Bloch Theory for 1D-FLC Aperiodic Media

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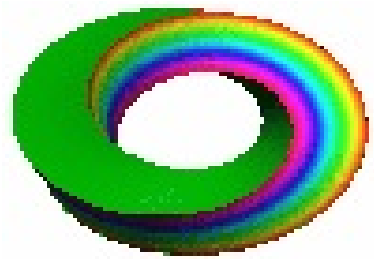

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I - GAP-graphs

J. E. Anderson, I. Putnam,
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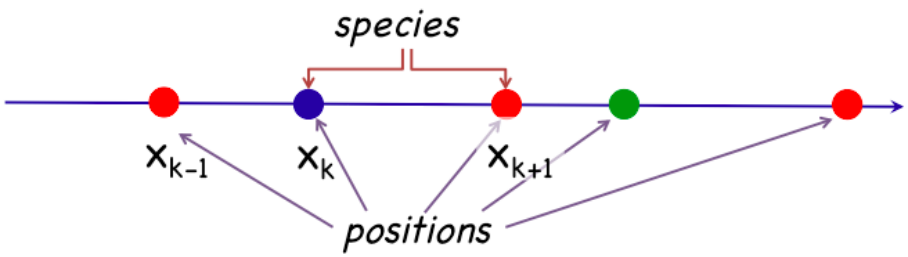
One-Dimensional FLC Atomic Sets



- 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*

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

Collared Proto-points and Proto-tiles

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

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

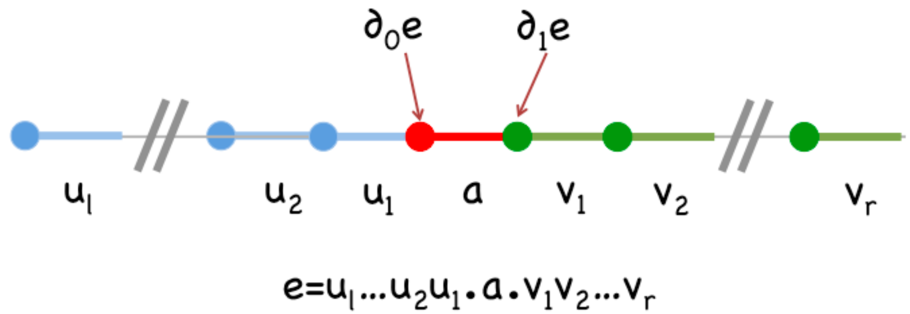
- $\mathcal{E}_{l,r}$ is the set of (l,r)-*collared proto-tiles*, namely, a dotted word $u \cdot a \cdot v$ with

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

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:** $\mathcal{G}_{l,r} = (\mathcal{V}_{l,r}, \mathcal{E}_{l,r}, \partial)$ 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* $\mathcal{G}_n$

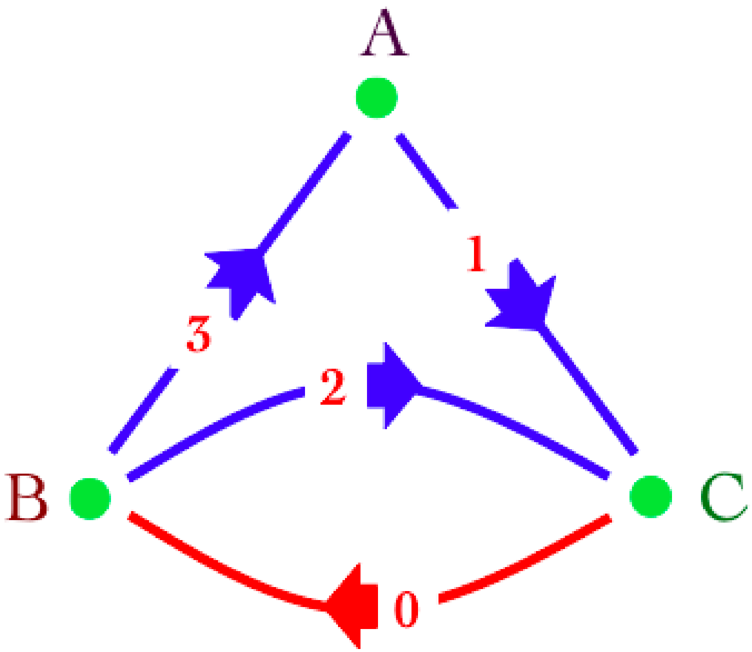
- *Any GAP-graph is connected without dandling vertex*

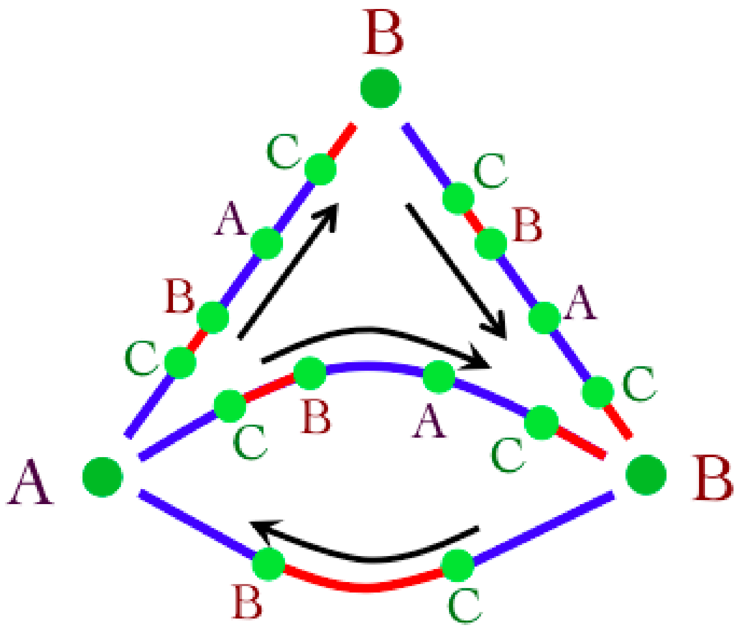
- **Loops are Growing:** *if* $\mathcal{L}$ *is aperiodic the minimum size of a loop in* $\mathcal{G}_n$ *grows as* $n \to \infty$

II - Examples of GAP-graphs

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 $b \cdot a$

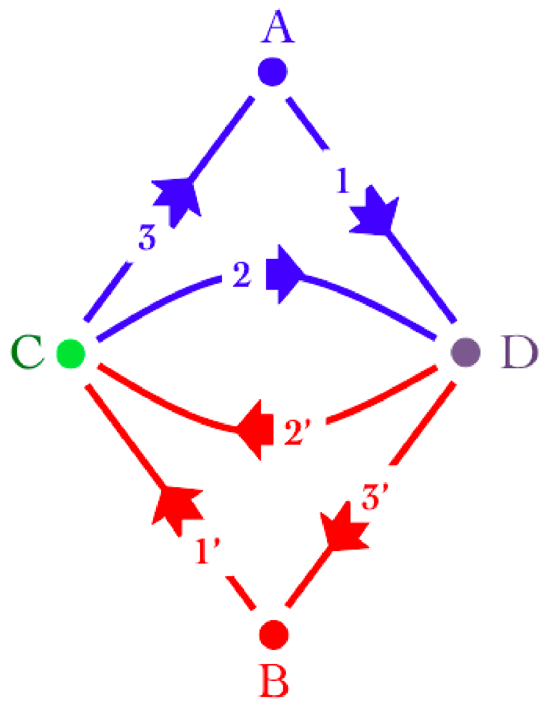




Left: $\mathcal{G}_{1,1}$ *Right:* $\mathcal{G}_{8,8}$

The Thue-Morse Tiling

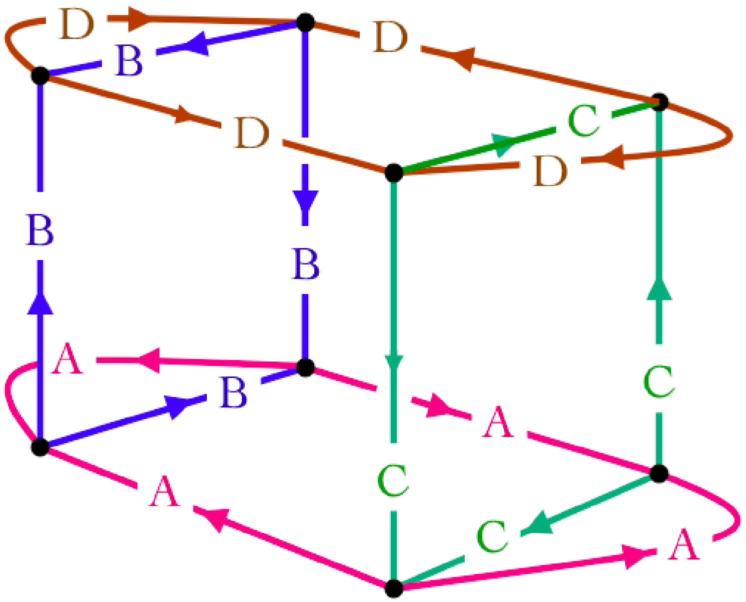
- **Alphabet:** $\mathcal{A} = \{a, b\}$
- **Thue-Morse sequences:** generated by the *substitution* $a \to ab$, $b \to ba$ starting from either $a \cdot a$ or $b \cdot a$



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

The Rudin-Shapiro Tiling

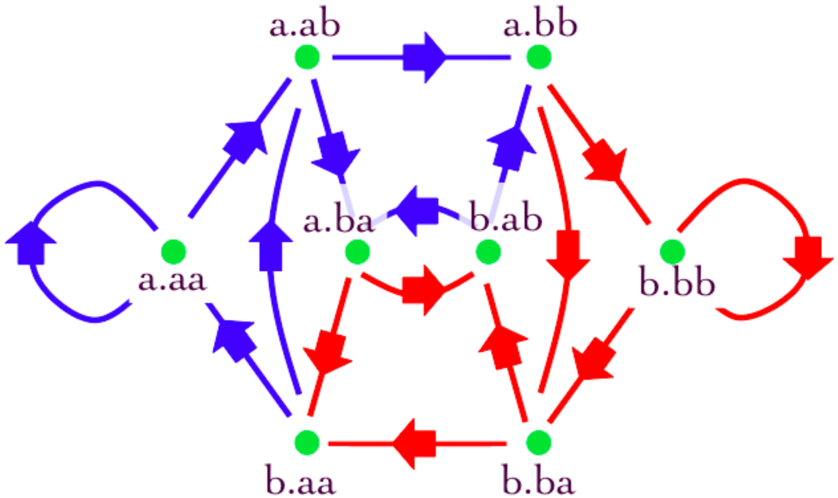
- **Alphabet:** $\mathcal{A} = \{a, b, c, d\}$
- **Rudin-Shapiro sequences:** generated by the *substitution* $a \to ab\,,\ b \to ac\,,\ c \to db\,,\ d \to dc$ starting from either $b \cdot a\,,\ c \cdot a$ or $b \cdot d\,,\ c \cdot d$



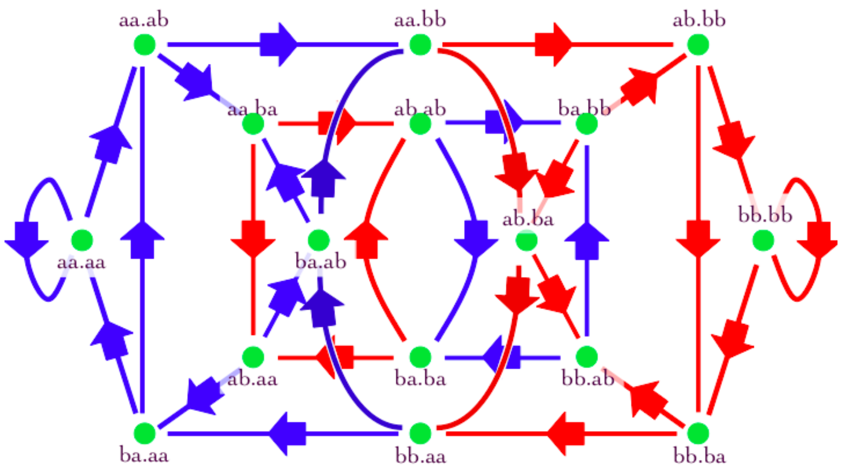
Rudin-Shapiro $\mathcal{G}_{1,1}$

The Full Shift on Two Letters

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



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



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

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

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

- 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

- 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 $p(n+1) - p(n)$
- *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 $n \to \infty$*

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

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

- *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* $s_a : \Xi(\cdot a) \to \Xi(a\cdot)$ *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 with unit space Ξ.

The Lagarias group

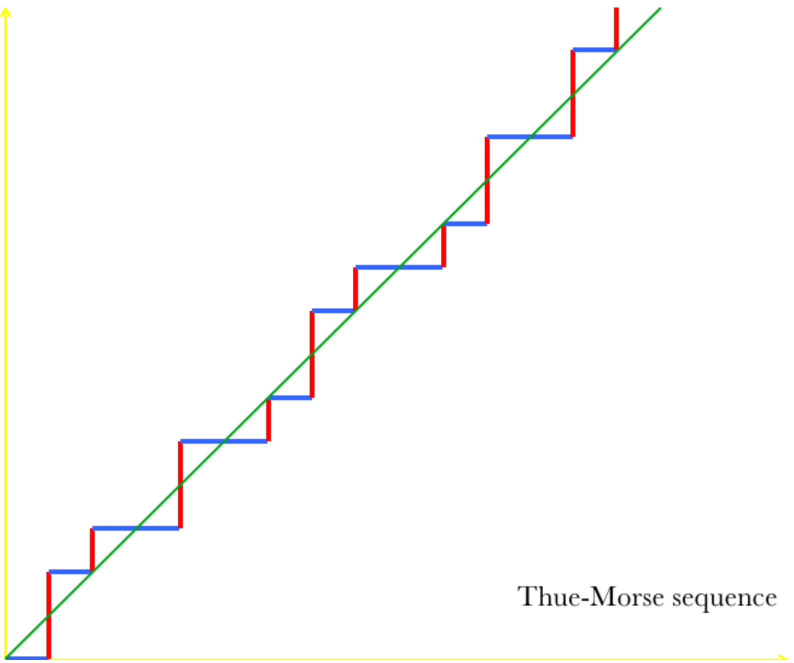
- The *Lagarias group* $\mathbb{L}$ is the free abelian group generated by the alphabet $\mathcal{A}$. *By FLC,* $\mathbb{L}$ *has finite rank.*
- Given a GAP-graph $\mathcal{G}_n$, $\mathbb{L}_n \subset \mathbb{L}$ is the subgroup generated by the words representing the union of edges separating two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

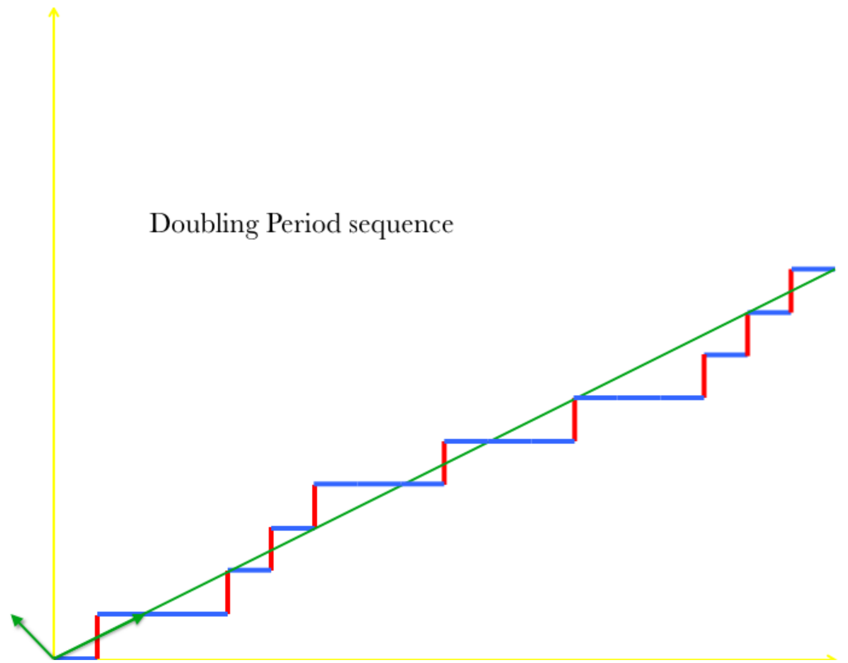
$$\mathbb{B}_n = \mathrm{Hom}\{\mathbb{L}_n, \mathbb{T}\}$$

- **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 $\xi \in \Xi$ let $\mathcal{L}_\xi$ 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

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

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

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

Hilbert Spaces

- Through *Fourier transform* $\mathcal{K} = \ell^2(\mathbb{L}) \simeq L^2(\mathbb{B})$.

- 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

$$v \neq w \;\Rightarrow\; P_\xi(v) \perp P_\xi(w) \qquad\qquad \sum_{v \in \mathcal{V}_{l,r}} P_\xi(v) = \Pi_\xi$$

Wannier Transform

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

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

- **Parseval Formula:**

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

- 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

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

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

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

A Strategy For Spectral Theory

- Let $H = H^*$ be a *polynomial* *w.r.t* the shift operators $\{S(a)\,;\, a \in \mathcal{A}\}$ and let H_ξ be its representative in $\mathcal{H}_\xi$:

How can one get its spectral properties ?

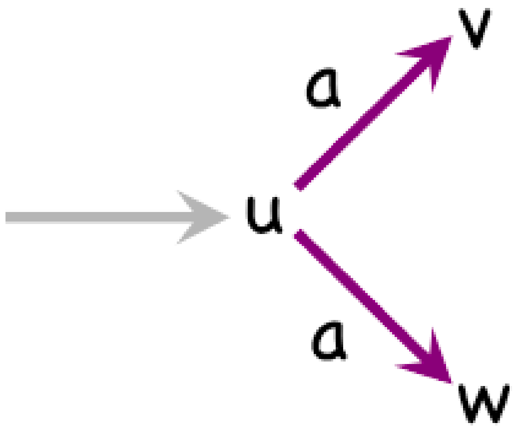
- **The Main Idea:**
  - *Replace H by the corresponding polynomial in the matrices* $S_{v,w}(a;\kappa)$*,*
  - *Compute the spectrum (band spectrum)*
  - *Let* $(l, r) \to \infty$

  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 submatrixs

$$T = e^{\imath\kappa\cdot a} \begin{matrix} u \to \\ v \to \\ w \to \end{matrix} \overbrace{\begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}}^{u \;\; v \;\; w} \Rightarrow \|T^*T\| = 2$$



- 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

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

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

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

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

GAP-Algebras

- Let then $\mathcal{A}_{l,s}$ be the *GAP-Algebra*, namely the C*-algebra generated by the matrix valued functions $(\kappa, \chi) \mapsto S(a; \kappa, \chi)$ defined before.
- Just as for the GAP-graphs $\mathcal{A}_{l,s} \sim \mathcal{A}_{l+1,r-1}$ so as it will be denoted by $\mathcal{A}_n$ if $n = l + r$.
- **Expected Result:**
  - *The family $\mathcal{A}_n$ converges to a C*-algebra $\mathcal{A}_\infty$, in the sense of continuous field of algebras.*
  - *There is an exact sequence $0 \to \mathcal{J} \to \mathcal{A}_\infty \to C^*(\Gamma) \to 0$ where the ideal $\mathcal{J} \sim C(X) \otimes K$ for some completely disconnected space X.*
  - *The nature of X is entirely described by the complexity of the AP-graphs. In particular, if the number of branching points is bounded X is finite.*

Expected Spectral Consequences

- If H is a polynomial in the $S(a)$'s, then it defines a *continuous field* $n \mapsto H_n \in \mathcal{A}_n$ of selfadjoint elements.
- Each H_n has a band spectrum with a *finite number of bands*.
- **Spectral Gaps:** If the expected results hold, then the spectrum of H_∞ is the *limit* (Hausdorff metric) of the spectra of the H_n's.
- **Branching Defect Ideal:** the ideal $\mathcal{J}$ represents the impact of *defects* coming from the branching points boundary conditions.
- The spectrum of H_∞ contains the spectrum of H_ξ, the rest being due to *defects*. In particular, if the number of branching points is bounded, the residual part is made of *a finite number of eigenvalues of finite multiplicities* in each gap.

Expected Spectral Consequences

- **Strong Convergence:** If $f \in \ell^2(\mathcal{L}_\xi)$ has a finite support, then it can be seen as vector in $\ell^2(\mathcal{V}_n)$ for n large enough. It becomes possible to express the concept of *strong convergence*.
- Then the spectral measure of H_n relative to f *weak*-converges* to the spectral measure of H_∞.
- **Traces:** there is a natural trace $\mathcal{T}_n$ on each $\mathcal{A}_n$, another $\mathcal{T}$ on $C^*(\Gamma)$ and $\mathcal{T}_\infty$ on $\mathcal{A}_\infty$. This field of traces is also *continuous* and $\mathcal{T}$ is obtained from $\mathcal{T}_\infty$ by projection.
- $\mathcal{T}_\infty$ *vanishes on the Branching Defect Ideal* $\mathcal{J}$.

Expected Spectral Consequences

- **Density of States:** The DOS is the measure on the real line defined by

$$\int_{-\infty}^{+\infty} g(E)\, d\mathcal{N}_*(E) = \mathcal{T}_*\left(g(H_*)\right) \qquad\qquad * = n, \infty, \cdot$$

  Hence the DOS is expected to comes from the limit if the corresponding measures on each of the $\mathcal{A}_n$.

- In particular, the DOS of H_∞ should *coincide* with the one of H.

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*.