“Tomorrow’s hardest problems”

Guttmann 2025 - 80 and (still) counting

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30.06.2025

our insights to self-avoiding polygons

A *self-avoiding loop* on a graph is a cycle where no edges nor nodes repeat (apart from external nodes).

- Tony and Iwan have been counting these on the square lattice for fixed perimeter, particularly according to enclosed area (modulo translation).
- We observed in 2001 that the area law for large perimeter is perfectly fit by the area limit law of staircase polygons (Airy distribution)!

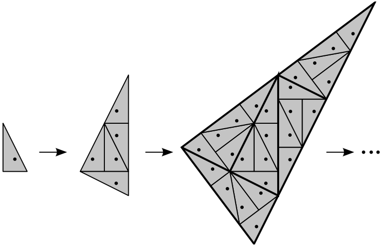
Planar self-avoiding loops (polygons) are a toy model for vesicles. Depending on pressure, they look inflated, deflated or "critical".

- The Airy distribution describes the area in the critical phase.
- This involves a prediction for the scaling function, which also describes the crossover from the inflated to the deflated phase.
- We tested the crossover behaviour numerically in 2004.

Federation Square (Paul Bourke)

pinwheel tiling (Conway-Radin 94)

- prototile: marked triangle of side lengths 1, 2, $\sqrt{5}$
- triangle orientations dense in $\mathbb{S}^1$

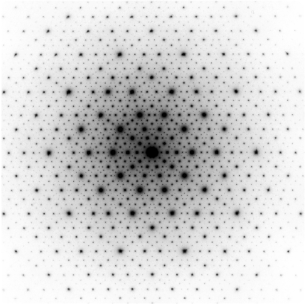


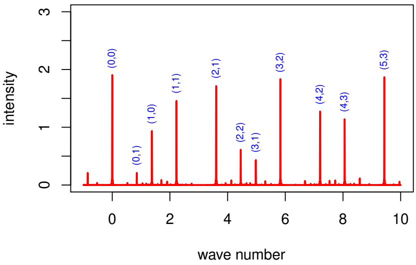
study (dis)order of point set by diffraction (Moody-Postnikoff-Strungaru 06)

- circular symmetric diffraction, single Bragg peak at origin
- continuous part of diffraction unknown

quasicrystal diffraction

AlMnPd quasicrystal (C. Beeli) versus Fibonacci set sample (size 100)

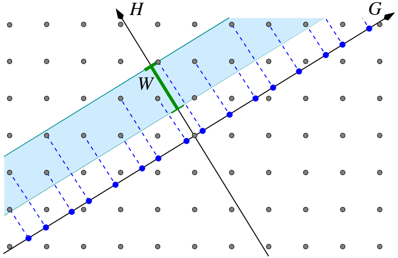




X-ray diffraction picture suggests:

- pure point diffractive, ten-fold symmetric (hence not periodic)
- dense set of Bragg peaks at $(m, n) \mathrel{\widehat{=}} c \cdot (m + n\tau)$
- above any given small intensity uniformly discrete, relatively dense

cut-and-project construction of regular model sets



- *G physical space*, *H internal space*, $\mathcal{L} \subset G \times H$ lattice
- project lattice points inside strip $G \times W$ down to G
- *regular model set*: boundary of W has volume 0
- $\mathcal{L}$ in generic position (projects densely to H and injectively to G)

model sets from translated strips all have the same diffraction

diffraction of a finite sample

physicist's recipe

$$\omega = \delta_\Lambda = \sum_{x\in\Lambda} \delta_x \xrightarrow{\;\widehat{\ }\;} \widehat{\omega}(k) = \sum_{x\in\Lambda} e^{-ikx} \xrightarrow{|\cdot|^2} k \mapsto \Big| \sum_{x\in\Lambda} e^{-ikx} \Big|^2$$

convolution formula suggests alternative computation

$$\begin{array}{ccc} \omega & \xrightarrow{\;*\;} & \omega * \widetilde{\omega} \\ {\scriptstyle \widehat{\ }}\big\downarrow & & \big\downarrow{\scriptstyle \widehat{\ }} \\ \widehat{\omega} & \xrightarrow{|\cdot|^2} & \widehat{\omega * \widetilde{\omega}} \end{array}$$

- convolve ω with its reflected version $\widetilde{\omega} = \delta_{-\Lambda}$
- autocorrelation $\omega * \widetilde{\omega}$ counts frequencies of interatomic distances
- diffraction intensity is FT of autocorrelation

diffraction of infinite point sets

idea

- restrict to balls $\omega_n = \delta_{\Lambda \cap B_n}$ and take proper limit
- compare Wiener's 1930 time series analysis (generalized HA)

diffraction measure

- autocorrelation measure γ_ω of ω is a vague accumulation point of

$$\left(\frac{1}{|B_n|} \omega_n * \widetilde{\omega_n} \right)_{n \in \mathbb{N}}$$

  exists if Λ has finite upper uniform density

  useful if Λ has positive lower uniform density
- diffraction measure $\widehat{\gamma_\omega}$ is FT of the positive definite measure γ_ω

pure point diffraction

- ω pure point diffractive if $\widehat{\gamma_\omega}$ is a point measure

Which distribution of matter diffracts?

pure point diffraction might arise from "almost periodicity" of Λ

- Recall that $f \in C_u(G)$ is *Bohr almost periodic* if for every $\varepsilon > 0$ the set $\{t \in G : \|f - T_t f\|_\infty < \varepsilon\}$ is relatively dense in G.
- A measure μ is *strongly almost periodic* if $\mu * \varphi$ is Bohr almost periodic for all $\varphi \in C_c(G)$.
- SAP measures have finite upper uniform density.
- SAP measures have a unique pure point diffraction.

restrict to *FLC sets*: finitely many local configurations (mod translation)

Theorem (Kellendonk-Lenz 13)

Let $\Lambda \subset \mathbb{R}^n$ be uniformly discrete, relatively dense and FLC. Then δ_Λ is SAP if and only if Λ is an ideal crystal.

Here, Λ is an ideal crystal if $\Lambda = \Gamma + F$ for lattice Γ and finite $F \neq \varnothing$.

Meyer sets ...

... are certain uniformly discete and relatively dense FLC sets.

Definition (Meyer set)

A relatively dense Λ is a Meyer set if $\Lambda - \Lambda$ is uniformly discrete.

- Every relatively dense subset of a lattice is a Meyer set.
- Thus Meyer sets may have very different diffraction properties.

Theorem (Meyer 72)

Let Λ be relatively dense. Then Λ is a Meyer set if and only if Λ is a subset of a regular model set.

- Meyer provided a cut-and-project construction for Meyer sets.

… and substitution tilings

many (counter-) examples of point sets arise from substitution tilings

- substitution S with finitely many prototiles (mod translation)

Definition (Pisot substitution)

S is *Pisot* if its substitution matrix is primitive, with λ_{PF} an algebraic integer > 1 and all its algebraic conjugates $|(\lambda_{PF})'| < 1$.

- Mark the prototiles to obtain a point set Λ_S.
- If S is Pisot, then Λ_S is a Meyer set.

Conjecture (Pisot conjecture)

Let S be any Pisot substitution. Then Λ_S is a regular model set.

- holds true on binary alphabets (Hollander-Solomyak 03)
- no counter-example known, see the review Akiyama et al 15

Which Meyer sets are regular model sets?

The following is due to Meyer (2012).

- A real measure ϱ is *generalized-almost-periodic* if for every $\varepsilon > 0$ we have $\mu_\varepsilon \le \varrho \le \nu_\varepsilon$ for SAP measures $\mu_\varepsilon, \nu_\varepsilon$ satisfying

$$\limsup_{n\to\infty} \frac{(\nu_\varepsilon - \mu_\varepsilon)(B_n)}{|B_n|} < \varepsilon \; .$$

- Λ is an *almost periodic pattern* if δ_Λ is g-a-p.
- Any regular model set is an almost periodic pattern (approximate 1_W from below and from above in $C_c(H)$).

Every g-a-p measure has a unique pure point diffraction.

Theorem (Lenz-R-Strungaru 24)

Let Λ be a Meyer set. Then Λ is a regular model set if and only if Λ is an almost periodic pattern.

Fourier quasicrystals $\Lambda = \{x \in \mathbb{R} : p(x) = 0\}$

- p trigonometric polynomial having real simple roots
- always arises from Lee-Yang polynomial (Alon-Cohen-Vinzant 24)
- assume that Λ is aperiodic

Theorem (cf Olevskii-Ulanovskii 20)

δ_Λ is SAP with locally finite support and finite upper uniform density. Moreover, its distributional Fourier transform has locally finite support of infinite density.

- new class of pure point diffractive points sets
- No regular model set is an aperiodic FQC and vice versa.
- some FQC are "curved model sets" (Meyer 23)

modulated lattices $\Lambda = \{n + f(n) : n \in \mathbb{Z}\}$

- $\Lambda \subset \mathbb{R}$ is called modulation of $\mathbb{Z}$ with modulation function f.
- Assume here $f : \mathbb{R} \to \mathbb{R}$ Bohr almost periodic. Then δ_Λ is SAP.

Theorem (Favorov 23)

Let $\Lambda \subset \mathbb{R}$ be locally finite. If δ_Λ is SAP, then Λ is a modulated lattice.

a cut-and-project scheme $(G, H, \mathcal{L})$ associated to Λ (LLRSS 20)

- $G = \mathbb{R}$, $H = \overline{\{T_t f : t \in G\}}^{\infty}$ is a compact abelian group
- $\mathcal{L} = \{(n, n^\star) : n \in \mathbb{Z}\}$ is a lattice in $G \times H$, where $n^\star = T_n f$.
- $\mathbb{Z}$ is a regular model set in G with trivial window $W = H$.
- $f(n) = F(n^\star)$ for $F \in C(H)$, the evaluation at 0.

some references

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