Bloch Theory
for 1D-FLC
Aperiodic Media

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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 \( A \) of colored proto-tiles is finite, it plays the role of an *alphabet*.
- The atomic *configuration* \( L \) is represented by a *dotted infinite word*

\[
\cdots \ a_{-3} \ a_{-2} \ a_{-1} \bullet \ a_0 \ a_1 \ a_2 \ \cdots
\]

\( \bullet = \text{origin} \)
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
  
  $$uv \in \mathcal{W} \quad |u| = l \quad |v| = r$$

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

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

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

$e = u_1 \ldots u_2 u_1 \cdot a \cdot v_1 v_2 \ldots v_r$
• **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^\mathcal{V}(l,r) \leftarrow (l', r'), \pi^\mathcal{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 $(l, r) \leq (l', r') \iff l \leq l', r \leq r'$)
GAP-graphs Properties

• **Theorem** If \( n = l + r = l' + r' \) then \( G_{l,r} \) and \( G_{l',r'} \) are isomorphic graphs. They all might be denoted by \( G_n \)

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

• **Loops are Growing:** if \( L \) is aperiodic the minimum size of a loop in \( G_n \) grows as \( n \to \infty \)
II - Examples of GAP-graphs
The Fibonacci Tiling

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

Left: \( G_{1,1} \)

Right: \( G_{8,8} \)
The Thue-Morse Tiling

- **Alphabet:** \( A = \{a, b\} \)
- **Thue-Morse sequences:** generated by the substitution \( a \to ab, b \to ba \) starting from either \( a \cdot a \) or \( b \cdot a \)
The Rudin-Shapiro Tiling

- **Alphabet:** $A = \{a, b, c, d\}$

- **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 $b \cdot d$, $c \cdot d$
The Full Shift on Two Letters

- **Alphabet:** $\mathcal{A} = \{a, b\}$ all possible word allowed.
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
  \[
  h = \lim_{n \to \infty} \sup \frac{\ln(p(n))}{n}
  \]
- **Amenable sequence** have zero configurational entropy
Branching Points of a GAP-graph

- A vertex \( v \) of \( G_{l,r} \) 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 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 \( G_n \) becomes eventually negligible as \( n \to \infty \).
- If the configurational entropy \( h \) is positive the ratio of the number of branching points in \( G_n \) 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
  \[
  \Xi = \lim_{\leftarrow} \left( \mathcal{V}_{l, r}, \pi^0_{(l, r) \leftarrow (l', r')} \right)
  \]
- The Tiling Space of \( \mathcal{L} \) is compact and completely disconnected. If no element of \( \Xi \) is periodic then \( \Xi \) 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 $a \in A$, let $\Xi(\cdot a)$ (resp. $\Xi(a\cdot)$) be the set of points in $\Xi$ 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 $\{s_a ; a \in A\}$ generates a locally compact étale groupoid $\Gamma$ with unit space $\Xi$. 
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

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

• **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 $\xi$, 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 $\mathcal{IL}$. Through the address map, $\mathcal{L}_\xi \subset \mathcal{IL}$.

- For a proto-point of the form $v = a_{-l} \cdots a_{-1} \cdot a_1 \cdots a_r$ 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 $\mathcal{K} = \ell^2(\mathbb{L}) \cong L^2(\mathbb{B})$.

• Let $\mathcal{H}_\xi = \ell^2(\mathcal{L}_\xi) \subset \mathcal{K}$ with orthogonal projection $\Pi_\xi$.

• $\mathcal{H}_\xi(v) = \ell^2(\mathcal{L}_\xi(v)) \subset \mathcal{H}_\xi$ with projection $P_\xi(v)$. Then

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

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

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

- **Parseval Formula**:

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

- 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 \( v \overset{a}{\rightarrow} w \), 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

\[
\mathcal{W}_\xi P_\xi(w) S_\xi(a) P_\xi(v) W_{\xi}^{-1} = \begin{cases} 
  e^{i\kappa \cdot a} & \text{if } v \overset{a}{\rightarrow} w \\
  0 & \text{otherwise}
\end{cases}
\]

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

\[
S_{v,w}(a; \kappa) = \begin{cases} 
  e^{i\kappa \cdot a} & \text{if } v \overset{a}{\rightarrow} w \\
  0 & \text{otherwise}
\end{cases}
\]
A Strategy For Spectral Theory

• Let $H = H^*$ be a polynomial w.r.t the shift operators $\{S(a); a \in A\}$ and let $H_\xi$ 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 $(l, r) \rightarrow \infty$

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 submatrixs

$$
T = e^{i\kappa \cdot a} 
\begin{bmatrix}
0 & 0 & 0 \\
1 & 0 & 0 \\
1 & 0 & 0
\end{bmatrix}
\Rightarrow \|T^*T\| = 2
$$

• 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 $\chi_e$ so that

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

• This requires the formal elements $\chi_e$'s to commute and satisfy

$$\chi_e^2 = \chi_e = \chi_e^* \quad \sum_{e;\partial_0e=u} \chi_e = 1 \quad \sum_{e;\partial_1e=u} \chi_e = 1$$

• This edge algebra is commutative and finite dimensional with spectrum given by the set of branching points $\mathcal{B}_{l,r}$. 
• 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 $0 \to \mathcal{I} \to \mathcal{A}_\infty \to C^*(\Gamma) \to 0$ where the ideal $\mathcal{I} \sim C(X) \otimes K$ 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 self-adjoint 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 $H_\infty$ is the limit (Hausdorff metric) of the spectra of the $H_n$’s.

• **Branching Defect Ideal:** the ideal $J$ represents the impact of defects coming from the branching points boundary conditions.

• The spectrum of $H_\infty$ contains the spectrum of $H_\xi$, 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 a 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 $H_\infty$.

- **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 $\mathcal{I}$. 
Expected Spectral Consequences

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

\[
\int_{-\infty}^{+\infty} g(E) \, dN_\star(E) = T_\star (g(H_\star)) \quad \star = n, \infty, \cdot
\]

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

• In particular, the DOS of \( H_\infty \) 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 $\mathcal{C}^*$-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.**