Approaches to the study of substitutive quasicrystals

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Outline

Historical introduction

Fundamental approach to aperiodic systems (for today's talk)
- Making aperiodic order using 'substitution' processes
- The "hull": a dynamical systems approach

Matrices and the information they carry
- Beginning bookkeeping: The substitution matrix
- Intermediate bookkeeping: The digit matrix

Renormalization approach to diffraction analysis
- A whirlwind review of mathematical diffraction theory
- Advanced bookkeeping: the Fourier matrix

Setting

- Our objects: a class of aperiodic tilings of Euclidean space
- These tilings display hierarchical structure that is highly ordered yet not periodic.
- The way we study them originates in fields as disparate as logic, geometry, and chemistry.
- I offer a story from each field for motivation.

Story 1 (Logic): The domino problem

- Imagine square tiles whose edges come in given combinations of labelfs.
- You are only allowed to put two tiles next to each other if the edge labels match.

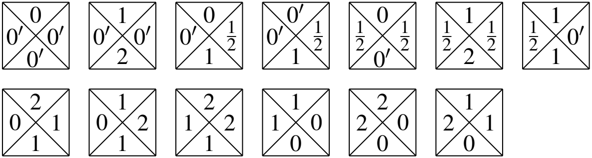

Figure: Jeandel and Rao's aperiodic set (2019).

- Immediate question: Can you make an infinite tiling of the plane with these tiles? (That's the "domino problem".)

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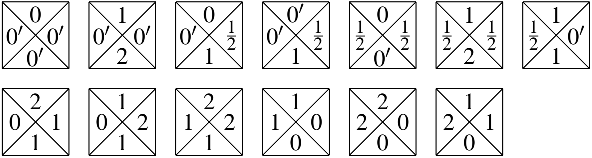


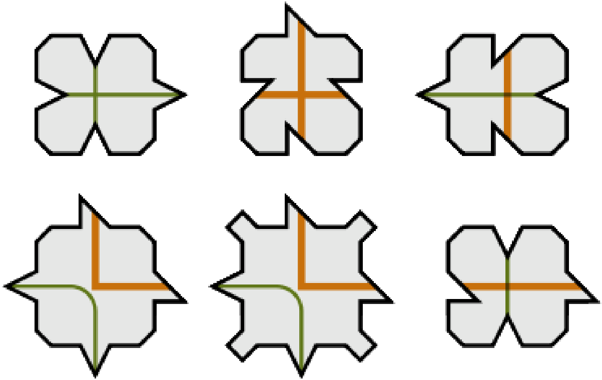
Figure: Jeandel and Rao's aperiodic set (2019).

- Deep question: can you make a Turing machine that answers that question for any finite tile set?
  - This is the question logician Hao Wang was considering in 1961 [**Wang**].

Undecidability of the domino problem

- Can you make a machine that answers that question for any finite tile set?
- The answer depended on whether an *aperiodic prototile set* exists, i.e. a set of tiles that can tile the plane, but only nonperiodicaly.
- In 1966 Wang's student Rober Berger found an aperiodic set of tiles with over 20000 tiles.
- In 1971 Raphael Robinson published an aperiodic set with only 6 tiles.

Robinson's aperiodic tile set



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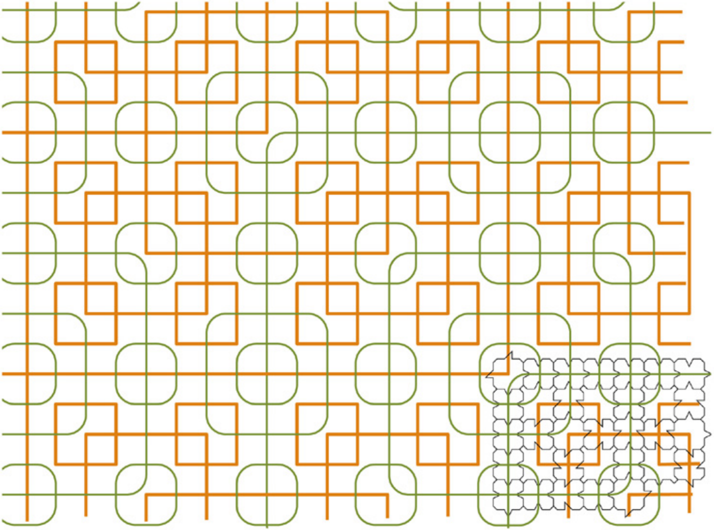
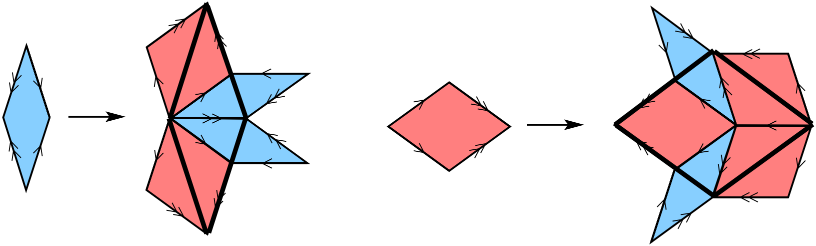
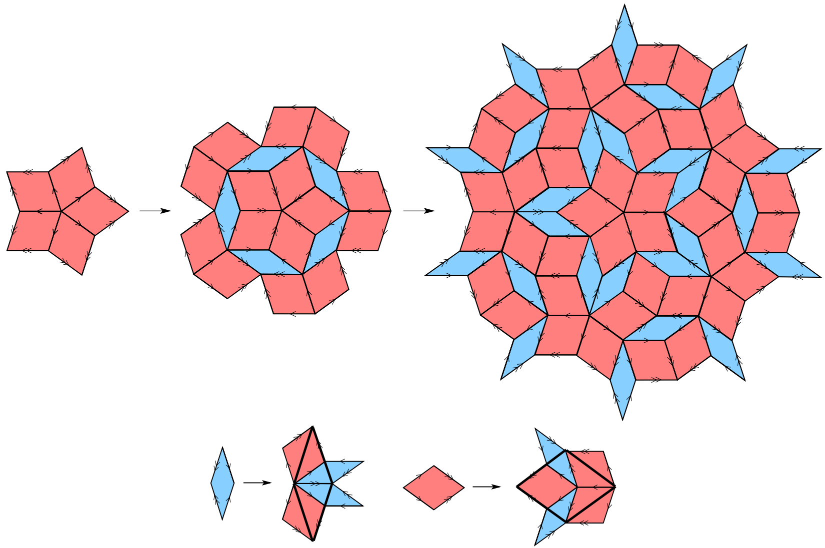


Story 2 (Geometry): Penrose's aperiodic set of two tiles

- Roger Penrose began to develop an interest in tiling questions in part because of Hilbert's Problem 18.
- Also he (and his father) began a collaboration with M. C. Esher.
- Penrose was trying to create a hierarchical tiling and found his original tiling by experimentation.
- He succeeded! There are several equivalent versions of Penrose tilings.
- I recommend Penrose's foreword to Baake/Grimm's **Aperiodic Order** for his telling of the history.





The 2011 Nobel Prize in Chemistry

Daniel Shechtman

"For the discovery of quasicrystals"

‘Impossible’ diffraction image

- Shechtman’s colleague at U.S. NIST made an aluminum-magnesium alloy
- Shechtman did a diffraction analysis and found contradictory properties
  - it had bright spots indicative of a periodic (crystal) atomic structure
  - had symmetries impossible for such a structure

Original diffraction image

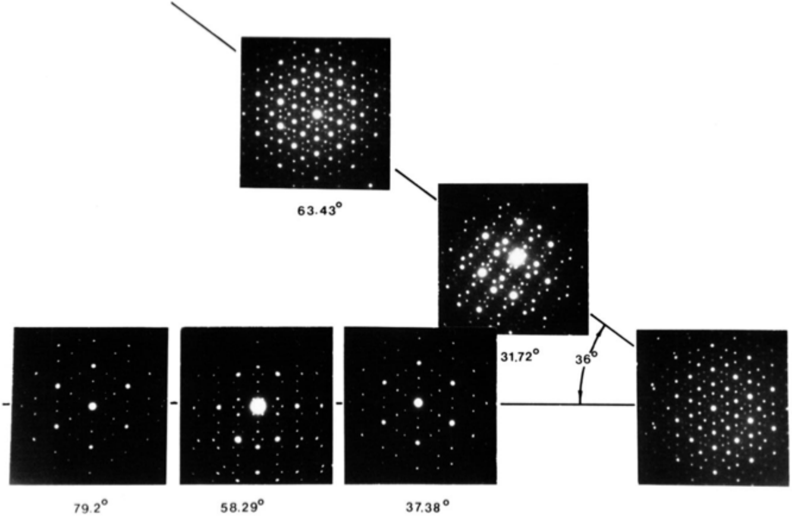
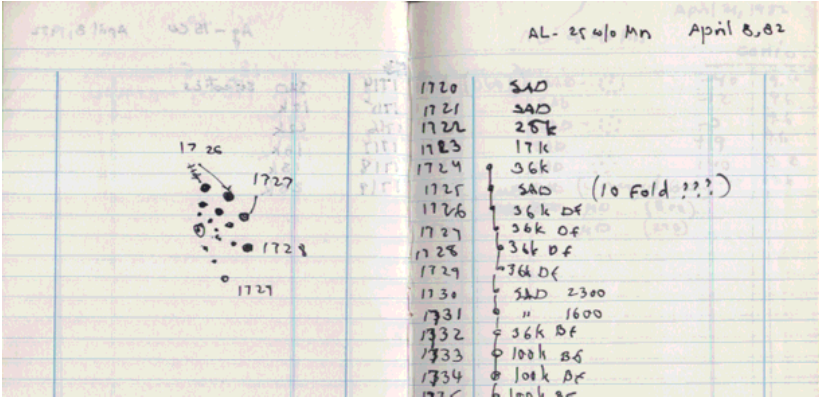
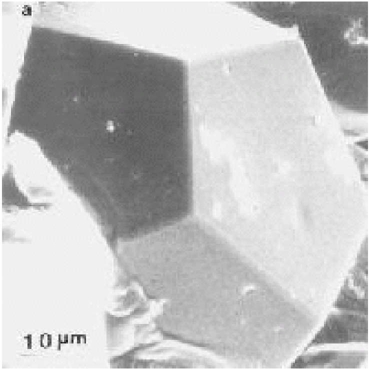


FIG. 2. Selected-area electron diffraction patterns taken from a single grain of the icosahedral phase. Rotations match those in Fig. 1.

Shechtman's original notebook

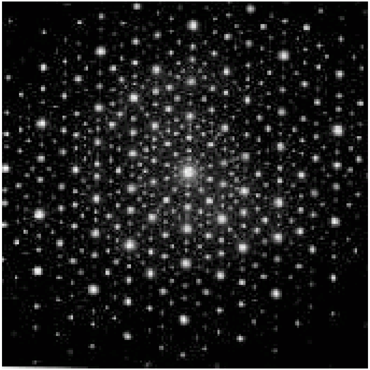


Discovery of Quasicrystals



Single grain of icosahedral Al–Pd–Mn phase

source: A. P. Tsai



Diffraction image of Al6Mn

www.ph.melb.edu.au/diffraction/image/fivefold.html

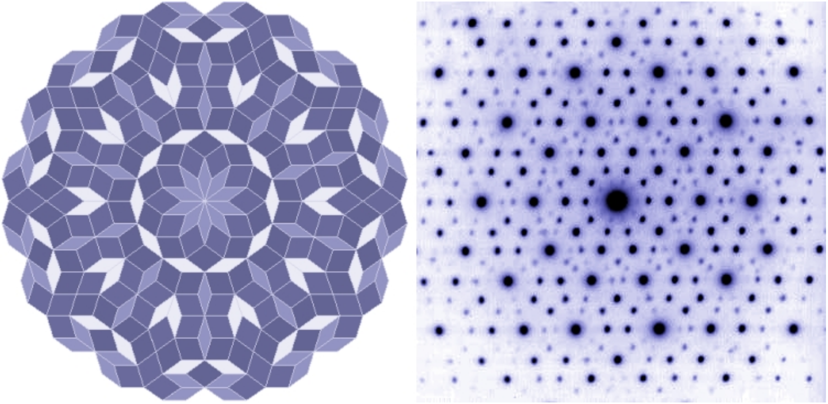


Image source: Oxford Dept. of Chemistry http://www.xtl.ox.ac.uk/tag/penrose-tiling.html

Left: A patch of a Penrose tiling. Right: An electron diffraction pattern of Zn-Mg-Ho alloy.

Connections

- Diffraction image of Penrose tiling (computed by Mackay in 1982) looked like Shechtman's images
- Tilings like the Penrose tiling might be good models for quasicrystals
- Penrose tiles have matching rules like the Robinson tiling
- (Note: there was already a field of one-dimensional supertile construction methods: substitution)
- Some of us analyze the diffraction and/or dynamical spectrum of tilings

An Aperiodic Order community arises

- Mathematical physicists
- Theoretical computer scientists
- Mathematicians with training in ergodic theory and dynamical systems, topology, discrete geometry, functional analysis, and more

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A simple substitution rule

Alphabet $\mathcal{A} = \{1, 2\}$.

Define $\mathcal{S} : \mathcal{A} \to \mathcal{A}^*$ by

$$\boxed{\mathcal{S}(1) = 1222; \quad \mathcal{S}(2) = 1}$$

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A simple tiling substitution rule

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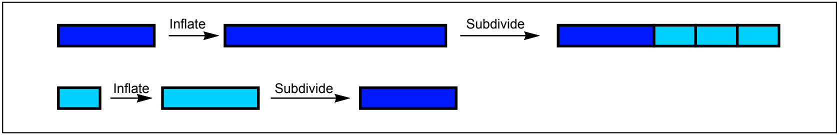

Lengths are $\gamma = \frac{1+\sqrt{13}}{2}$ and 1.

Expansion is by γ.

Self-similar tilings

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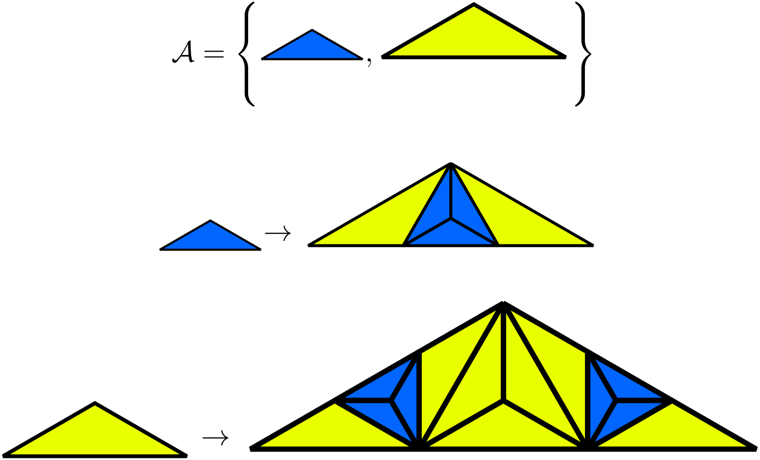
(Expanded support of $\mathfrak{t}$ = Union of supports of its subtiles)

Danzer's "T2000" inflate-and-subdivide rule.



Tiling self-similarity

We can extend $\mathcal{S}$ to tiles, patches, and tilings:

- If $t = \mathfrak{t} - x$ for $\mathfrak{t} \in \mathcal{A}$ and $x \in \mathbb{R}^d$ we define

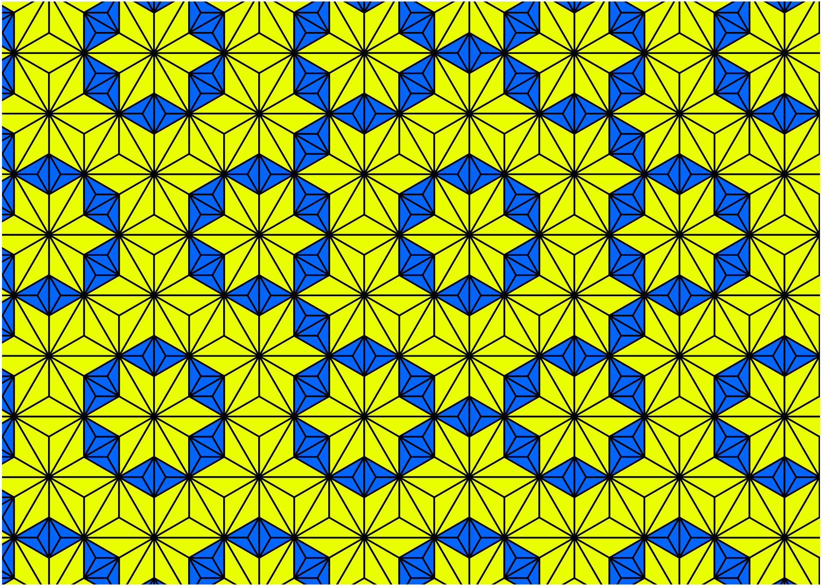
$$\mathcal{S}(t) := \mathcal{S}(\mathfrak{t}) - \phi(x)$$

- $\mathcal{Q}$ patch or tiling:

$$\mathcal{S}(\mathcal{Q}) = \bigcup_{t \in \mathcal{Q}} \mathcal{S}(t)$$

- Lingo: an *n-supertile* is a patch of the form $\mathcal{S}^n(t)$

A tiling $\mathcal{T}$ is said to be **self-similar** if $\mathcal{S}(\mathcal{T}) = \mathcal{T}$.



Outline

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- The metric topology is the product topology
- The action of the dynamics is “shift your sequence one unit to the left”
- Since the metric is origin-centric, the shift action allows us to “see” parts of a sequence that are far away by shifting them to the origin.
- *Subshifts* are closed shift-invariant subspaces

The big ball metric for tilings

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Definition

Let $R(\mathcal{T}, \mathcal{T}')$ be the supremum of all $r \geq 0$ such that there exists $\vec{x}, \vec{y} \in \mathbb{R}^d$ with

1. $|\vec{x}| < 1/2r$ and $|\vec{y}| < 1/2r$, and
2. On the ball of radius r around the origin, $(\mathcal{T} - \vec{x}) \cap B_r(0) = (\mathcal{T}' - \vec{y}) \cap B_r(0)$.

We define

$$d(\mathcal{T}, \mathcal{T}') := \min\left\{\frac{1}{R(\mathcal{T},\ T')}, 1\right\}$$

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The distance between $\mathcal{T}$ and $\mathcal{T}'$ is determined by the largest origin-centered ball the tilings agree on up to a small translation.

Tiling spaces

- $\Omega_{\mathcal{P}}$ = the space of all $\mathcal{P}$-tilings
  - Note: Elements of $\mathcal{A}^{\mathbb{Z}}$ are infinite sequences, likewise elements of $\Omega_{\mathcal{P}}$ are infinite tilings of $\mathbb{R}^d$.

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- We write $(\Omega, \mathbb{R}^d)$ for the dynamical system under the action of translation
  - Unlike the symbolic case, the action is continuous
- There are two particularly nice ways to make tiling spaces:
  - The "hull" of a tiling $\mathcal{T}$
  - The set of all tilings made of specified patches

Two tiling space constructions

To study a given tiling $\mathcal{T}$: The *hull of the tiling* $\mathcal{T}$ is the orbit closure of $\mathcal{T}$:

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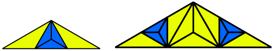
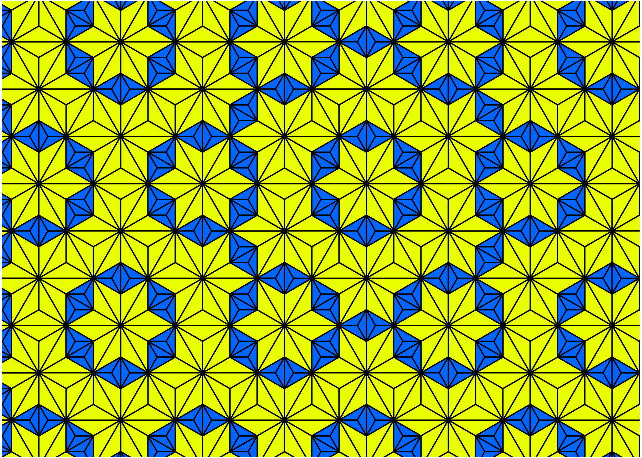
To restrict the patch types: Let $\mathcal{R}$ be a set of $\mathcal{P}$-patches to be used as a 'language'.

We say that $\mathcal{T} \in \Omega_{\mathcal{P}}$ is *allowed* by $\mathcal{R}$ if every patch in $\mathcal{T}$ is translation-equivalent to a subpatch of an element of $\mathcal{R}$.

The tiling space $\Omega_{\mathcal{R}}$ is the set of all allowed tilings.





Basic topology of tiling spaces

LEMMA. Under mild conditions, Ω is connected. Each tiling in Ω defines a path component that is homeomorphic to $\mathbb{R}^d$, and there are uncountably many path components.

LEMMA. If $\Omega \subset \Omega_{\mathcal{P}}$ is closed and of finite local complexity, then Ω is complete and compact.

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The substitution[1] matrix $\mathcal{M}$.

We define the $|\mathcal{A}| \times |\mathcal{A}|$ matrix $\mathcal{M}$ by:

$$\boxed{\mathcal{M}_{i,j} = \text{ the number of occurrences of a tile of type } i \text{ in } \mathcal{S}(j)}$$

Ex. For $1 \to 1222;\ 2 \to 1$ we obtain

$$\mathcal{M} = \begin{pmatrix} 1 & 1 \\ 3 & 0 \end{pmatrix}$$

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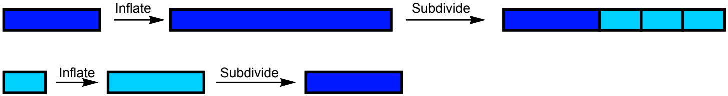

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  - In one dimension, this gives the natural tile lengths that make a symbolic substitution into a self-similar tiling.
- The right PF eigenvector tells us the relative frequencies of the tile types.

Outline

The digit[2] matrix $\mathcal{D}$.

We define the $|\mathcal{A}| \times |\mathcal{A}|$ **set-valued** matrix $\mathcal{D}$ by:

$$\boxed{\mathcal{D}_{i,j} = \text{ locations of left endpoints of all tiles of type } i \text{ in } \mathcal{S}(j)}$$

Ex. For $1 \to 1222;\ 2 \to 1$ and tile lengths $\gamma = \frac{1+\sqrt{13}}{2}$ and 1:

$$\mathcal{D} = \begin{pmatrix} \{0\} & \{0\} \\ \{\gamma, \gamma+1, \gamma+2\} & \emptyset \end{pmatrix}$$

[2] A.k.a. displacement or location matrix

Digit matrix construction of supertiles

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And puts tiles of type 2 at $\boxed{\lambda x + \mathcal{D}_{2,1}}$. (and so on.)

Digit matrix recursion for Delone sets

Let $\Lambda_i \subset \mathbb{R}^d$ be the locations of all tiles of type i in our self-similar tiling $\mathcal{T}$.

If there is a type 1 tile at x, then there are tiles of type i at $\boxed{\lambda x + \mathcal{D}_{i,1}}$;

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This allows a renormalization approach to diffraction.

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Diffraction: the Dirac comb

- $\mathbf{\Lambda} = \bigcup \Lambda_i$ represents our set of scatterers from $\mathcal{T}$
- Choose scattering strengths $a_i \in \mathbb{C}$ for each tile type
- We have the *weighted Dirac comb*

$$\omega = \sum a_i \delta_{\Lambda_i} = \sum a_i \sum_{x \in \Lambda_i} \delta_x$$

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Waves passing through this Dirac comb display patterns of interference that help us understand the long-range order properties of the tiling.

The autocorrelation and diffraction measures

The autocorrelation is defined to be

$$\begin{aligned}\gamma_\omega &= \lim_{R\to\infty} \frac{1}{Vol(B_R(0))} \left(\omega|_{B_R(0)} * \tilde{\omega}|_{B_R(0)}\right) \\ &= \sum_{i,j\le m} a_i \overline{a_j} \sum_{z\in\Lambda_i-\Lambda_j} \nu_{ij}(z)\delta_z,\end{aligned}$$

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where the *pair correlation coefficient* ν_{ij} is:

$$\nu_{ij}(z) = \lim_{R\to\infty} \frac{1}{Vol(B_R(0))} \#\{x \in \Lambda_i \cap B_R(0) \text{ and } x - z \in \Lambda_j\}$$

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Definition

When the autocorrelation measure γ_ω exists, the *diffraction measure* of $\mathcal{T}$ is defined to be its Fourier transform $\widehat{\gamma_\omega}$.

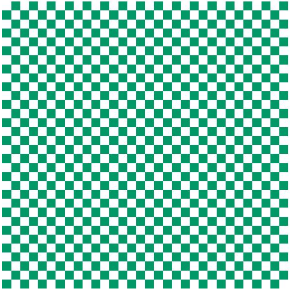
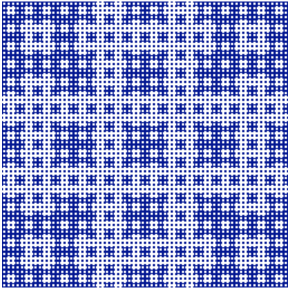
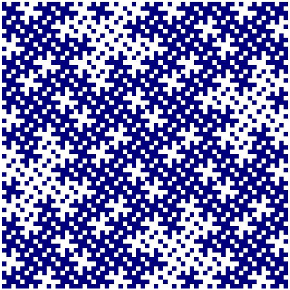
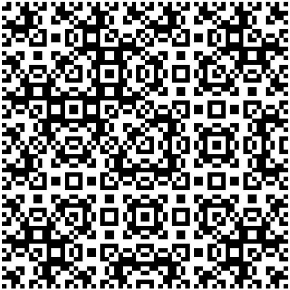
The diffraction measure, briefly interpreted

The measure $\widehat{\gamma_\omega}$ tells us how much intensity is scattered into a given volume.

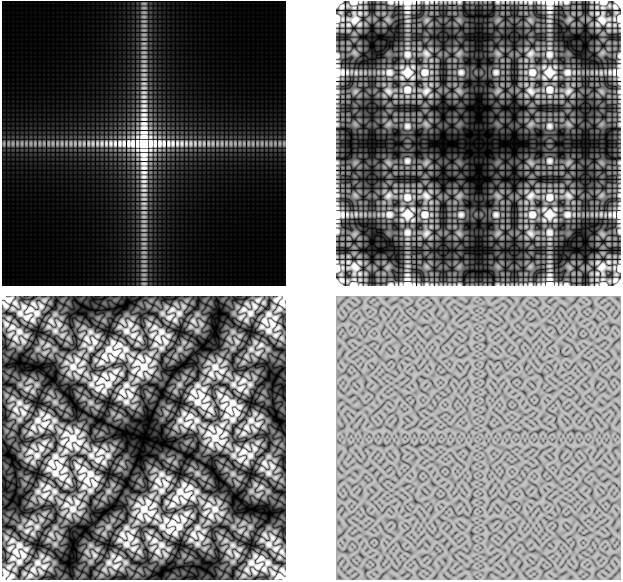
$$\widehat{\gamma_\omega} = (\widehat{\gamma_\omega})_{pp} + (\widehat{\gamma_\omega})_{sc} + (\widehat{\gamma_\omega})_{ac}.$$

The pure point part tells us the location of the 'Bragg peaks'; the degree of disorder in the solid is quantified by the continuous parts.

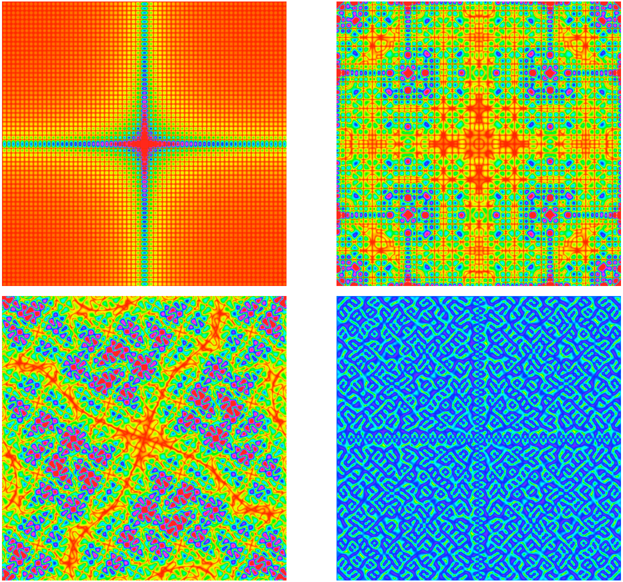
The singular continuous part is rare (or hard?) to observe in physical experiments ( )

Simulated diffraction images for four tilings



With a fun colormap



Outline

Historical introduction

Fundamental approach to aperiodic systems (for today's talk)

- Making aperiodic order using 'substitution' processes
- The "hull": a dynamical systems approach

Matrices and the information they carry

- Beginning bookkeeping: The substitution matrix
- Intermediate bookkeeping: The digit matrix

Renormalization approach to diffraction analysis

- A whirlwind review of mathematical diffraction theory
- Advanced bookkeeping: the Fourier matrix

Renormalization programme: pair coefficients.

Recall the *pair correlation coefficient* ν_{ij} is:

$$\nu_{ij}(z) = \lim_{R\to\infty} \frac{1}{Vol(B_R(0))} \#\{x \in \Lambda_i \cap B_R(0) \text{ and } x - z \in \Lambda_j\}$$

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From $\Lambda_i = \bigcup_j \lambda\Lambda_j + \mathcal{D}_{ij}$ we obtain the renormalization relation :

$$\boxed{\nu_{ij}(z) = \frac{1}{\lambda} \sum_{m,n} \sum_{r\in\mathcal{D}_{im}} \sum_{s\in\mathcal{D}_{jn}} \nu\left(\frac{z-r+s}{\lambda}\right)}$$

Renormalization programme: pair correlation measures

Decompose the autocorrelation by pair correlation:

$$\boxed{\Upsilon_{ij} = \sum_{z \in \Lambda_i - \Lambda_j} \nu_{ij}(z)\delta_z}$$

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where the matrix of Dirac combs $\delta_{\mathcal{D}}$ is given by

$$(\delta_{\mathcal{D}})_{ij} = \sum_{x \in \mathcal{D}_{ij}} \delta_x$$

The Fourier matrix $\mathcal{F}$.

Since the goal is diffraction, we're going to Fourier transform all of those delta functions anyway. Why not do it early?

The Fourier matrix $\mathcal{F}$ is given by the f.t. of the combs:

$$\mathcal{F}_{ij}(k) = \sum_{x \in \mathcal{D}_{ij}} \exp(2\pi i k x)$$

$$\boxed{\Upsilon = \frac{1}{\lambda}\left(\widetilde{\delta_{\mathcal{D}}} \otimes^{*} \delta_{\mathcal{D}}\right) * (f.\Upsilon)}$$

Fourier matrix cocycle

Recall $\mathcal{M}$ is the matrix of the substitution; one can check that $\mathcal{M}^n$ is the matrix for the substitution applied n times.

The Fourier matrix for $\mathcal{M}^n$ can be obtained via a matrix cocycle:

$$\mathcal{F}^{(n)}(k) = \mathcal{F}(k)\mathcal{F}(\lambda k) \cdots \mathcal{F}(\lambda^n(k))$$

Maximal Lyapunov exponent:

$$\chi^{\mathcal{F}}(k) := \limsup_{n\to\infty} \frac{1}{n} \log ||\mathcal{F}^{(n)} k||$$

Fourier matrix cocycle

$$\chi^{\mathcal{F}}(k) := \limsup_{n\to\infty} \frac{1}{n} \log ||\mathcal{F}^{(n)} k||$$

Only known examples with a.c. spectrum have

$$\chi^{\mathcal{F}}(k) = 1/2 \log(\lambda)$$

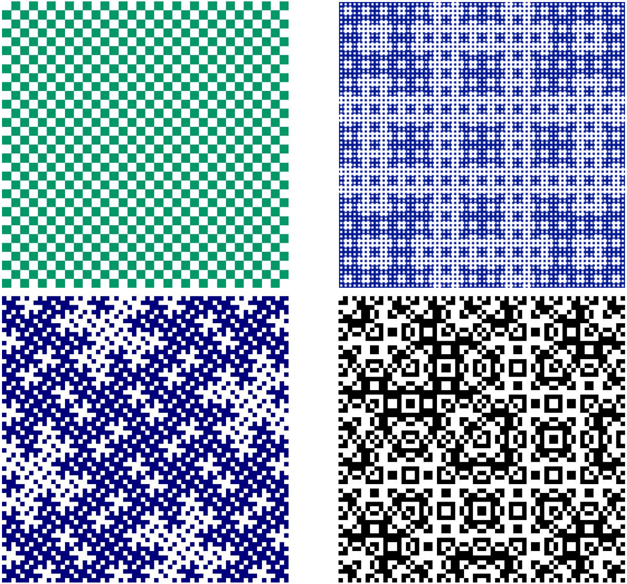
Thm. (Baake, various coauthors.) If there is some $\epsilon > 0$ s.t. for a.e. $k \in \mathbb{R}$ we have

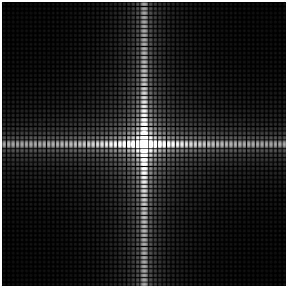
$$\chi^{\mathcal{F}}(k) \leq 1/2 \log \lambda - \epsilon,$$

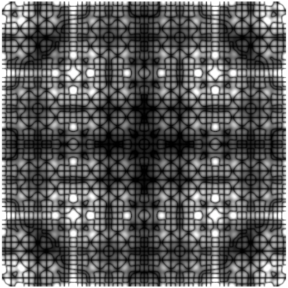
then there is no a.c. part to the diffraction.

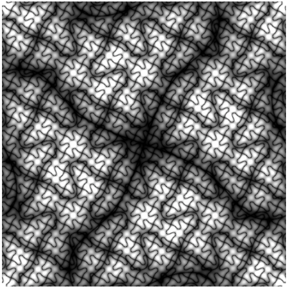
Renormalization programme: applications

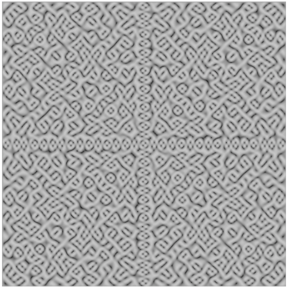
- ‘Spectral purity’ results
- In mixed spectrum examples, conditions for nonexistence of a.c. spectrum
- For pure point examples, explicit and efficient direct computation of diffraction measure
- In higher dimensions the programme works too
- Tilings with infinite local complexity can be approached; with singular spectrum identified
- All of it requires a high degree of technical prowess











Thank you for your attention