some $N \in \mathbb{N}$ such that if $n > N$ then $\Gamma_{n,\gamma}$ is included in \mathcal{U} .

Continuous Field of Algebras

- The C^* -algebra $C^*(\widehat{\Gamma})$ can be seen as a *continuous field* of C^* -algebras $(C^*(\Gamma_{n,\gamma}))_{n \in \mathbb{N}, \gamma \in \mathcal{O}_n}$.
- Given a letter $a \in \mathcal{A}$ the partial map s_a induces a *partial isometry* $S(a)$ in $C^*(\widehat{\Gamma})$, and consequently, evaluating it on each (n, γ) gives a partial isometry in each of the $C^*(\Gamma_{n,\gamma})$'s.
- The family $\{S(a); a \in \mathcal{A}\}$ generates $C^*(\widehat{\Gamma})$.
- Consequently if $H = H^*$ is a *Hamiltonian* constructed from the $S(a)$'s gives rise to a family $(H_{n,\gamma})_{n \in \mathbb{N}, \gamma \in \mathcal{O}_n}$ of Hamiltonians, which is a *continuous vector field* for the continuous field of C^* -algebras including a family $(H_\xi)_{\xi \in \Xi}$ in the limit $n \rightarrow \infty$.

Convergence Results

J. DIXMIER, *Les C*-algèbres et leurs représentations*, Editions Jacques Gabay, 1969

Definition *Let T be a topological space. A family $(A_t)_{t \in T}$ of self-adjoint operators on a Hilbert space \mathcal{H} is called continuous if the maps $t \in T \mapsto \|p(A_t)\|$ are continuous for each polynomial p .*

Theorem *If $(A_t)_{t \in T}$ is a continuous family of self-adjoint operators on the Hilbert space \mathcal{H} , then the spectrum edges and the gap edges of the spectrum of A_t are continuous w.r.t. $t \in T$.*

Convergence Results

Corollary *The spectrum edges and the gap edges of the field $(H_{n,\gamma})_{n \in \mathbb{N}, \gamma \in \mathcal{O}_n}$ converges to the spectrum edges and the corresponding gap edges of H_ξ as $n \rightarrow \infty$.*

Proposition *The spectral measures of the field $(H_{n,\gamma})_{n \in \mathbb{N}, \gamma \in \mathcal{O}_n}$ converges weakly to the corresponding spectral measures of H_ξ as $n \rightarrow \infty$.*

VII - Lipschitz Continuity

Lipshitz Constant

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

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

- If $f : T \rightarrow \mathbb{C}$ is Lipshitz continuous its *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 Lipschitz continuous if the maps $t \in T \mapsto \|A_t^2 + aA_t + b\|$ are uniformly Lipschitz for a, b in a compact subset of \mathbb{R} .

Theorem If $(A_t)_{t \in T}$ is a Lipschitz 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 Lipschitz continuous w.r.t. $t \in T$ as long as the corresponding gap is open, and Hölder continuous of exponent $1/2$ otherwise.

Lipshitz Continuity of the Norm

Let (T, d) be a *complete metric space*. Let $(A_t)_{t \in T}$ be a family of operators on a Hilbert space \mathcal{H} . Let $D = (D_t)_{t \in T}$ be a family of self adjoint operator on \mathcal{H} such that A_t *leaves the domain* of D_t invariant for all $t \in T$.

Definition *The family $(A_t)_{t \in T}$ is called weakly Lipshitz continuous w.r.t. D whenever each states $\psi \in \mathcal{H}$ the Lipshitz constant of the map $t \in T \mapsto \langle \psi | A_t \psi \rangle$ is bounded by*

$$\| \langle \psi | A_t \psi \rangle \|_{Lip} \leq \sup_{t \in T} \| [D, A_t] \| < \infty$$

Theorem *If $(A_t)_{t \in T}$ is a weakly Lipshitz continuous family of operators on (\mathcal{H}, D) , then $t \in T \mapsto \|A_t\|$ is Lipshitz continuous.*

Ultrametric

- To us the previous arguments, the *augmented tiling space* $\widehat{\mathbb{E}}$ is endowed with an ultrametric d .
- **Remark:** *Let d be an ultrametric. If $F : [0, \infty) \rightarrow [0, \infty)$ is increasing and $F(0) = 0$, then $F(d)$ is an ultrametric.*
- It becomes possible to choose d such that the distance from a loop $\gamma \in \mathcal{O}_n$ to \mathbb{E} is exponentially small in n .

Spectral Triples

A standard construction (I. Palmer '10), leads to a *spectral triple*, namely $(C(\widehat{E}), \mathcal{H}, D)$ where

- \mathcal{H} is a Hilbert space,
- $C(\widehat{E})$ is represented faithfully on \mathcal{H}
- D is a self-adjoint operator on \mathcal{H} with *compact resolvent*
- for $f \in C(\widehat{E})$ Lipschitz continuous, then

$$\|[D, f]\| = \|f\|_{Lip}$$

Metric Bundle Construction

- Including the \mathbb{Z} -action requires an additional construction, called the *metric bundle construction* (Bellissard, Marcolli, Reihani '10).
- This leads to a new spectral triple $(\mathcal{B}, \widehat{\mathcal{H}}, \widehat{D})$, where \mathcal{B} is a C^a -algebra on which the original observable algebra \mathcal{A} acts as *bounded multipliers*.

- The result is

Definition $H = H^*$ is called *pattern equivariant* if it is given by a polynomial in the $S(a)$'s

If $H = H^*$ is a pattern equivariant Hamiltonian then the field $(H_{n,\gamma})_{n \in \mathbb{N}, \gamma \in \mathcal{O}_n}$ is weakly Lipschitz continuous w.r.t. \widehat{D}

Convergence Results

Theorem *The spectral and gap edges of any pattern equivariant Hamiltonian is approximate exponentially fast w.r.t. the period by the spectral and gap edges of its periodic approximants*

Conclusion

Interpretation

- **Noncommutative Geometry versus Combinatoric:** 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.
- **Worms in Quasicrystals:** Such defects actually exist in quasicrystals under the names of *flip-flops, worms or phason modes*. They responsible for the continuous background in the diffraction spectrum.
- **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*.