Towards spectral analysis of self-similar tilings via a renormalization approach

Michael Baake[1] Natalie P. Frank[2] Uwe Grimm[3] E. Arthur Robinson Jr.[4]

[1]University of Bielefeld

[2]Vassar College

[3]Open University

[4]George Washington University

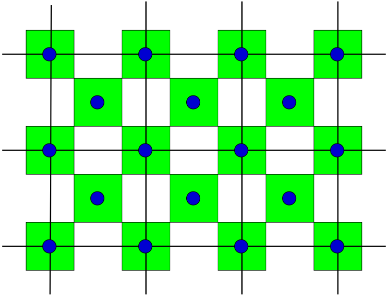
Special Session on Dynamical Systems, January 5 2017

Tilings of Euclidean Space.

- Begin with a finite set of closed topological disks in $\mathbb{R}^n$
  - We call these *prototiles*
  - Prototiles can carry labels, markings, or colors
- In one dimension, tiles are just closed intervals; in higher dimensions they can have interesting geometry
- Tilings are coverings of $\mathbb{R}^n$ by isometric copies of the prototiles, intersecting only on their boundaries

Tilings as models for atomic structures.

- Prototile types can represent atom types.
- Mark certain points in tiles to represent the location of atoms in the solid.

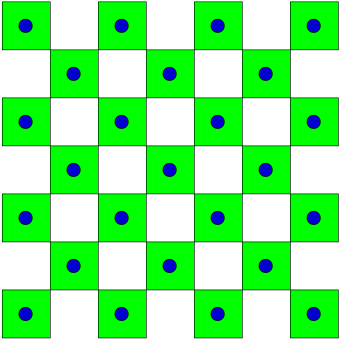


-

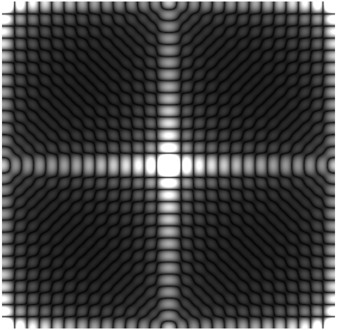
Diffraction.

- A diffraction experiment passes rays of appropriate wavelength through the solid.
- The rays bounce off the atoms and combine with constructive and destructive interference.
- I'll describe how it is modeled mathematically via the Fourier transform of autocorrelations.

Simulated diffraction pattern of diamond tiling



Cleavage plane tiling of diamond



Simulated diffraction image

Quasicrystalline solids and tiling models.

- In the 1980s, Daniel Shechtman discovered a quasicrystalline solid via its diffraction pattern.
- It was quickly realized that the Penrose tilings had a similar diffraction pattern.
- In 2011, Shechtman was awarded the Nobel Prize in Chemistry

  "For the discovery of quasicrystals"

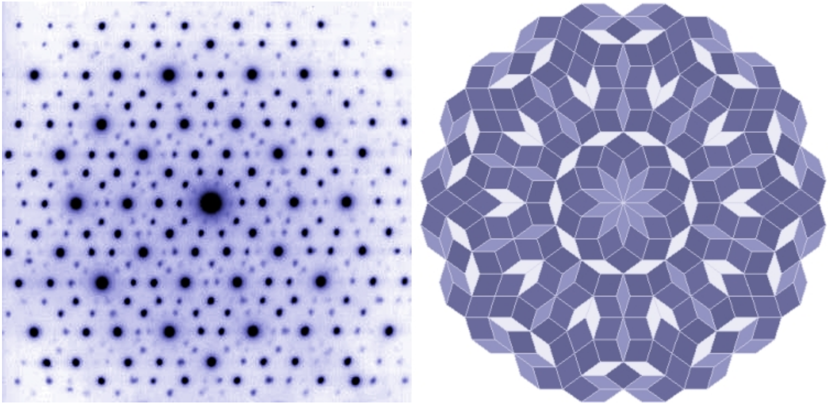


Image source: Oxford Dept. of Chemistry http://www.xtl.ox.ac.uk/tag/penrose-tiling.html

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

Summary of this talk's universe

- Quasicrystals are fascinating
- One way to identify and analyze them is through diffraction
- You can construct tilings that model them
- Dynamical systems theory analyzes tiling models
  - Especially through spectral measures, which include diffraction
- This particular talk is our attempt to analyze the diffraction of a specific one-dimensional quasicrystalline tiling

Our Goal: Identify This Tiling's Spectral Type.

- Symbolically: $0 \to 0111$, $1 \to 0$
- The inflation constant is $\lambda = \frac{1+\sqrt{13}}{2}$, non-Pisot

- Infinite tilings look like:

Our Goal: Identify This Tiling's Spectral Type.

- Symbolically: $0 \to 0111$, $1 \to 0$
- The inflation constant is $\lambda = \frac{1+\sqrt{13}}{2}$, non-Pisot

- Infinite tilings look like:

What's known in general

- Tiling dynamical systems:
  - Take all translates of the tiling
  - Close it up to make the tiling space X
  - $(X, \mathbb{R})$ is a dynamical system under translation
- Spectral analysis of $L^2(X)$ yields measures on the circle
- Eigenfunctions yield atomic measures on the circle (Bragg peaks)
- The diffraction measure $\widehat{\Upsilon}$ is also a measure on the circle
  - it is dominated by the maximal spectral type of the dynamical system

What's known for our example

- Dynamical result of Solomyak shows there are no nonconstant eigenfunctions
- Thus the maximal spectral type has no atoms other than the trivial one at 0
- Thus there are no Bragg peaks either, except at 0
- The diffraction measure $\widehat{\Upsilon}$ is continuous with respect to Lebesgue measure.

Our Conjecture and Approach

- Conjecture: $\widehat{\Upsilon}$ is Singular Continuous with respect to Lebesgue measure.
- Approach: Use a Renormalization scheme
  - Capitalizes on the self-similar structure of the tiling
  - Uses the fact that the expansion constant is not Pisot
  - Eliminates the possibility that $\widehat{\Upsilon}$ is absolutely continuous in certain examples

Dirac comb scatterer

Dirac comb scatterer

- Recall: tile lengths are $\lambda = \frac{1+\sqrt{13}}{2}$ and 1.
- We use the left endpoints of tiles as our diffraction set:

$$\Lambda = \{..., -1-3\lambda, -3\lambda, -2\lambda, -\lambda, 0, \lambda, 1+\lambda, 2+\lambda, 3+\lambda, 3+2\lambda...\}$$

- To simulate atoms at the endpoints we use the Dirac comb

$$\delta_\Lambda = \sum_{x \in \Lambda} \delta_x$$

Dirac comb two-point autocorrelation

- The autocorrelation measure γ is defined by

$$\gamma = \lim_{r \to \infty} \frac{\delta_{\Lambda_r} * \delta_{-\Lambda_r}}{2r}$$

where $\Lambda_r = \Lambda \cap [-r, r]$

- We can express γ as a weighted Dirac comb via

$$\gamma = \sum_{\Lambda - \Lambda} \eta(z) \delta_z,$$

where

Dirac comb two-point autocorrelation

- The autocorrelation measure γ is defined by

$$\gamma = \lim_{r\to\infty} \frac{\delta_{\Lambda_r} * \delta_{-\Lambda_r}}{2r}$$

where $\Lambda_r = \Lambda \cap [-r, r]$

- We can express γ as a weighted Dirac comb via

$$\gamma = \sum_{\Lambda-\Lambda} \eta(z)\delta_z,$$

where

$$\eta(z) = \lim_{r\to\infty} \frac{card(\Lambda_r \cap (z + \Lambda_r))}{2r}$$

The Diffraction Measure

- The diffraction measure $\widehat{\gamma}$ is the Fourier transform of the autocorrelation measure γ
- It is a finite measure on the torus.
- As such, it breaks into three parts: atomic, singular, and absolutely continuous
- Quasicrystals have a nontrivial atomic part; random structures have absolutely continuous parts
- What about singular continuous spectrum?

Pair correlation functions.

- Because we have two tile types it is easier to compute using $\Lambda^{(i)}$, the set of left endpoints of tiles of type i. Then

$$\Lambda = \Lambda^{(0)} \cup \Lambda^{(1)}$$

- $\nu_{ij}(z)$ is the frequency with which an i is followed z units later by a j:
- $$\nu_{ij}(z) = \lim_{r\to\infty} \frac{card(\Lambda_r^{(i)} \cap \Lambda_r^{(j)} - z)}{dens(\Lambda_r)}$$

  where $\Lambda_r^{(i)}$ is the set of points labelled i in $\Lambda \cap [-r, r]$

Pair Correlation and Autocorrelation

- The pairwise Dirac comb

$$\Upsilon_{ij} := \sum_{\Lambda^{(j)} - \Lambda^{(i)}} \nu_{ij}(z)\delta_z$$

- becomes the autocorrelation via

$$\gamma = dens(\Lambda) \sum_{i,j \in \{0,1\}} \Upsilon_{ij}$$

Diffraction Measure.

- We can obtain the diffraction $\widehat{\gamma}$ via

$$\widehat{\gamma} = dens(\Lambda) \sum_{i,j \in \{0,1\}} \widehat{\Upsilon}_{ij}$$

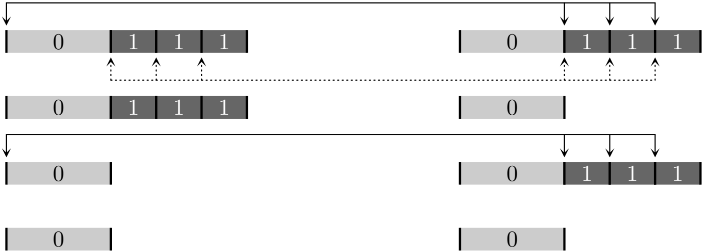
- Our renormalization approach works at the level of ν_{ij}, Υ_{ij}, and $\widehat{\Upsilon}_{ij}$

Tracking correlations via supertiles

- Recall $\nu_{ij}(z) :=$ frequency with which we see an i followed by a j at a distance of z
- This can be recursively computed if you know frequencies of supertiles at a distance of about z/λ

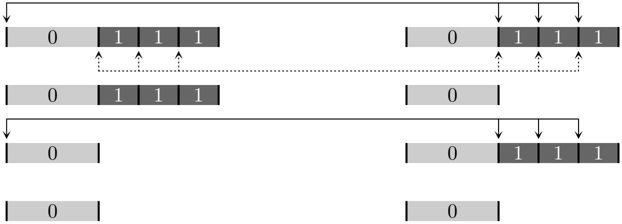
Tracking correlations via supertiles

- Recall $\nu_{ij}(z) :=$ frequency with which we see an i followed by a j at a distance of z
- This can be recursively computed if you know frequencies of supertiles at a distance of about z/λ



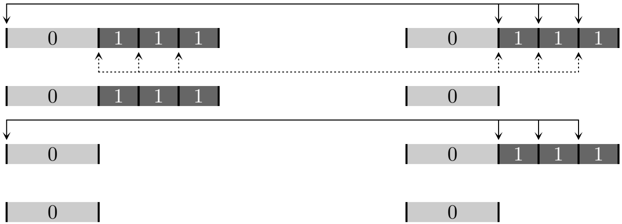
Tracking correlations via supertiles

Example: Among supertiles, we see a 0 followed by a 1 at a distance z in six distinct ways.



Tracking correlations via supertiles

Example: Among supertiles, we see a 0 followed by a 1 at a distance z in six distinct ways.



$$\nu_{01}(z) = \frac{1}{\lambda}\left(\nu_{00}\left(\frac{z-\lambda}{\lambda}\right) + \nu_{00}\left(\frac{z-\lambda-1}{\lambda}\right) + \nu_{00}\left(\frac{z-\lambda-2}{\lambda}\right) + \nu_{10}\left(\frac{z-\lambda}{\lambda}\right) + \nu_{10}\left(\frac{z-\lambda-1}{\lambda}\right) + \nu_{10}\left(\frac{z-\lambda-2}{\lambda}\right)\right)$$

Renormalization for pair correlations

We obtain four total renormalization equations:

$$\nu_{00}(z) = \frac{1}{\lambda}\left(\nu_{00}\left(\frac{z}{\lambda}\right) + \nu_{10}\left(\frac{z}{\lambda}\right) + \nu_{01}\left(\frac{z}{\lambda}\right) + \nu_{11}\left(\frac{z}{\lambda}\right)\right)$$

$$\nu_{01}(z) = \frac{1}{\lambda}(\nu_{00}\left(\frac{z-\lambda}{\lambda}\right) + \nu_{00}\left(\frac{z-\lambda-1}{\lambda}\right) + \nu_{00}\left(\frac{z-\lambda-2}{\lambda}\right) + \nu_{10}\left(\frac{z-\lambda}{\lambda}\right) + \nu_{10}\left(\frac{z-\lambda-1}{\lambda}\right) + \nu_{10}\left(\frac{z-\lambda-2}{\lambda}\right))$$

$$\nu_{10}(z) = \ldots$$

$$\nu_{11}(z) = \ldots$$

Renormalization on autocorrelation measure

- Recall that

$$\Upsilon_{ij} := \sum \nu_{ij}(z)\delta_z$$

- The renormalization on ν_{ij} passes to the Υ_{ij} with a bit of calculation
- It turns out that the matrix of Dirac combs related to the original substitution is essential:

$$\delta_T = \begin{pmatrix} \delta_0 & \delta_0 \\ \delta_\lambda + \delta_{\lambda+1} + \delta_{\lambda+2} & 0 \end{pmatrix}$$

- and we obtain...

Renormalization for the autocorrelation measure.

$$\Upsilon = \frac{1}{\lambda}(\delta_{-T} \otimes^{*} \delta_T) * (f.\Upsilon)$$

- where $*$ denotes convolution of measures,
- $f(x) = \lambda x$,
- and $\otimes^{*}$ is the Kronecker product of convolution of measures.

Renormalization for the Diffraction Measure.

$$\widehat{\Upsilon} = \frac{1}{\lambda^2} A(.)(f^{-1}.\widehat{\Upsilon})$$

- where $f(x) = \lambda x$,
- and $A(k)$ is the Fourier transform of the matrix $\delta_{-T} \otimes^* \delta_T$, i.e. $A(k)$ is a four-by-four matrix of exponentials that are transforms of delta functions in δ_T.

Eliminating Absolutely Continuous Diffraction

1. Let h represent the Radon-Nikodym derivative of $\widehat{\Upsilon}$.
2. Renormalization translates to the equation:

$$h\left(\frac{k}{\lambda}\right) = \frac{1}{\lambda} A\left(\frac{k}{\lambda}\right) h(k)$$

3. Iteration implies

$$h\left(\frac{k}{\lambda^n}\right) = \frac{1}{\lambda^n} A\left(\frac{k}{\lambda^n}\right) \cdots A\left(\frac{k}{\lambda}\right) h(k)$$

4. The eigenvalues of $A(z)$ for small z are very close to λ^2
5. This 'blow-up' at 0 implies that away from a thin set, h must be identically 0.
6. We are still dealing with the thin set but hope to prove $h \equiv 0$.

The Distribution Function