Mathematical diffraction theory of deterministic and stochastic structures

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Menue

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- PP spectra
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  - Model sets
- SC spectra
  - Cantor
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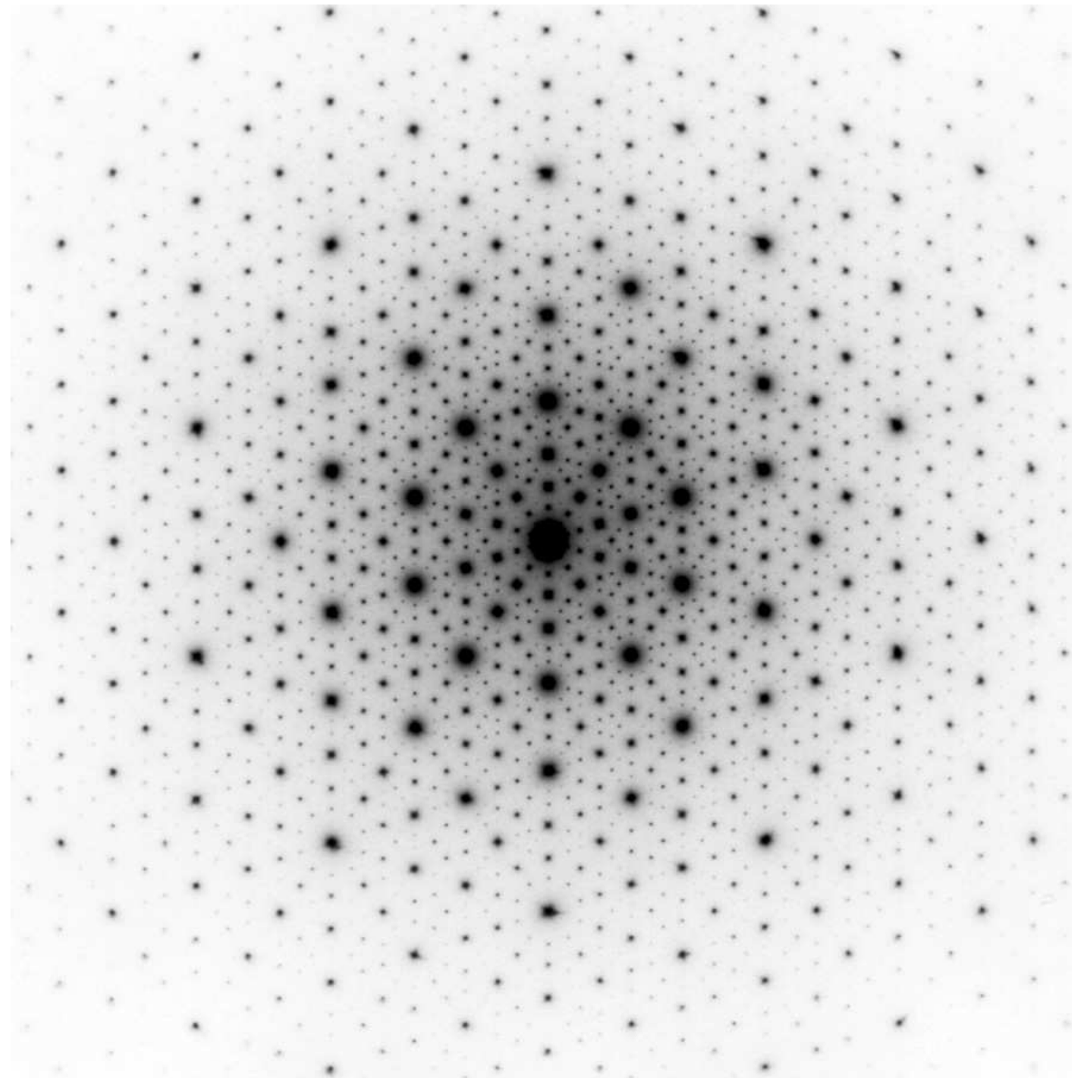
- AC spectra
  - Bernoulli
  - Rudin-Shapiro
- Further Directions
  - Algebraic systems
  - Random systems



Diffraction theory

Structure: translation bounded measure ω

assumed 'amenable'

Autocorrelation: $$\gamma = \gamma_\omega = \omega \circledast \widetilde{\omega} := \lim_{R\to\infty} \frac{\omega|_R * \widetilde{\omega|_R}}{\mathrm{vol}(B_R)}$$

Diffraction: $$\boxed{\widehat{\gamma} = \widehat{\gamma}_{\mathsf{pp}} + \widehat{\gamma}_{\mathsf{sc}} + \widehat{\gamma}_{\mathsf{ac}}}$$ (relative to λ)

- pp: Bragg peaks
- ac: diffuse scattering with density
- sc: whatever remains ...

Diffraction theory, ctd

Setting: $\omega \quad \curvearrowright \quad \gamma = \omega \circledast \widetilde{\omega} \quad \curvearrowleftright \quad \widehat{\gamma} \quad \not\curvearrowright \quad \omega$

Dirac comb on $\mathbb{Z}$:

$$\omega = \sum_{n\in\mathbb{Z}} w(n)\, \delta_n \qquad \curvearrowright \qquad \gamma = \sum_{m\in\mathbb{Z}} \eta(m)\, \delta_m$$

Autocorrelation coefficients:

$$\eta(m) = \lim_{N\to\infty} \frac{1}{2N+1} \sum_{n=-N}^{N} w(n)\, \overline{w(n-m)}$$

(similar for lattices)

Pure point spectra

Point measures: $\delta_x \, , \quad \delta_S := \sum_{x \in S} \delta_x$

Poisson summation formula: $\boxed{\widehat{\delta_{\varGamma}} = \mathrm{dens}(\varGamma)\, \delta_{\varGamma^*}}$

for lattice $\varGamma$, dual lattice $\varGamma^*$

Perfect crystals: $\omega = \mu * \delta_{\varGamma}$ (μ finite)

$$\Longrightarrow \quad \gamma = \mathrm{dens}(\varGamma)\, (\mu * \widetilde{\mu}) * \delta_{\varGamma}$$

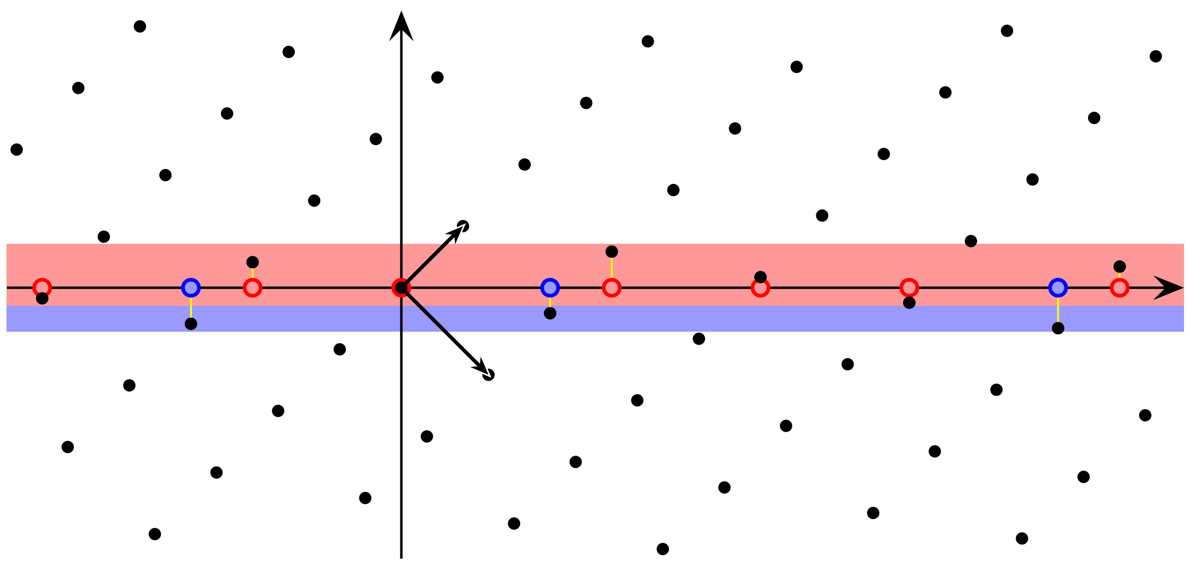
$$\Longrightarrow \quad \boxed{\widehat{\gamma} = \big(\mathrm{dens}(\varGamma)\big)^2 \, \big|\widehat{\mu}\big|^2 \, \delta_{\varGamma^*}}$$

pure point

Pure point spectra, ctd

Silver mean substitution: $a \mapsto aba,\ b \mapsto a \qquad (\lambda_{\mathrm{PF}} = 1 + \sqrt{2})$

Silver mean point set: $\varLambda = \bigl\{ x \in \mathbb{Z}[\sqrt{2}\,] \mid x' \in [-\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}\,] \bigr\}$



Pure point spectra, ctd

CPS:

$$\begin{array}{ccccc}
\mathbb{R}^d & \xleftarrow{\;\pi\;} & \mathbb{R}^d \times \mathbb{R}^m & \xrightarrow{\;\pi_{\mathrm{int}}\;} & \mathbb{R}^m \\
\cup & & \cup & & \cup \text{ dense} \\
\pi(\mathcal{L}) & \xleftarrow{\;1-1\;} & \mathcal{L} & \longrightarrow & \pi_{\mathrm{int}}(\mathcal{L}) \\
\| & & & & \| \\
L & & \xrightarrow{\qquad\star\qquad} & & L^\star
\end{array}$$

Model set: $\boxed{\varLambda = \{x \in L \mid x^\star \in W\}}$ (assumed regular)

with $W \subset \mathbb{R}^m$ compact, $\lambda(\partial W) = 0$

Diffraction: $\boxed{\widehat{\gamma} = \sum_{k \in L^{\circledast}} |A(k)|^2 \, \delta_k}$ pure point !! $(\omega = \delta_\varLambda)$

with $L^{\circledast} = \pi(\mathcal{L}^*)$ (Fourier module of $\varLambda$)

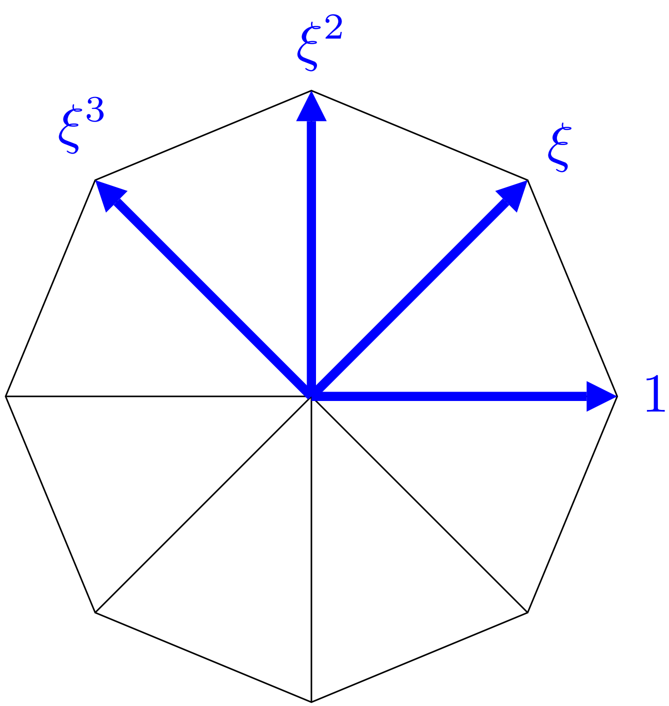
and amplitude $A(k) = \frac{\mathrm{dens}(\varLambda)}{\mathrm{vol}(W)} \, \widehat{1_W}(-k^\star)$

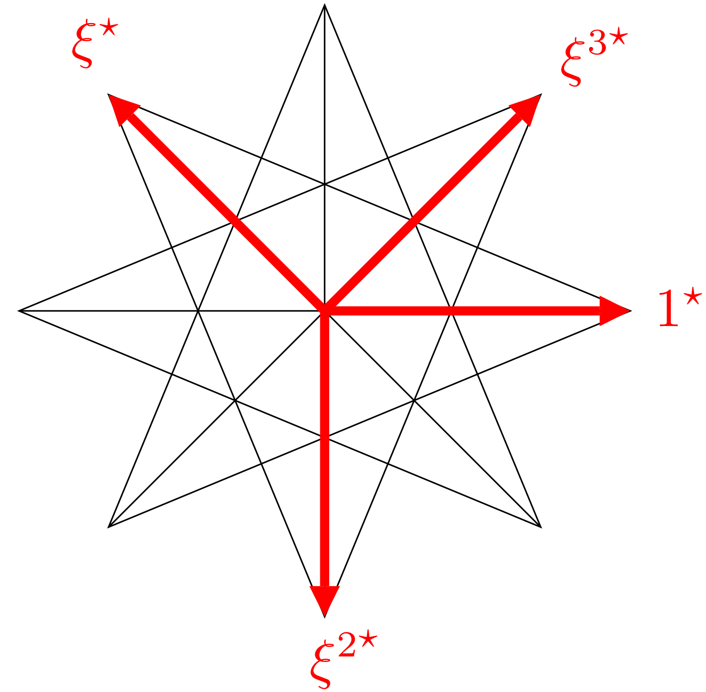
Example: Ammann-Beenker

$L = \mathbb{Z}[\xi]$ $\quad$ $\mathcal{L} \sim \mathbb{Z}^4 \subset \mathbb{R}^2 \times \mathbb{R}^2$ $\quad$ O: octagon

$\xi = \exp(2\pi i/8)$ $\quad$ $\phi(8) = 4$ $\quad$ $\star$-map: $\xi \mapsto \xi^3$

$$\Lambda_{\mathrm{AB}} = \left\{ x \in \mathbb{Z}1 + \mathbb{Z}\xi + \mathbb{Z}\xi^2 + \mathbb{Z}\xi^3 \mid x^\star \in O \right\}$$





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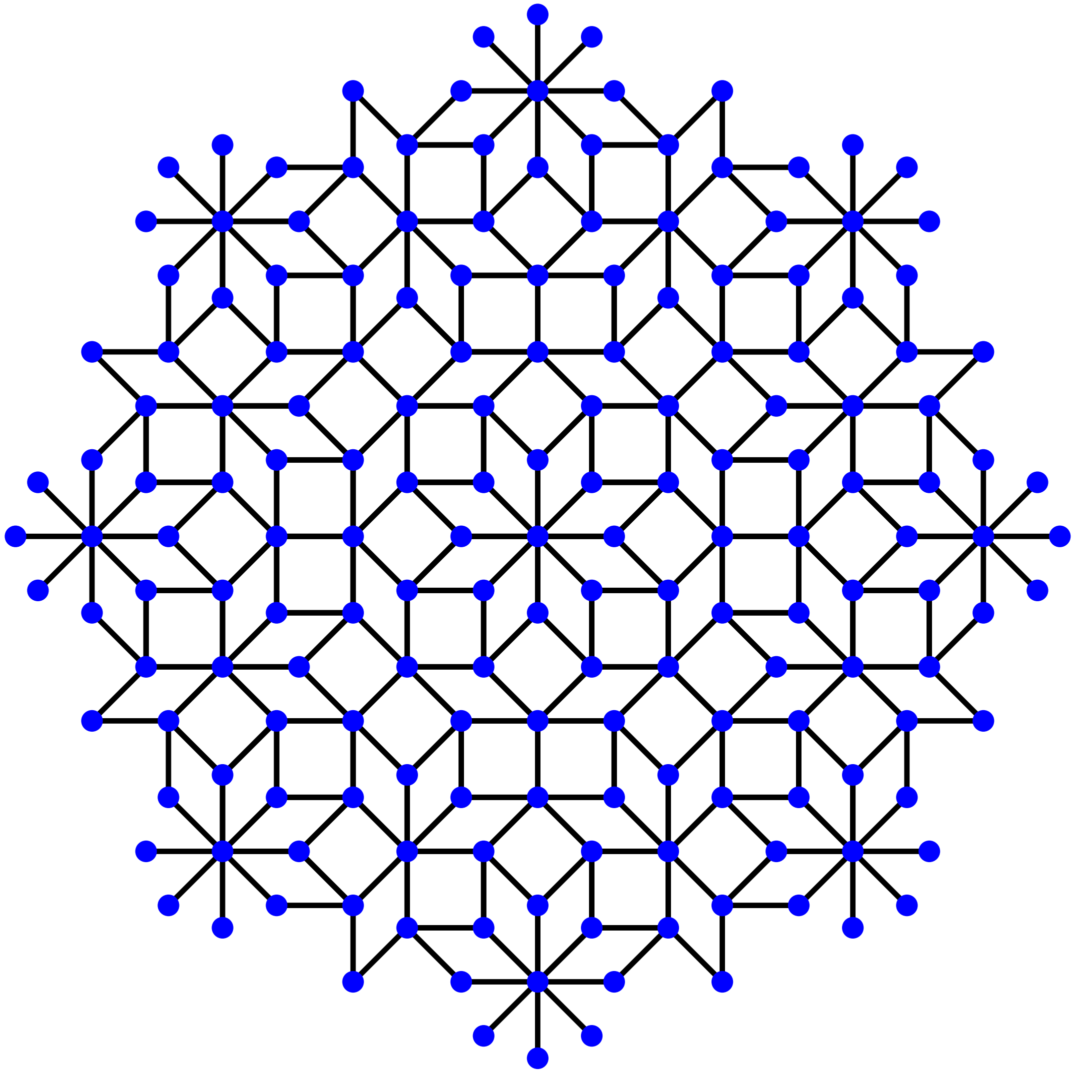
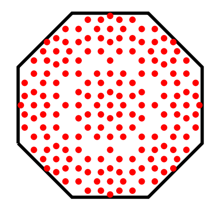
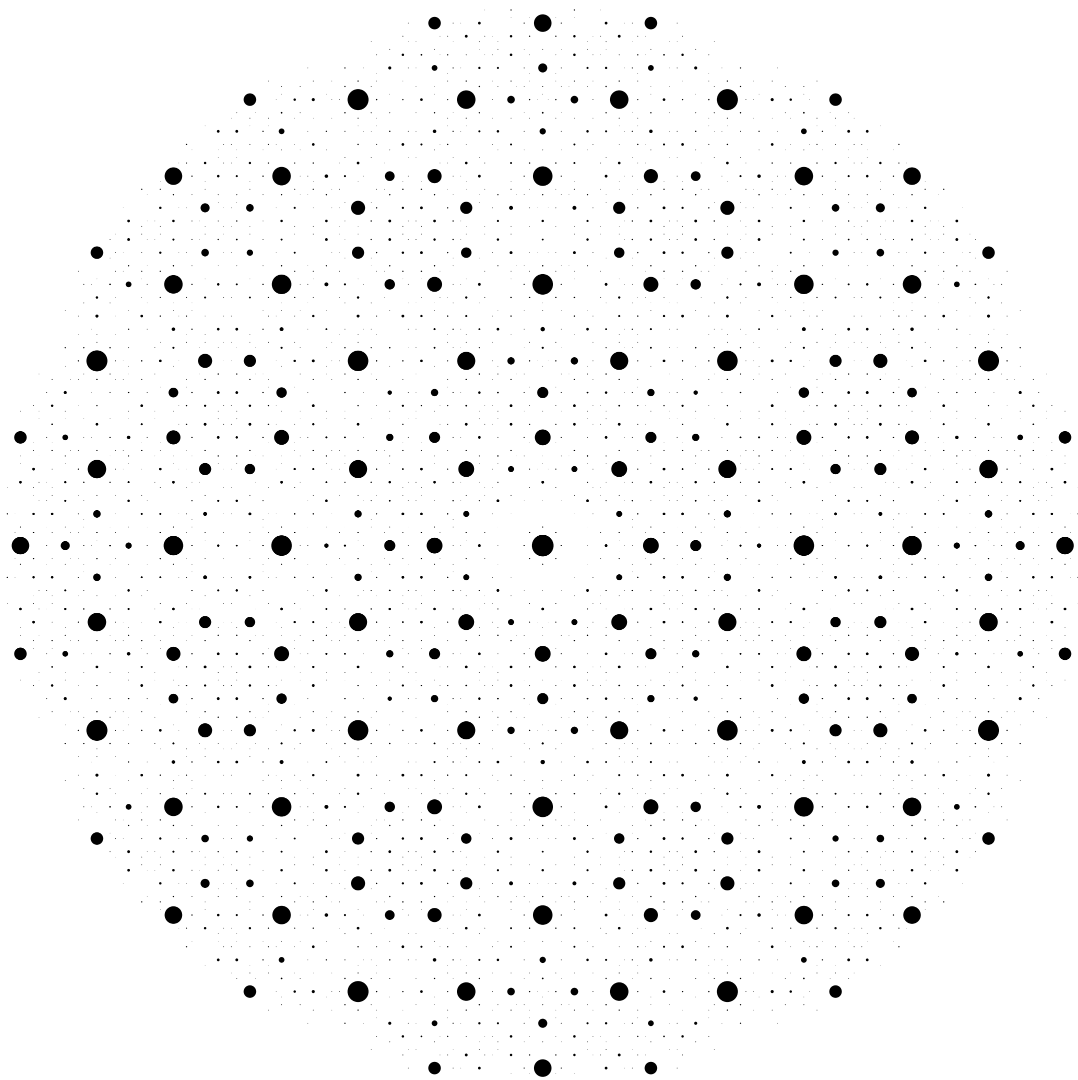


physical space



internal space

Example: Ammann-Beenker



Interlude: Homometry

Problem: distinct structures with identical autocorrelation

Example 1: $\delta_{6\mathbb{Z}} * \sum_{j=0}^{5} c_j \, \delta_j$

j	0	1	2	3	4	5
c_j	11	25	42	45	31	14
c_j	10	21	39	46	35	17

same correlations up to order 5 (Grünbaum & Moore)

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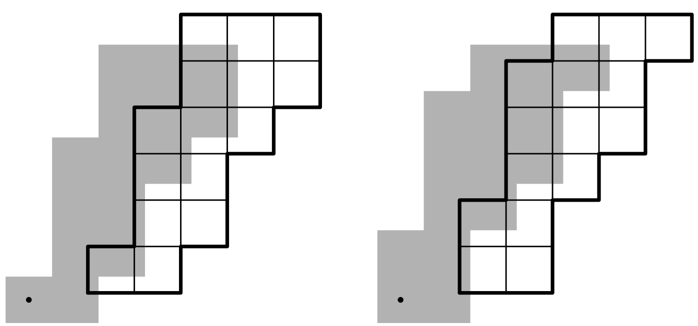
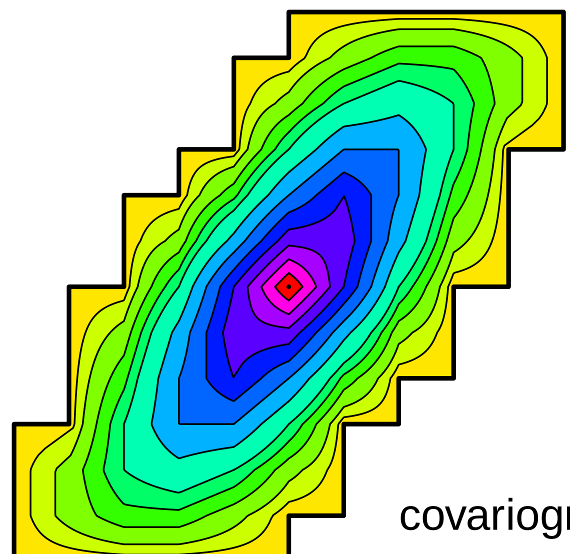
Example 2: homometric models sets with distinct windows



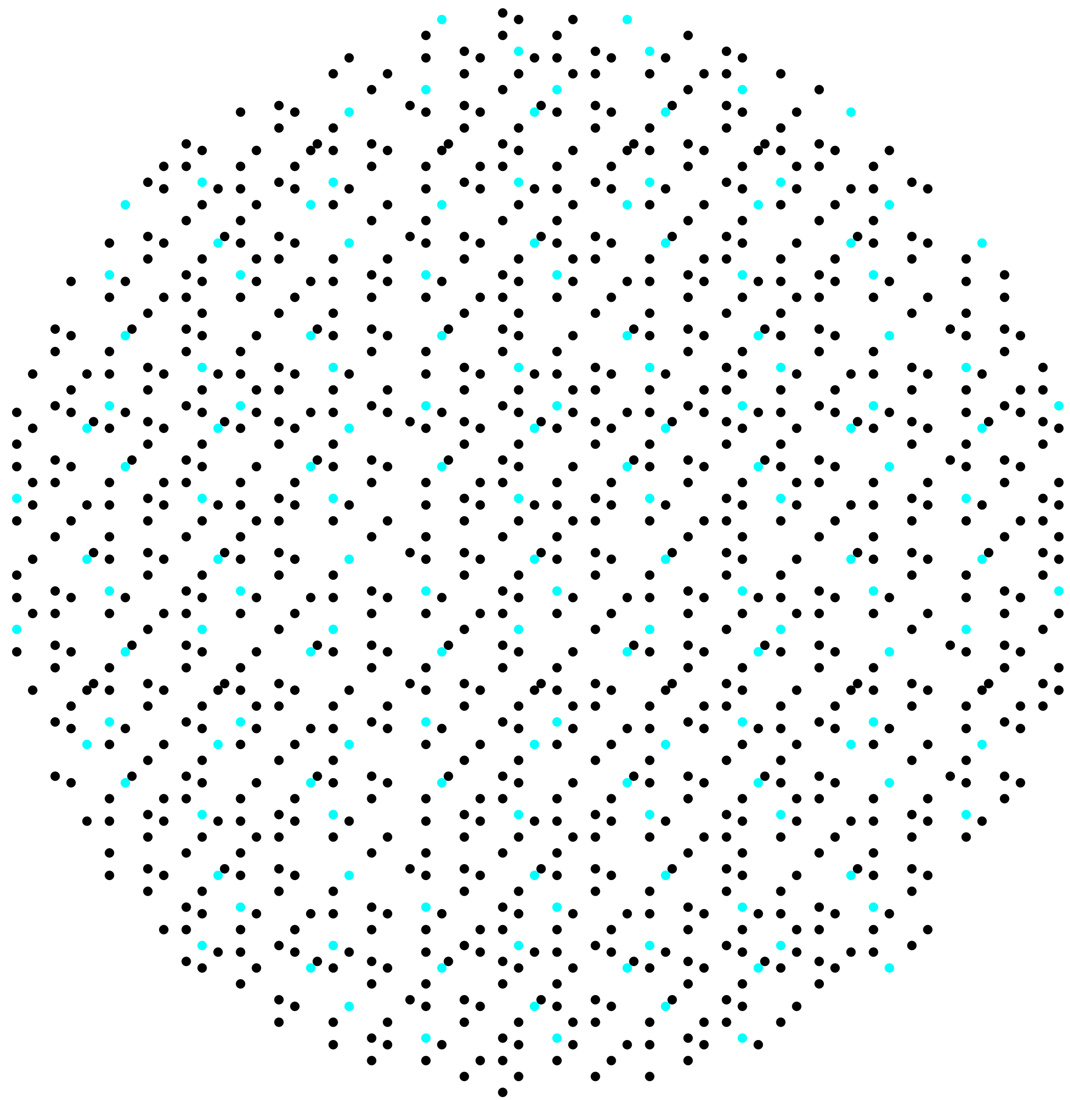
windows



covariogram

$\eta(z) \sim \mathrm{cvg}(z^\star)$

Interlude: Homometry



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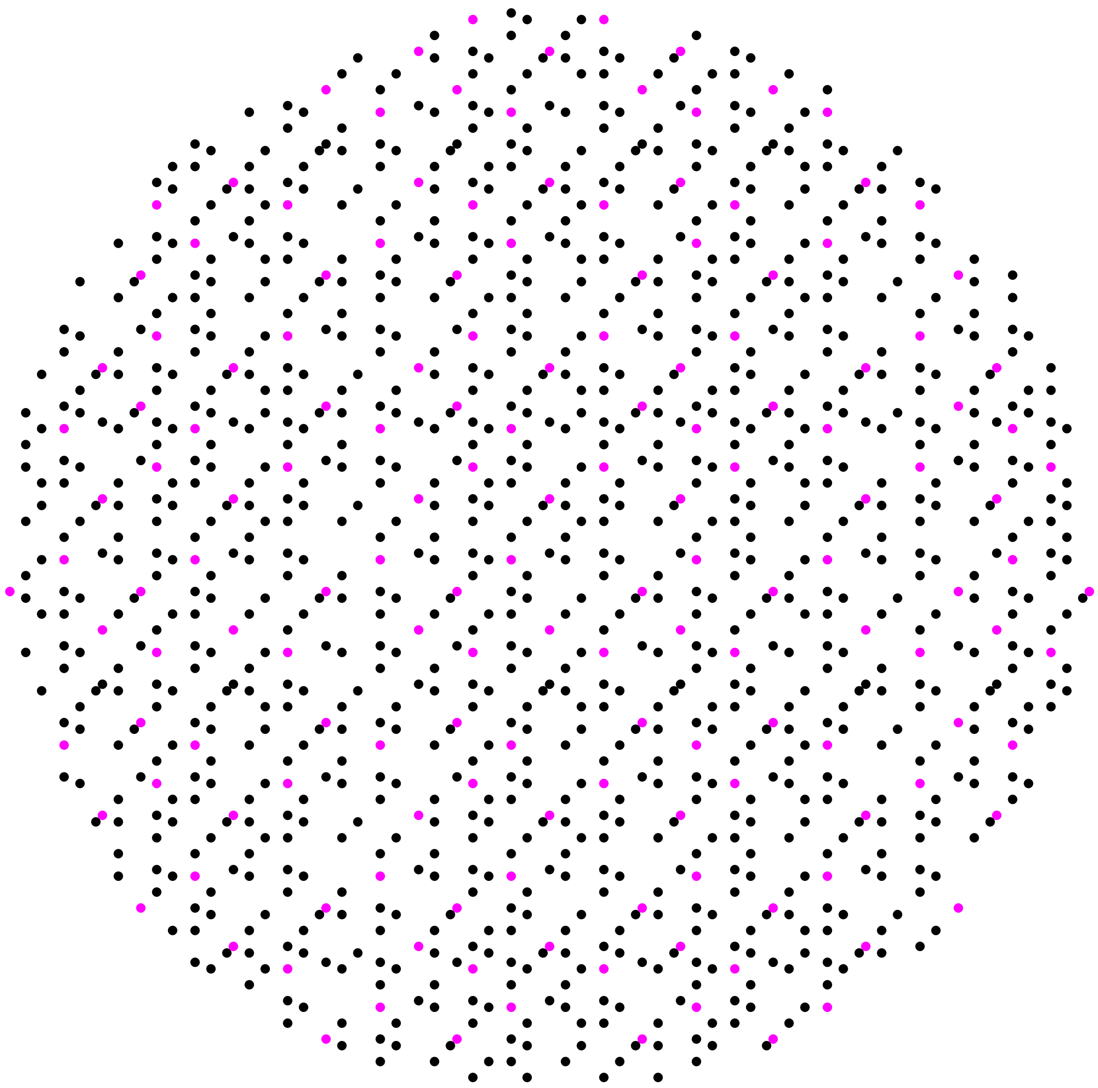

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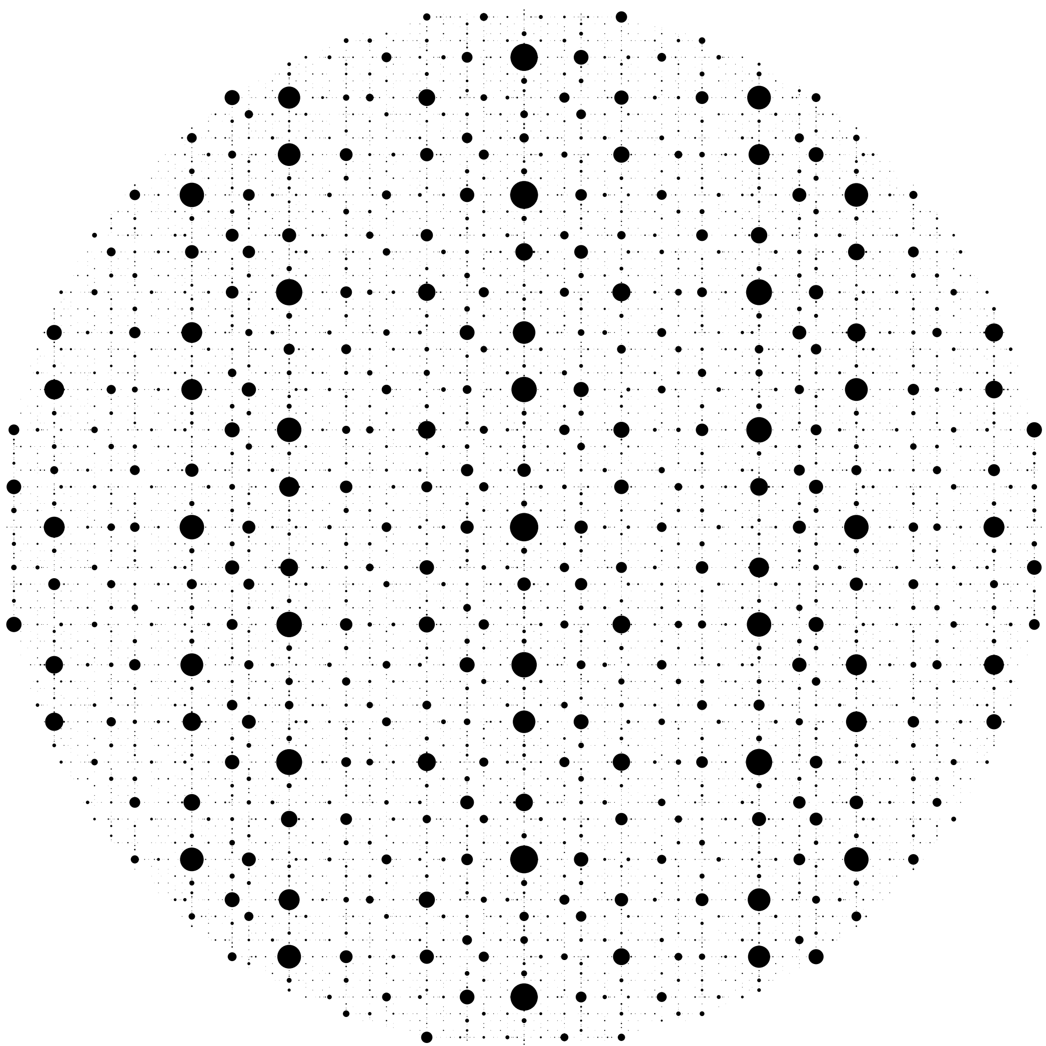
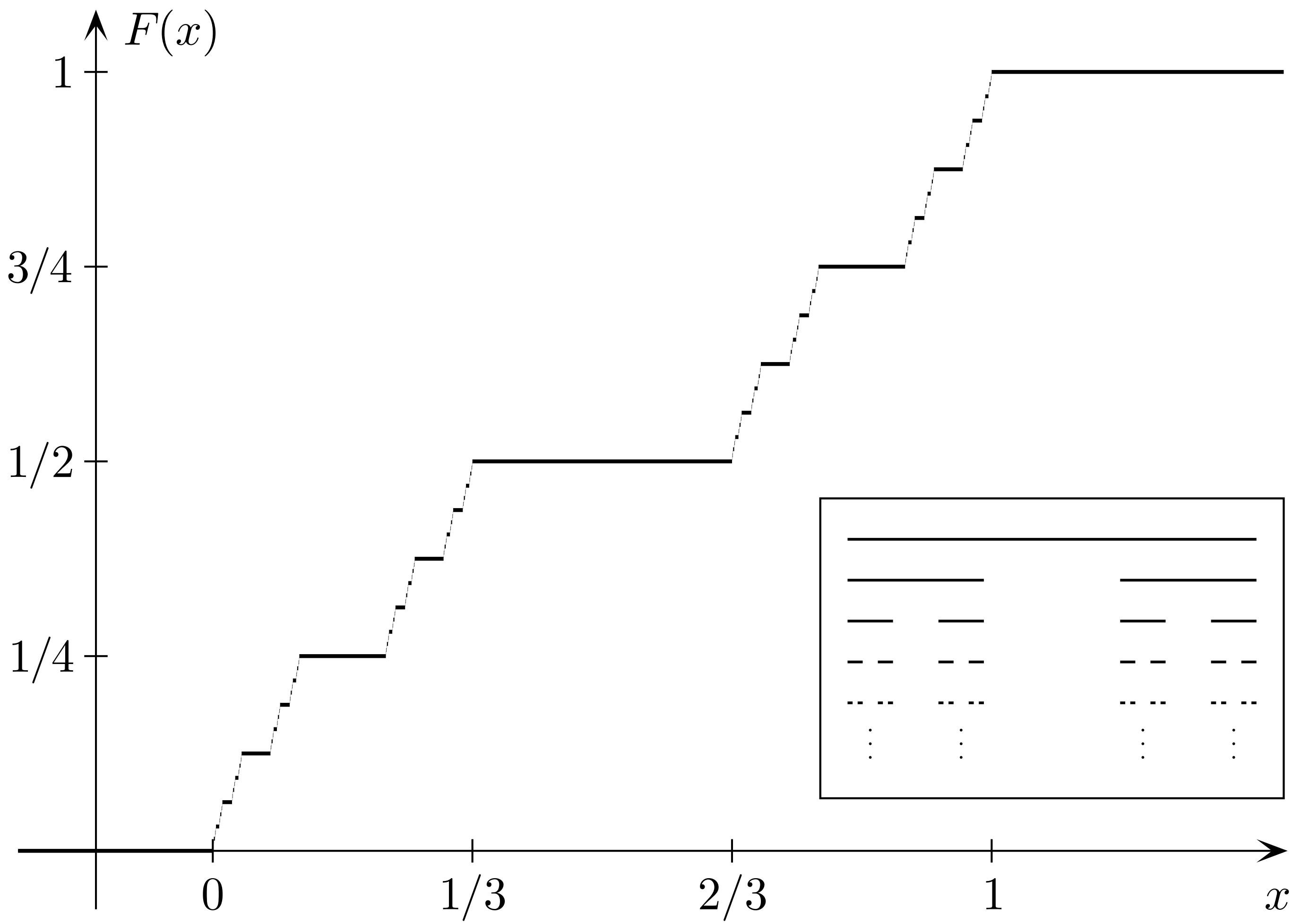


Singular spectra



Thue-Morse chain

Substitution: $\varrho : \begin{array}{l} 1 \mapsto 1\bar{1} \\ \bar{1} \mapsto \bar{1}1 \end{array}$ $\quad (\,\bar{1} \,\hat{=}\, -1\,)$

Iteration and fixed point:

$$1 \mapsto 1\bar{1} \mapsto 1\bar{1}\bar{1}1 \mapsto 1\bar{1}\bar{1}1\bar{1}11\bar{1} \mapsto \ldots \longrightarrow v = \varrho(v) = v_0 v_1 v_2 v_3 \ldots$$

- $\boxed{v_{2i} = v_i}$ and $\boxed{v_{2i+1} = \bar{v}_i}$
- $v_i = (-1)^{\text{sum of the binary digits of } i}$
- v is (strongly) cube-free
- hull of v is aperiodic and strictly ergodic

Two-sided version: $w_i = \begin{cases} v_i, & \text{for } i \geq 0 \\ v_{-i-1}, & \text{for } i < 0 \end{cases}$

TM: Autocorrelation

Structure: $\gamma = \sum_{m\in\mathbb{Z}} \eta(m)\,\delta_m = \eta\,\delta_{\mathbb{Z}}$

with $\eta(m) = \lim_{n\to\infty} \frac{1}{n}\sum_{i=0}^{n-1} v_i\, v_{i+m}$

and $\eta(-m) = \eta(m)$ for $m \geq 0$

Recursion: $\eta(0) = 1$, $\eta(1) = -\frac{1}{3}$ and, for all $m \geq 0$,

$$\boxed{\eta(2m) = \eta(m)} \quad \text{and} \quad \boxed{\eta(2m+1) = -\tfrac{1}{2}\big(\eta(m) + \eta(m+1)\big)}$$

(also valid for all $m \in \mathbb{Z}$)

Observation: $\operatorname{supp}(\gamma) \subset \mathbb{Z} \implies \delta_1 * \widehat{\gamma} = \widehat{\gamma}$

Diffraction: Absence of pp part

$$\boxed{\widehat{\gamma} = \mu * \delta_{\mathbb{Z}}} \quad \text{with} \quad \mu = \widehat{\gamma}\big|_{[0,1)} \quad \text{and} \quad \eta(m) = \int_0^1 \mathrm{e}^{2\pi \mathrm{i} m y} \,\mathrm{d}\mu(y)$$

(Herglotz-Bochner)

Wiener's criterion: $\mu_{\mathsf{pp}} = 0 \iff \Sigma(N) = o(N)$

where $\Sigma(N) = \sum_{m=-N}^{N} \bigl(\eta(m)\bigr)^2$

Argument: $\Sigma(4N) \leq \frac{3}{2} \Sigma(2N)$ (by recursion for η)

$$\Longrightarrow \quad \boxed{\mu = \mu_{\mathsf{cont}} = \mu_{\mathsf{sc}} + \mu_{\mathsf{ac}}}$$

Define: $F(x) = \mu\bigl([0,x]\bigr)$ for $x \in [0,1]$, where $F = F_{\mathsf{ac}} + F_{\mathsf{sc}}$

Diffraction: Absence of ac part

Functional relation:

$$\begin{aligned} \mathrm{d}F\left(\tfrac{x}{2}\right) + \mathrm{d}F\left(\tfrac{x+1}{2}\right) &= \mathrm{d}F(x) \\ \mathrm{d}F\left(\tfrac{x}{2}\right) - \mathrm{d}F\left(\tfrac{x+1}{2}\right) &= -\cos(\pi x)\, \mathrm{d}F(x) \end{aligned}$$

valid for F_{ac} and F_{sc} separately ($\mu_{\mathsf{ac}} \perp \mu_{\mathsf{sc}}$)

Define: $\eta_{\mathsf{ac}}(m) = \int_0^1 \mathrm{e}^{2\pi \mathrm{i} m x}\, \mathrm{d}F_{\mathsf{ac}}(x)$

$\curvearrowright$ same recursion as for $\eta(m)$, but $\eta_{\mathsf{ac}}(0)$ free

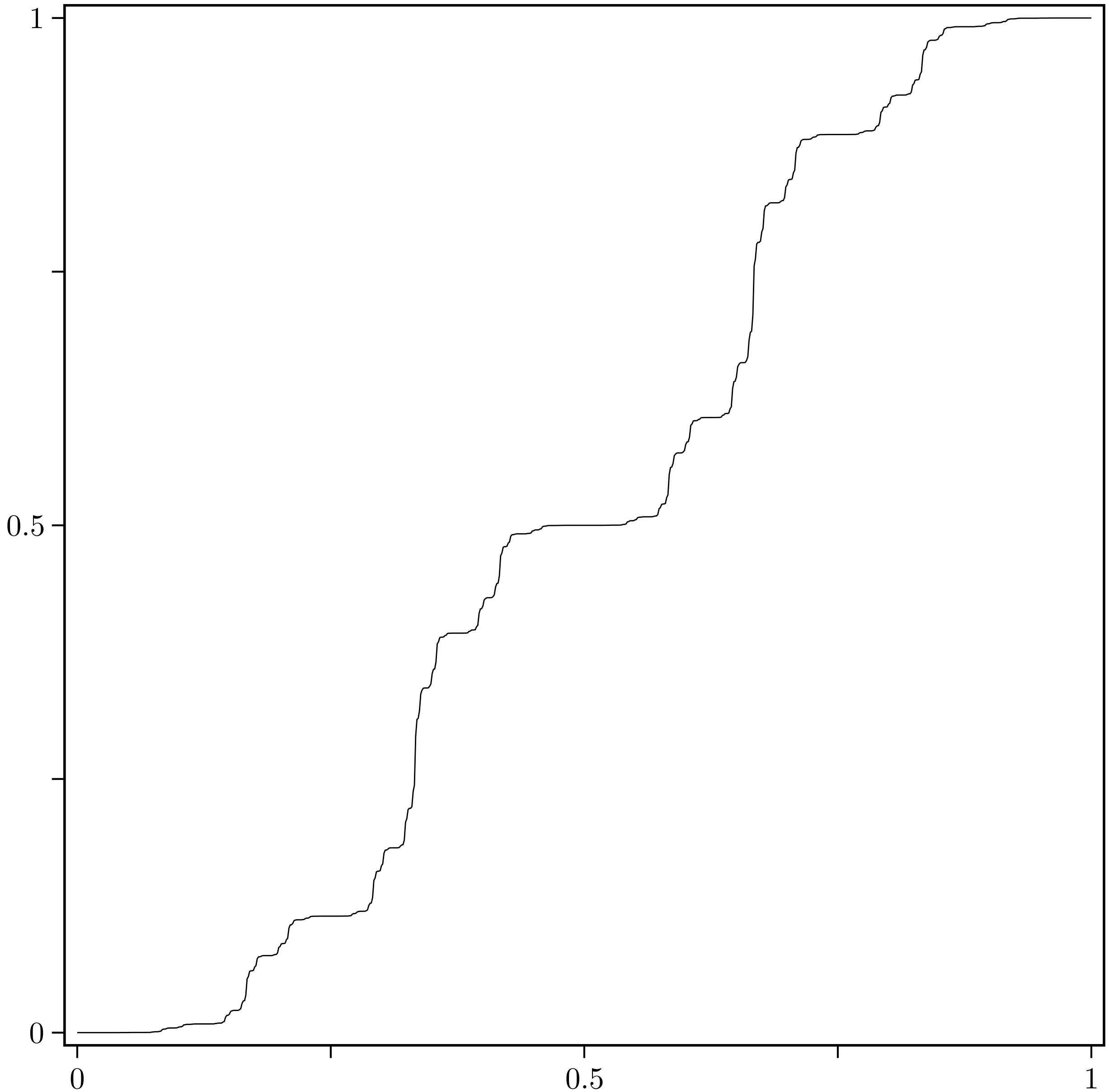
Riemann-Lebesgue lemma: $\lim_{m\to\pm\infty} \eta_{\mathsf{ac}}(m) = 0$

$\Longrightarrow \quad \eta_{\mathsf{ac}}(0) = 0 \quad \Longrightarrow \quad \eta_{\mathsf{ac}}(m) \equiv 0 \quad \Longrightarrow \quad F_{\mathsf{ac}} = 0$

(Fourier uniqueness thm)

Theorem: $\boxed{\mu = \mu_{\mathsf{sc}}}$ and $\widehat{\gamma}$ is purely sc.

TM measure



Fourier series and Volterra iteration

Functional equation: $F(1-x)+F(x)=1$ on $[0,1]$ and

$$F(x)=\frac{1}{2}\int_0^{2x}\big(1-\cos(\pi y)\big)\,\mathrm{d}F(y)\quad \text{for } x\in[0,\tfrac{1}{2}]$$

$$\Longrightarrow \quad \boxed{F(x)=x+\sum_{m\geq 1}\frac{\eta(m)}{m\pi}\,\sin(2\pi m x)}$$

uniform convergence

Define: $F_0(x)=x$ and

$$F_{n+1}(x)=\frac{1}{2}\int_0^{2x}\big(1-\cos(\pi y)\big)\,F_n'(y)\,\mathrm{d}y$$

for $n\geq 0$ and $x\in[0,\frac{1}{2}]$,

extension to $[0,1]$ by symmetry

Generalised Morse sequences

Substitution: $\varrho : \begin{array}{l} 1 \mapsto 1^k \, \bar{1}^\ell \\ \bar{1} \mapsto \bar{1}^k \, 1^\ell \end{array}$ (with $k, \ell \in \mathbb{N}$)

Fixed point: $v_0 = 1, \quad v_{m(k+\ell)+r} = \begin{cases} v_m, & \text{if } 0 \le r < k \\ \bar{v}_m, & \text{if } k \le r < k+\ell \end{cases}$

Coefficients: $\eta(0) = 1, \; \eta(\pm 1) = \frac{k+\ell-3}{k+\ell+1}$, and

$$\boxed{\eta\bigl((k+\ell)m + r\bigr) = \tfrac{1}{k+\ell}\bigl(\alpha_{k,\ell,r}\, \eta(m) + \alpha_{k,\ell,k+\ell-r}\, \eta(m+1)\bigr)}$$

with $m \in \mathbb{Z}, \; 0 \le r \le k+\ell-1$, and

$$\alpha_{k,\ell,r} = k + \ell - r - 2\min(k, \ell, r, k+\ell-r)$$

Generalised Morse sequences

Fourier series: $$F(x) = \widehat{\gamma}\big([0,x]\big)$$

$$= x + \sum_{m\geq 1} \frac{\eta(m)}{m\,\pi} \, \sin(2\pi m x)$$

(uniform convergence)

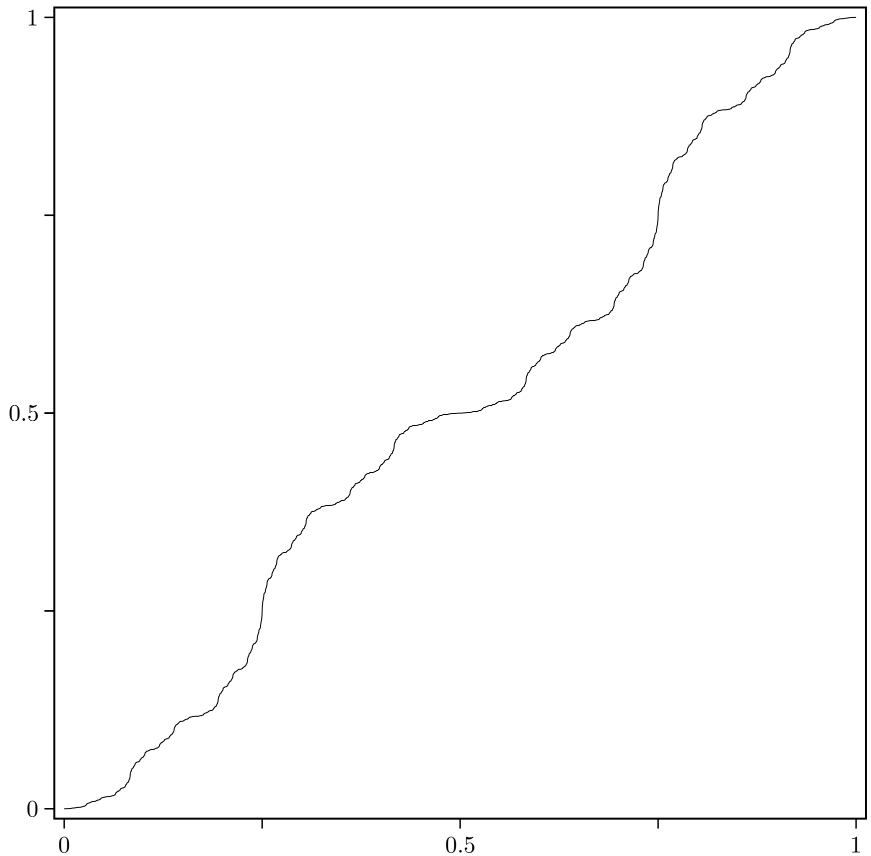
Riesz product: $$\prod_{n\geq 0} \vartheta\big((k+\ell)^n x\big)$$ with

$$\vartheta(x) = 1 + \frac{2}{k+\ell} \sum_{r=1}^{k+\ell-1} \alpha_{k,\ell,r} \, \cos(2\pi r x)$$

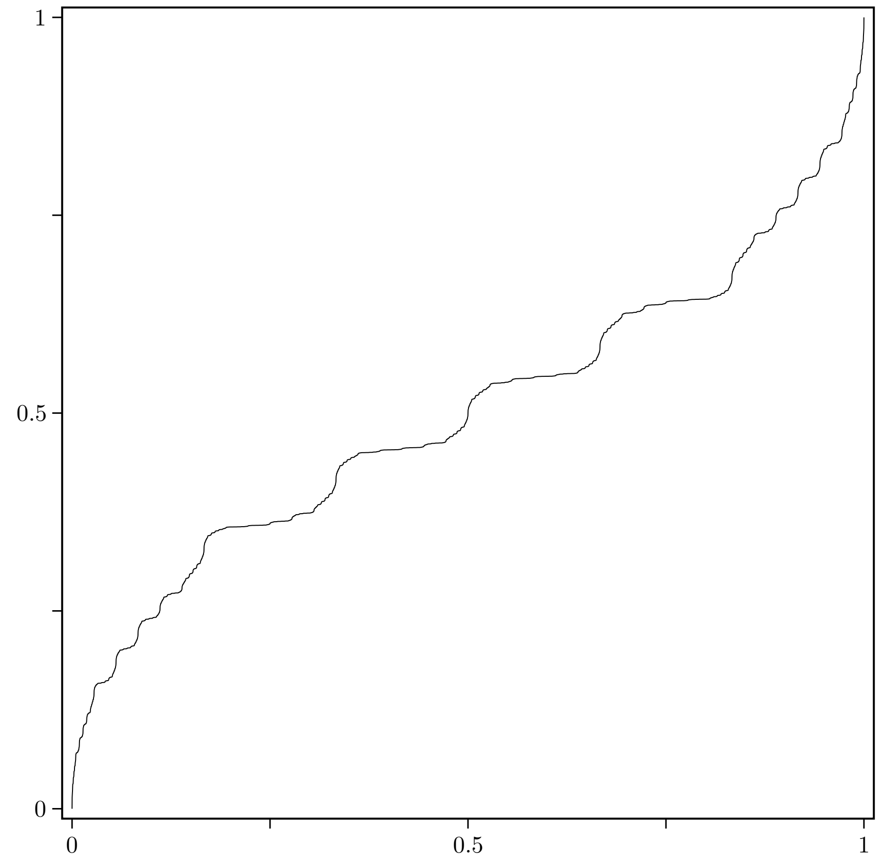
(vague convergence)

TM $(k=\ell=1)$: $$\prod_{n\geq 0} \big(1 - \cos(2^{n+1}\pi x)\big)$$

Further TM measures



$(2, 1)$



$(5, 1)$

Period doubling sequences

Block map: $\psi : \quad 1\bar{1}, \bar{1}1 \mapsto a, \quad 11, \bar{1}\bar{1} \mapsto b$

$\curvearrowright$ gen. period doubling: $\varrho' : \begin{array}{l} a \mapsto b^{k-1} a b^{\ell-1} b \\ b \mapsto b^{k-1} a b^{\ell-1} a \end{array}$

$\uparrow$

coincidence

$\Longrightarrow$ model set !!

(Dekking, BMS)

$$\begin{array}{ccc} \mathbb{X}_{\mathrm{TM}} & \xrightarrow{\;\varrho\;} & \mathbb{X}_{\mathrm{TM}} \\ \psi \big\downarrow & & \big\downarrow \psi \quad (2{:}1) \\ \mathbb{X}_{\mathrm{pd}} & \xrightarrow{\;\varrho'\;} & \mathbb{X}_{\mathrm{pd}} \\ \pi \big\downarrow & & \big\downarrow \pi \quad (\text{a.e. } 1{:}1) \\ \text{Sol} & \xrightarrow[\times\,(k+\ell)]{\times\,2} & \text{Sol} \end{array}$$

AC spectra: Coin tossing sequence

Sequence: i.i.d. random variables $W_n \in \{\pm 1\}$
with probabilities p and $1-p$

Metric entropy: $H(p) = -p\log(p) - (1-p)\log(1-p)$

Autocorrelation: $\gamma_{\mathrm{B}} = \sum_{m\in\mathbb{Z}} \eta_{\mathrm{B}}(m)\delta_m$ with

$$\eta_{\mathrm{B}}(m) := \lim_{N\to\infty} \frac{1}{2N+1} \sum_{n=-N}^{N} W_n W_{n+m} \overset{\text{(a.s.)}}{=} \begin{cases} 1, & m = 0 \\ (2p-1)^2, & m \neq 0 \end{cases}$$

(strong law of large numbers)

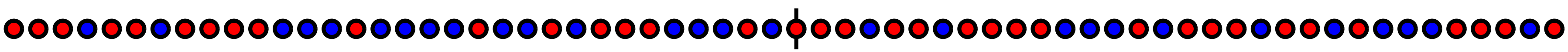
Diffraction measure: $\boxed{\widehat{\gamma_{\mathrm{B}}} \overset{\text{(a.s.)}}{=} (2p-1)^2\delta_{\mathbb{Z}} + 4p(1-p)\,\lambda}$

Rudin-Shapiro sequence

Substitution: $\varrho: \quad a \mapsto ac,\ b \mapsto dc,\ c \mapsto ab,\ d \mapsto db$

Fixed point: $b|a \xrightarrow{\varrho^2} dbab|acab \xrightarrow{\varrho^2} \ldots \longrightarrow u = \varrho^2(u)$

Reduction: $\varphi: \quad a, c \mapsto 1, \quad b, d \mapsto -1,$ $\boxed{w := \varphi(u)}$



Alternative description: $w(-1) = -1,\ w(0) = 1,$ and

$$w(4n+\ell) = \begin{cases} w(n), & \text{for } \ell \in \{0,1\} \\ (-1)^{n+\ell}\, w(n), & \text{for } \ell \in \{2,3\} \end{cases}$$

Autocorrelation: $\gamma_{\mathrm{RS}} = \sum_{m\in\mathbb{Z}} \eta(m)\delta_m$

RS: Autocorrelation

Define: $$\left.\begin{matrix}\eta(m)\\ \vartheta(m)\end{matrix}\right\} := \lim_{N\to\infty}\frac{1}{2N+1}\sum_{n=-N}^{N} w(n)\,w(n+m)\begin{cases}1\\(-1)^n\end{cases}$$

(all limits exist by Birkhoff's ergodic theorem)

Recursion: $\eta(0)=1,\ \vartheta(0)=0,$ and

$$\begin{aligned}
\eta(4m) &= \tfrac{1+(-1)^m}{2}\,\eta(m), \qquad \eta(4m+2) = 0,\\
\eta(4m+1) &= \tfrac{1-(-1)^m}{4}\,\eta(m) + \tfrac{(-1)^m}{4}\,\vartheta(m) - \tfrac{1}{4}\,\vartheta(m+1),\\
\eta(4m+3) &= \tfrac{1+(-1)^m}{4}\,\eta(m+1) - \tfrac{(-1)^m}{4}\,\vartheta(m) + \tfrac{1}{4}\vartheta(m+1),
\end{aligned}$$

$$\begin{aligned}
\vartheta(4m) &= 0, \qquad \vartheta(4m+2) = \tfrac{(-1)^m}{2}\,\vartheta(m) + \tfrac{1}{2}\,\vartheta(m+1),\\
\vartheta(4m+1) &= \tfrac{1-(-1)^m}{4}\,\eta(m) - \tfrac{(-1)^m}{4}\,\vartheta(m) + \tfrac{1}{4}\,\vartheta(m+1),\\
\vartheta(4m+3) &= -\tfrac{1+(-1)^m}{4}\,\eta(m+1) - \tfrac{(-1)^m}{4}\,\vartheta(m) + \tfrac{1}{4}\,\vartheta(m+1).
\end{aligned}$$

RS: Diffraction

Unique solution: $\vartheta(\pm 1) = 0 \;\; \curvearrowright \;\; \vartheta(m) = 0$ for all $m \in \mathbb{Z}$
and $\eta(m) = 0$ for all $m \neq 0$

Theorem: $\boxed{\gamma_{\mathrm{RS}} = \delta_0}$ and $\boxed{\widehat{\gamma_{\mathrm{RS}}} = \lambda}$

$\Longrightarrow$ homometric with coin tossing for $p = \frac{1}{2}$,
but zero entropy !

General weights: $h_{\pm}$ instead of ± 1:

$$\boxed{\widehat{\gamma_h} = \left| \frac{h_+ + h_-}{2} \right|^2 \delta_{\mathbb{Z}} + \left| \frac{h_+ - h_-}{2} \right|^2 \lambda}$$

Bernoullisation

Sequence: $S \in \{\pm 1\}^{\mathbb{Z}}$ (assumed ergodic)

with Dirac comb $\omega_S = \sum_{n\in\mathbb{Z}} S_n \, \delta_n$

and autocorrelation γ_S

Bernoullisation: $\omega := \sum_{n\in\mathbb{Z}} S_n W_n \, \delta_n \qquad \bigl(W_n \in \{\pm 1\}\bigr)$

Autocorrelation: $\gamma \overset{\text{(a.s.)}}{=} (2p-1)^2 \, \gamma_S + 4p(1-p) \, \delta_0$

(strong law of large numbers)

Application: Rudin-Shapiro, with $\gamma_S = \gamma_{\mathrm{RS}} = \delta_0$

$\curvearrowright$ $\gamma = \delta_0$ *independently* of p

$\curvearrowright$ diffraction $\boxed{\widehat{\gamma} \equiv \lambda}$

$\curvearrowright$ homometric, irrespective of entropy

Ledrappier's model

$$\mathbb{X}_{\rm L} = \big\{ w \in \{\pm 1\}^{\mathbb{Z}^2} \mid w_x w_{x+e_1} w_{x+e_2} = 1 \text{ for all } x \in \mathbb{Z}^2 \big\}$$

Properties:

closed subshift, Abelian group, Haar measure $\mu_{\rm L}$, rank 1 entropy

Dirac comb: $\omega = \sum_{x \in \mathbb{Z}^2} w_x \, \delta_x$ (balanced weights)

Theorem: $\boxed{\gamma = \delta_0}$ and $\boxed{\widehat{\gamma} = \lambda}$ ($\mu_{\rm L}$-almost surely)

$\curvearrowright$ homometric with 2D Bernoulli and Rudin-Shapiro

(but different 3-point function)

van Enter's example

Model: closed packed dimers on $\mathbb{Z}$

with random orientation: $\boxed{+\,-}$ or $\boxed{-\,+}$

Dirac comb with weights $w_i \in \{\pm 1\}$

Diffraction: $$\boxed{\widehat{\gamma_w} = \bigl(1 - \cos(2\pi k)\bigr)\lambda}$$ (purely ac)

Factor map: $$u_i = -w_i w_{i+1}$$

$$\Longrightarrow \quad \boxed{\widehat{\gamma_u} = \tfrac{1}{4}\delta_{\mathbb{Z}/2} + \tfrac{1}{2}\lambda}$$ (mixed)

$\curvearrowright$ similar to Thue-Morse versus period doubling !

Renewal process

Stationary process: $\varrho \in \mathcal{P}(\mathbb{R}_+)$ with mean 1

Autocorrelation: $\gamma = \delta_0 + \nu + \widetilde{\nu}$ with

$$\nu = \varrho + \varrho * \varrho + \varrho * \varrho * \varrho + \ldots$$

Renewal equations: $\nu = \varrho + \varrho * \nu$ and $(1 - \widehat{\varrho}\,)\,\widehat{\nu} = \widehat{\varrho}$

Theorem:

$$\boxed{\widehat{\gamma} = \bigl(\widehat{\gamma}\bigr)_{\mathsf{pp}} + (1-h) \cdot \lambda}$$

with $h(k) = \frac{2\left(|\widehat{\varrho}(k)|^2 - \mathrm{Re}(\widehat{\varrho}(k))\right)}{|1-\widehat{\varrho}(k)|^2}$ and

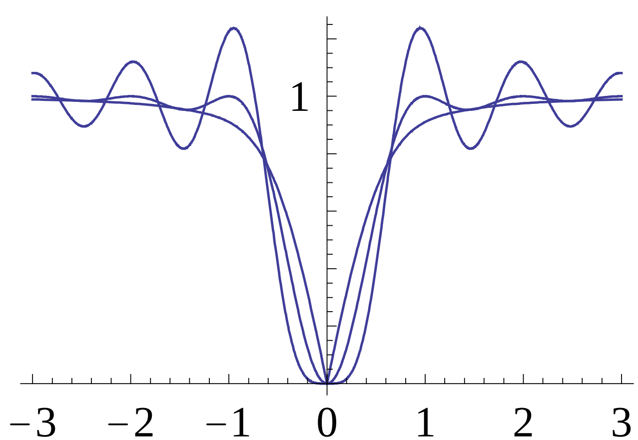
$$\bigl(\widehat{\gamma}\bigr)_{\mathsf{pp}} = \begin{cases} \delta_0, & \text{if } \mathrm{supp}(\varrho) \text{ is not a subset of a lattice,} \\ \delta_{\mathbb{Z}/b}, & \text{if } b\mathbb{Z} \text{ is the coarsest lattice that contains } \mathrm{supp}(\varrho). \end{cases}$$

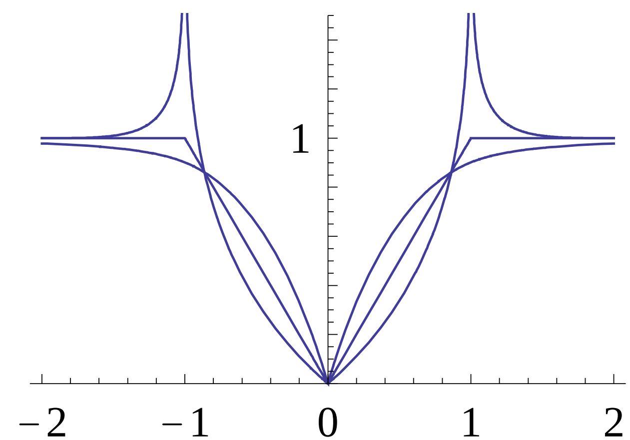
RME on the line

Setting: real eigenvalues of Dyson's random matrix ensembles

- symmetric ($\beta = 1$), Hermitian ($\beta = 2$), symplectic ($\beta = 4$) matrices
- semicircle law (with $r \sim \sqrt{\frac{2N}{\pi}}$), rescaling of central part (by $\sqrt{\frac{2N}{\pi}}$)
- stationary, ergodic point process of density 1 in the limit $N \to \infty$

Thm: $\gamma \overset{\text{(a.s.)}}{=} \delta_0 + \bigl(1 - f(|x|)\bigr)\lambda$ and $\widehat{\gamma} \overset{\text{(a.s.)}}{=} \delta_0 + h(k)\lambda$



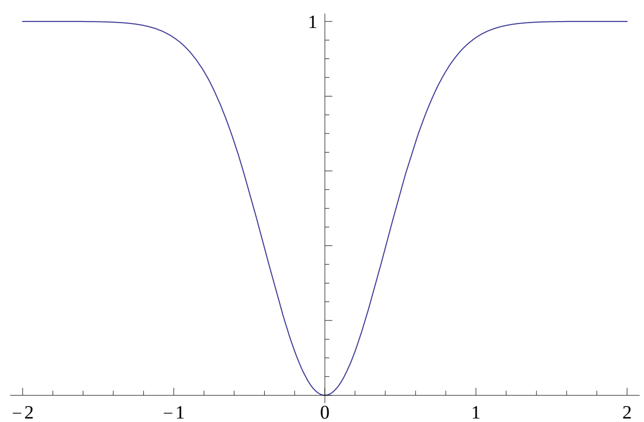


RME in the plane

Setting: eigenvalues of general, complex random matrices, viewed as point set in the plane (Ginibre's ensemble)

- uniform distribution in circle ($r \sim \sqrt{\frac{N}{\pi}}$), as $N \to \infty$
- Coulomb gas ($\beta = 2$), determinantal correlation functions
- stationary, ergodic point process of density 1 in the limit $N \to \infty$

Theorem: $$\widehat{\gamma} \overset{\text{(a.s.)}}{=} \delta_0 + \left(1 - e^{-\pi |k|^2}\right) \lambda$$ (self-dual)



Random clusters

Setting: $\varLambda$ FLC set, autocorrelation $\gamma = \sum_{z \in \varLambda - \varLambda} \eta(z)\, \delta_z$

Modification: $\boxed{\delta_{\varLambda}^{(\varOmega)} = \sum_{x \in \varLambda} \varOmega_x * \delta_x}$

$(\varOmega_x)_{x \in \varLambda}$ i.i.d. with law Q

$\mathbb{E}_Q\big(|\varOmega|\big)$ finite measure

$\mathbb{E}_Q\big((|\varOmega|(\mathbb{R}^d))^2\big) < \infty$

$$\Longrightarrow \quad \gamma^{(\varOmega)} \overset{\text{(a.s.)}}{=} \Big(\mathbb{E}_Q(\varOmega) * \widetilde{\mathbb{E}_Q(\varOmega)}\Big) * \gamma$$

$$+ \operatorname{dens}(\varLambda) \Big(\mathbb{E}_Q(\varOmega * \widetilde{\varOmega}) - \mathbb{E}_Q(\varOmega) * \widetilde{\mathbb{E}_Q(\varOmega)}\Big) * \delta_0$$

Theorem:

$$\boxed{\widehat{\gamma}^{(\varOmega)} \overset{\text{(a.s.)}}{=} \big|\mathbb{E}_Q(\widehat{\varOmega})\big|^2 \cdot \widehat{\gamma} \;+\; \operatorname{dens}(\varLambda) \Big(\mathbb{E}_Q(|\widehat{\varOmega}|^2) - |\mathbb{E}_Q(\widehat{\varOmega})|^2\Big) \cdot \lambda}$$

(analogous result holds for cluster processes)

Outlook

- Diffraction as useful tool
- Continuous spectra accessible
- Homometry more difficult
- Insensitivity to entropy
- Generalisation beyond lattice systems
- Extension to higher dimension
- Lower rank entropy (Ledrappier)
- Point process theory
- Randomness with interaction

Perspective

Harmonic Analysis				Dynamical Systems
	$\searrow$		$\swarrow$	
Algebra	$\rightarrow$	Aperiodic Order	$\leftarrow$	Topology
	$\nearrow$		$\nwarrow$	
Number Theory				Discrete Geometry

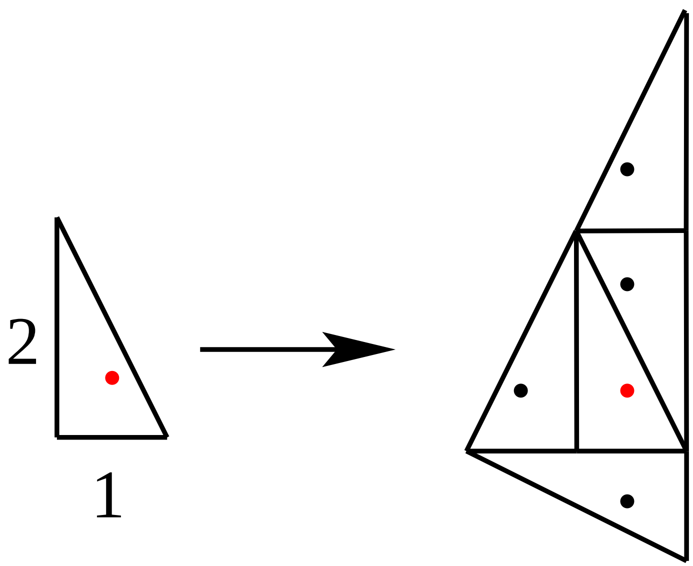
References

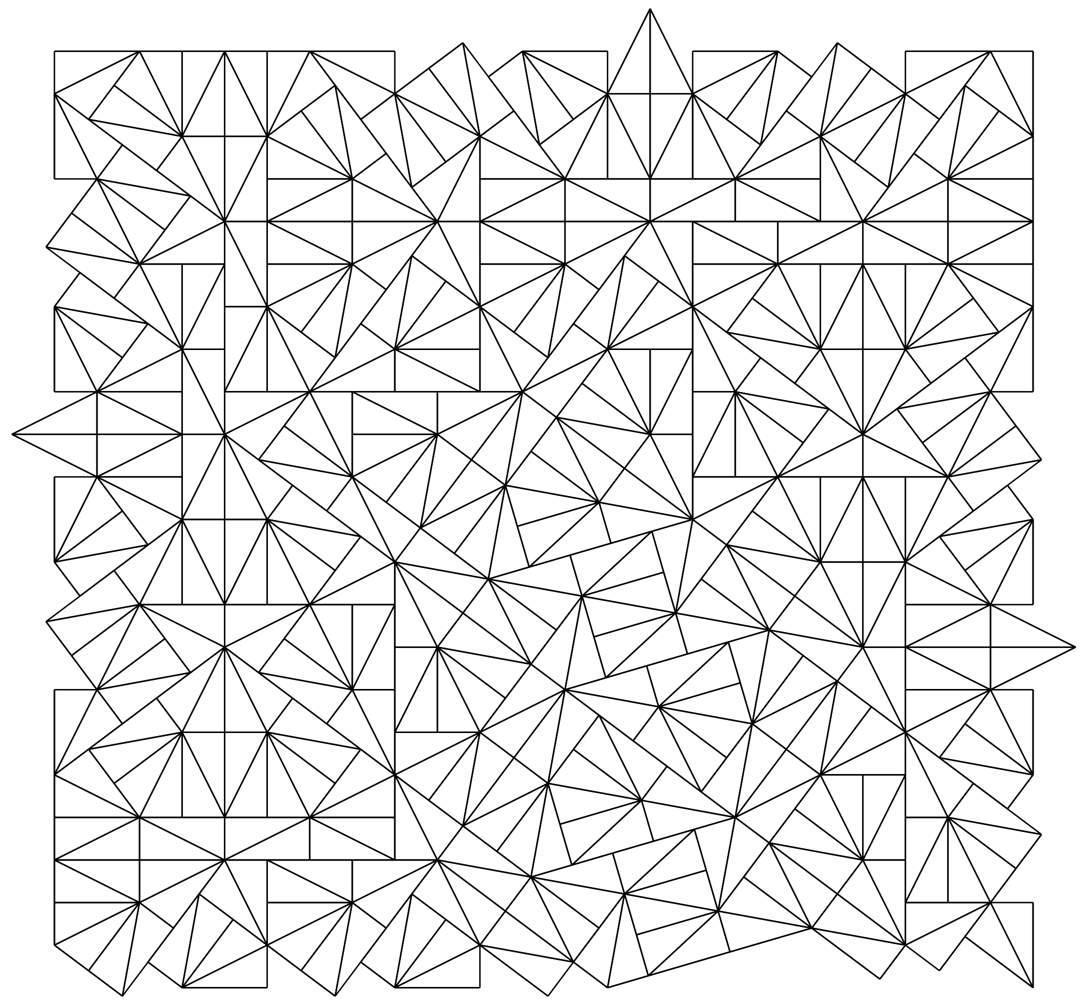
- N. Wiener, *The spectrum of an array and its application to the study of the translation properties of a simple class of arithmetical functions. Part I: The spectrum of an array,* J. Math. Massachusetts **6** (1927) 145–157
- K. Mahler, *— dto. — Part II: On the translation properties of a simple class of arithmetical functions*, J. Math. Massachusetts **6** (1927) 158–163
- M. Keane, *Generalized Morse sequences*, Z. Wahrscheinlichkeitsth. Verw. Gebiete **10** (1968) 335–353
- S. Kakutani, *Strictly ergodic symbolic dynamical systems*, in: *Proc. 6th Berkeley Symposium on Math. Statistics and Probability*, eds. L.M. LeCam, J. Neyman and E.L. Scott (eds.), Univ. of California Press, Berkeley (1972), pp. 319–326
- M. Queffélec, *Substitution Dynamical Systems — Spectral Analysis*, LNM 1294 (Springer, Berlin, 1987)
- M. Baake & U. Grimm, *The singular continuous diffraction measure of the Thue-Morse chain*, J. Phys. A.: Math. Theor. **41** (2008) 422001; `arXiv:0809.0580 (math.DS)`
- H.S. Shapiro, *Extremal Problems for Polynomials and Power Series*, Masters Thesis (MIT, Boston, 1951)
- W. Rudin, *Some theorems on Fourier coefficients*, Proc. AMS **10** (1959) 855–859

References, ctd

- F.M. Dekking, *The spectrum of dynamical systems arising from substitutions of constant length*, Z. Wahrscheinlichkeitsth. verw. Geb. **41** (1978) 221–239
- F.A. Grünbaum & C.C. Moore, *The use of higher-order invariants in the determination of generalized Patterson cyclotomic sets*, Acta Cryst. A **51** (1995) 310–323
- M. Höffe & M. Baake, *Surprises in diffuse scattering*, Z. Krist. **215** (2000) 441–444; `arXiv:math-ph/0004022`
- M. Baake & U. Grimm, *Homometric model sets and window covariograms*, Z. Krist. **222** (2007) 54–58; `arXiv:math.MG/0610411`
- U. Grimm & M. Baake, *Homometric point sets and inverse problems*, Z. Krist. **223** (2008) 777–781; `arXiv:0808.0094`
- M. Baake & U. Grimm, *Kinematic diffraction is insufficient to distinguish order from disorder*, Phys. Rev. B **79** (2009) 020203(R); `arXiv:0810.5750`
- X. Deng & R.V. Moody, *How model sets can be determined by their two-point and three-point correlations*, J. Stat. Phys. **135** (2009) 621–637; `arXiv:0901.4381`
- M. Baake, M. Birkner & R.V. Moody, *Diffraction of stochastic point sets: Explicitly computable examples*, Commun. Math. Phys. **293** (2010) 611–660; `arXiv:0803.1266`
- M. Baake & T. Ward, *Planar dynamical systems with pure Lebesgue diffraction spectrum*, J. Stat. Phys. **140** (2010) 90–102; `arXiv:1003.1536`

Pinwheel tiling





Pinwheel tiling

Autocorrelation is circularly symmetric,

$$\gamma_{\varLambda} \;=\; \delta_0 \;+ \sum_{r\in\mathcal{D}\setminus\{0\}} \eta(r)\mu_r \;=\; \sum_{r\in\mathcal{D}} \eta(r)\mu_r ,$$

with μ_r the normalised uniform distribution on $r\mathbb{S}^1$ and $\mu_0 = \delta_0$

R.V. Moody, D. Postnikoff and N. Strungaru, Circular symmetry of pinwheel diffraction,
Ann. H. Poincaré 7 (2006) 711–730

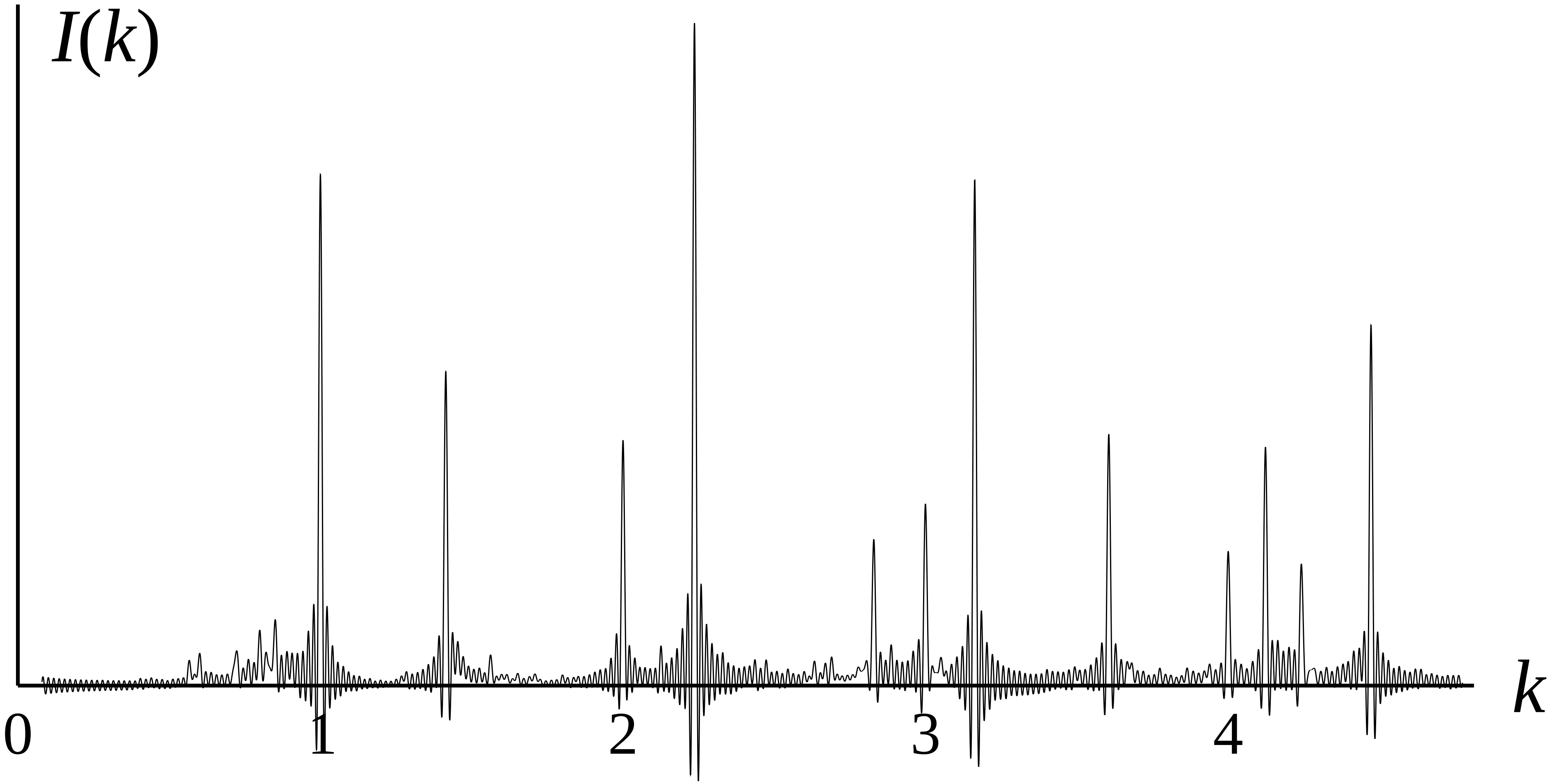
⟹ $\bigl(\widehat{\gamma_{\varLambda}}\bigr)_{\mathsf{pp}} \;=\; \bigl(\mathsf{dens}(\varLambda)\bigr)^2\,\delta_0 \;=\; \delta_0$

⟹ diffraction intensity on rings (singular component)

also *absolutely continuous* component?

Pinwheel tiling

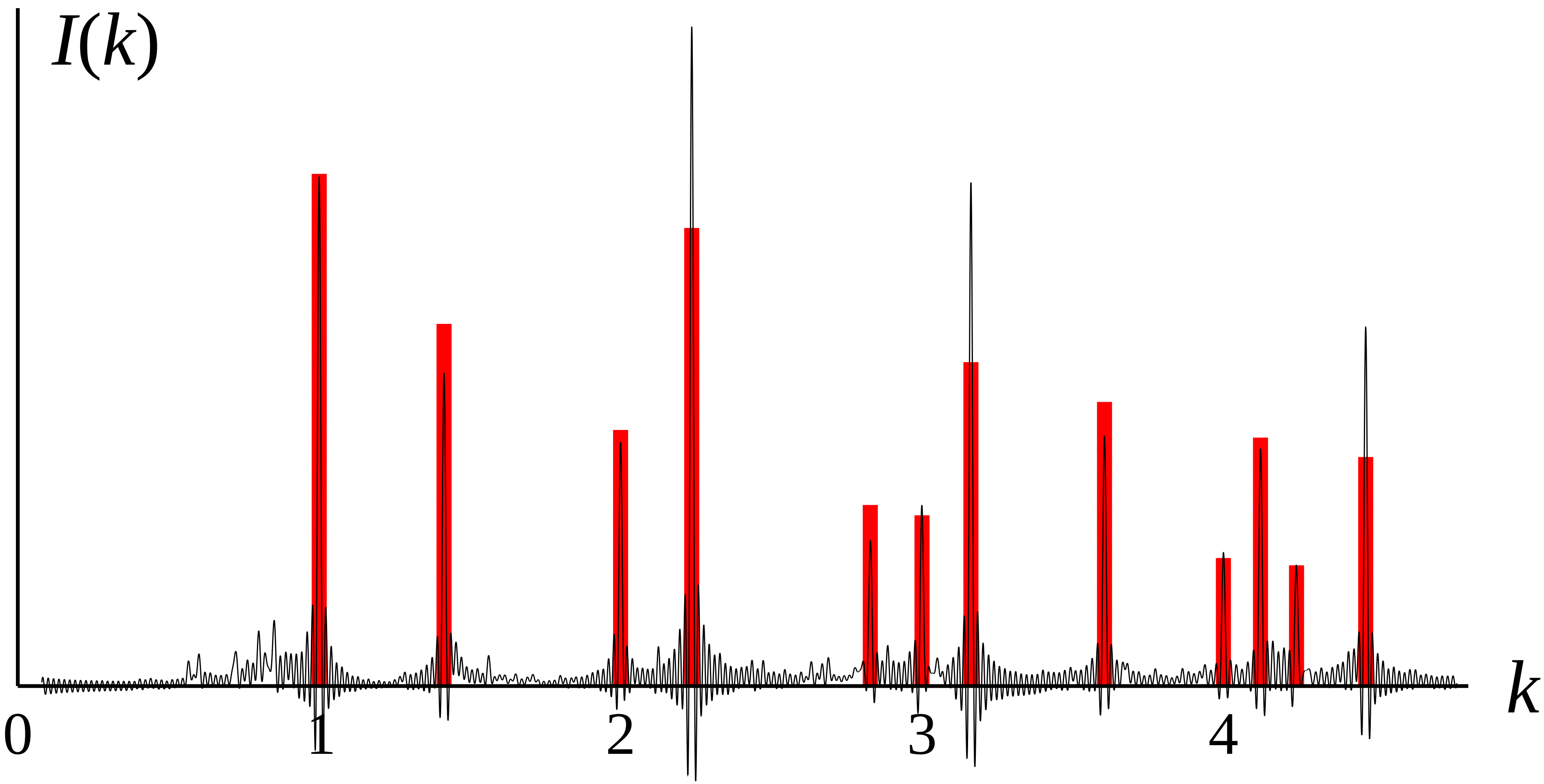
pinwheel radial intensity (numerical)



Pinwheel tiling

pinwheel radial intensity (numerical)

square lattice powder diffraction



(central intensity suppressed; relative scale chosen such peaks at $k = 1$ match)

Pinwheel tiling