Diffraction in Aperiodic Order

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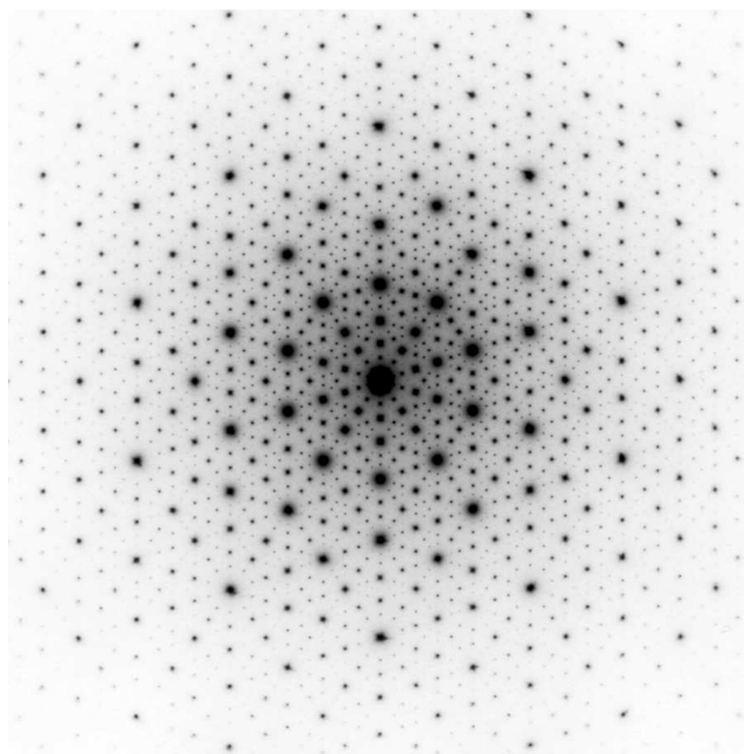
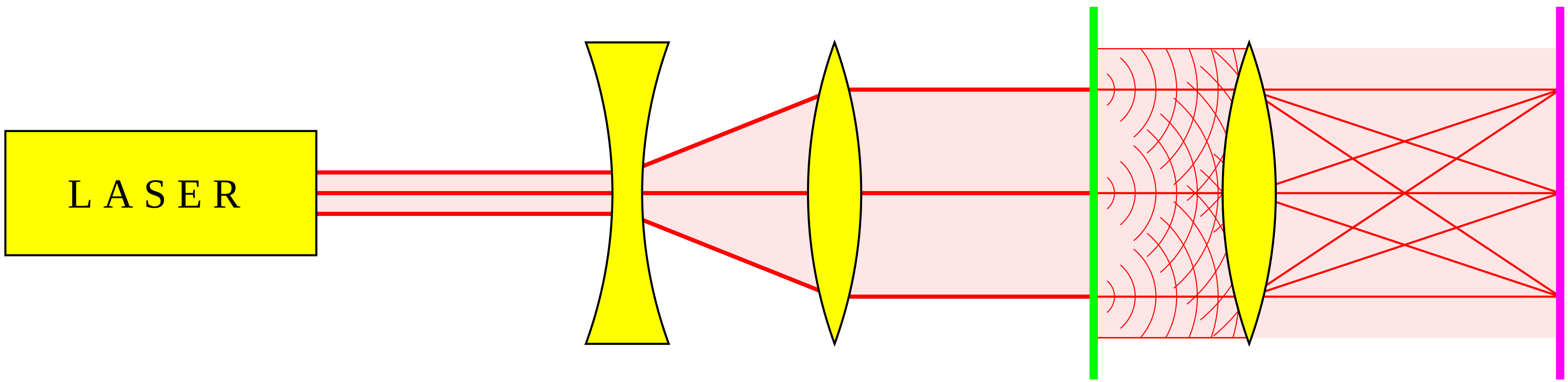


Diffraction

Optical diffraction:



Diffraction pattern:

- interference of scattered waves
- structure analysis
- X-ray, electron or neutron diffraction
- information on order and symmetry

Diffraction theory

Wiener diagram:

$$\begin{array}{ccc} g & \xrightarrow{\;\;*\;\;} & g * \widetilde{g} \\ {\scriptstyle \mathcal{F}}\big\downarrow & & \big\downarrow{\scriptstyle \mathcal{F}} \\ \widehat{g} & \xrightarrow{\;|.|^2\;} & |\widehat{g}|^2 \end{array}$$

commutative for integrable function g (with $\widetilde{g}(x) := \overline{g(-x)}$)

Kinematic diffraction:

diagonal map $g \mapsto |\widehat{g}|^2$

Mathematical diffraction theory:

use path via autocorrelation

for translation bounded measures

Diffraction theory

Structure: translation bounded measure ω
assumed ‘amenable’

Autocorrelation: $\gamma \;=\; \gamma_{\omega} = \omega \circledast \widetilde{\omega} \;:=\; \lim\limits_{R\to\infty} \dfrac{\omega|_R * \widetilde{\omega|_R}}{\mathrm{vol}(B_R)}$

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 ...

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

Perfect (conventional) crystals

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)

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

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

Perfect quasicrystals

CPS:

$$\begin{tikzcd}
\mathbb{R}^d & \mathbb{R}^d \times \mathbb{R}^m \arrow[l, "\pi"'] \arrow[r, "\pi_{\mathrm{int}}"] & \mathbb{R}^m \\
\cup & \cup & \cup \ \text{dense} \\
\pi(\mathcal{L}) & \mathcal{L} \arrow[l, "1-1"'] \arrow[r] & \pi_{\mathrm{int}}(\mathcal{L}) \\
\| & & \| \\
L \arrow[rr, "\star"] & & L^\star
\end{tikzcd}$$

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: $\boxed{\widehat{\gamma} = \sum_{k \in L^{\circledast}} |A(k)|^2 \, \delta_k}$

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

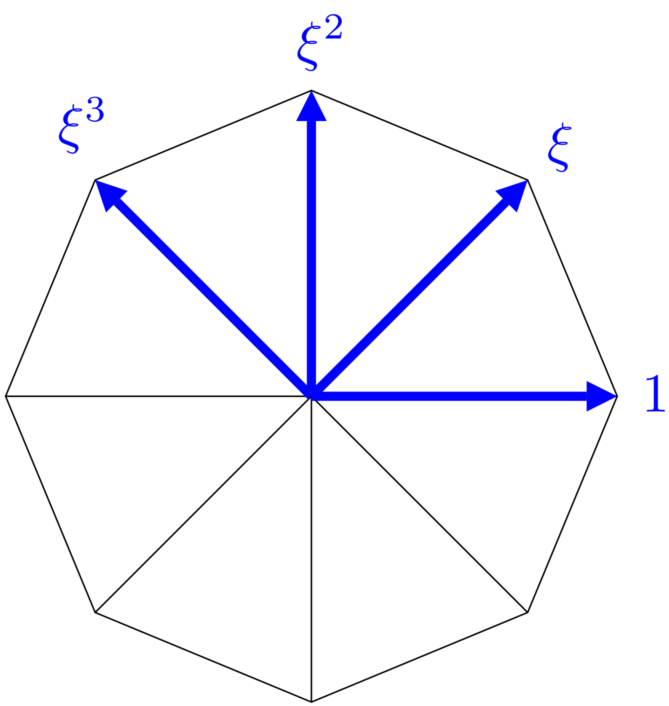
and amplitude $A(k) = \frac{\mathrm{dens}(\varLambda)}{\mathrm{vol}(W)} \, \widehat{1_W}(-k^\star)$

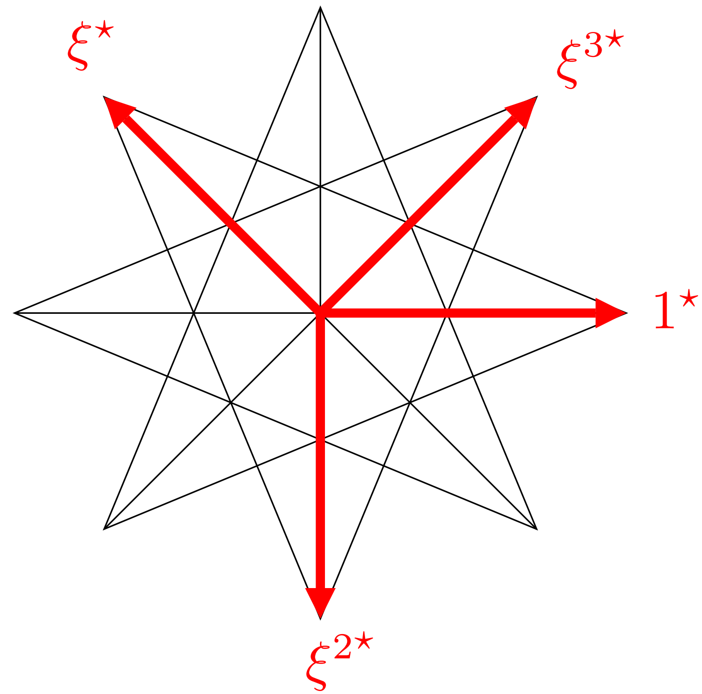
Example: Ammann–Beenker

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

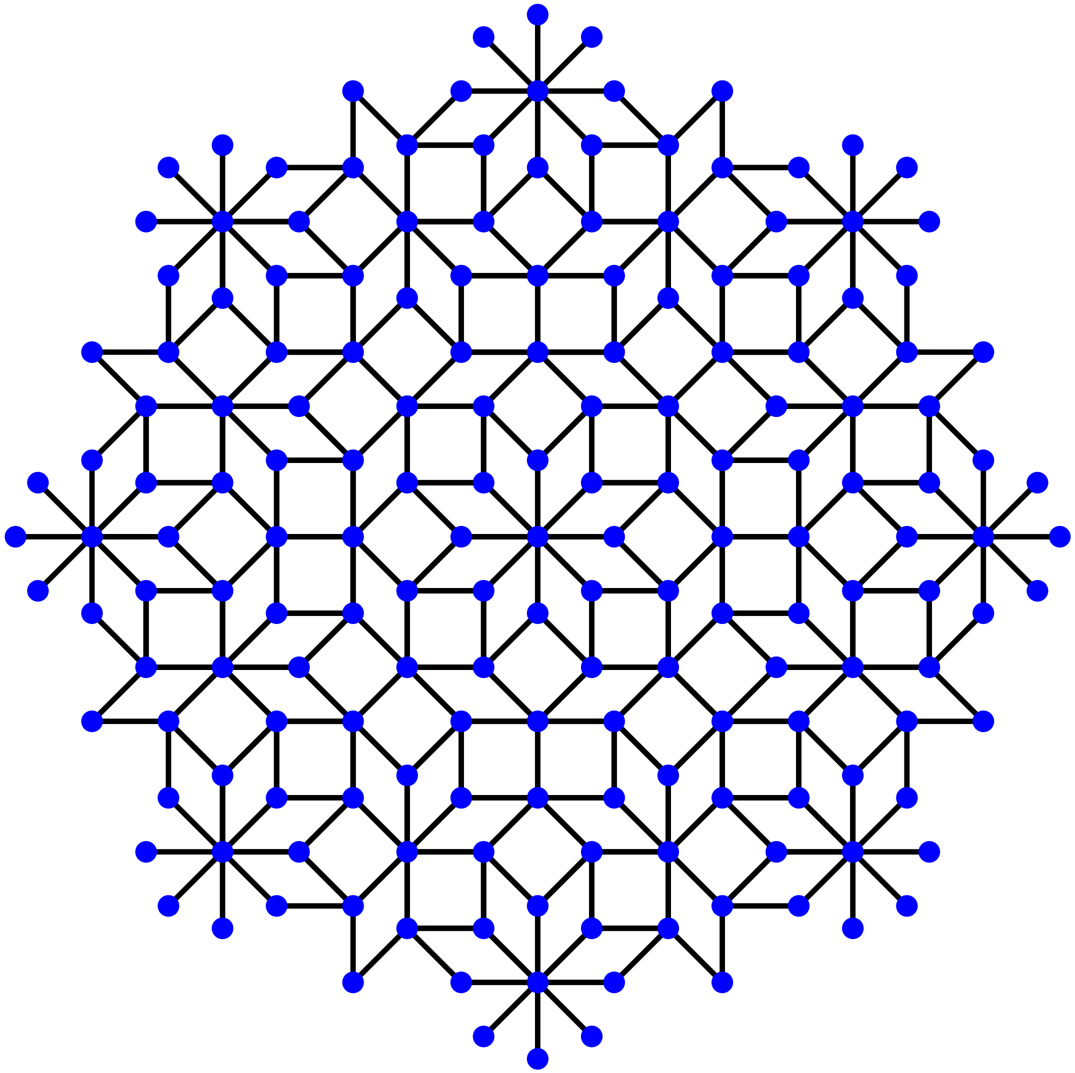
$\xi = \exp(2\pi \mathrm{i}/8)$ $\phi(8) = 4$ $\star$-map: $\xi \mapsto \xi^3$

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

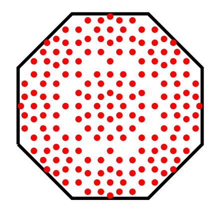




Example: Ammann–Beenker

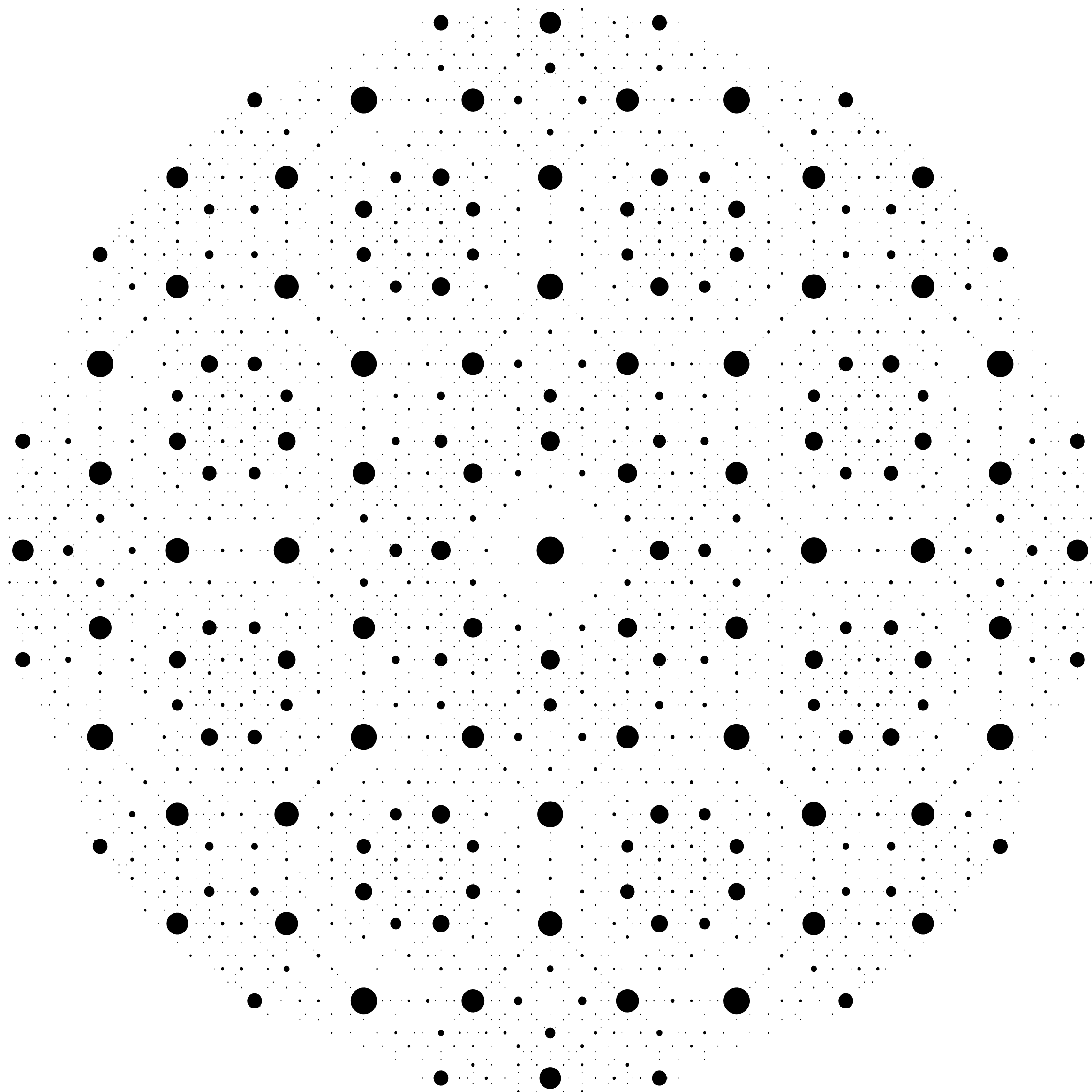


physical space



internal space

Example: Ammann–Beenker



Dirac combs on $\mathbb{Z}$

Weighted Dirac comb (on $\mathbb{Z}$)**:**

$$\omega \;=\; \sum_{n\in\mathbb{Z}} w(n)\,\delta_n$$

Autocorrelation:

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

Autocorrelation coefficients:

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

Diffraction:

$$\boxed{\widehat{\gamma} \;=\; \widehat{\gamma}_{\mathsf{pp}} + \widehat{\gamma}_{\mathsf{sc}} + \widehat{\gamma}_{\mathsf{ac}}}$$

SC spectra: Thue–Morse

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

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 $\boxed{v_{2i+1} = \bar{v}_i}$

—▷ **recursion for autocorrelation coefficients:**

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

for all $m \in \mathbb{Z}$, with $\eta(0) = 1$

—▷ **diffraction** is purely singular continuous

SC spectra: Thue–Morse

Exponential sum:

$$g_n(k) \;=\; \sum_{\ell=0}^{2^n-1} v_\ell \, e^{-2\pi i k \ell}$$

Recursion:

$$g_{n+1}(k) \;=\; \bigl(1 - e^{-2\pi i k 2^n}\bigr)\, g_n(k)$$

with $g_0(k) = 1$

(follows from $v^{(n+1)} = v^{(n)} \bar{v}^{(n)}$)

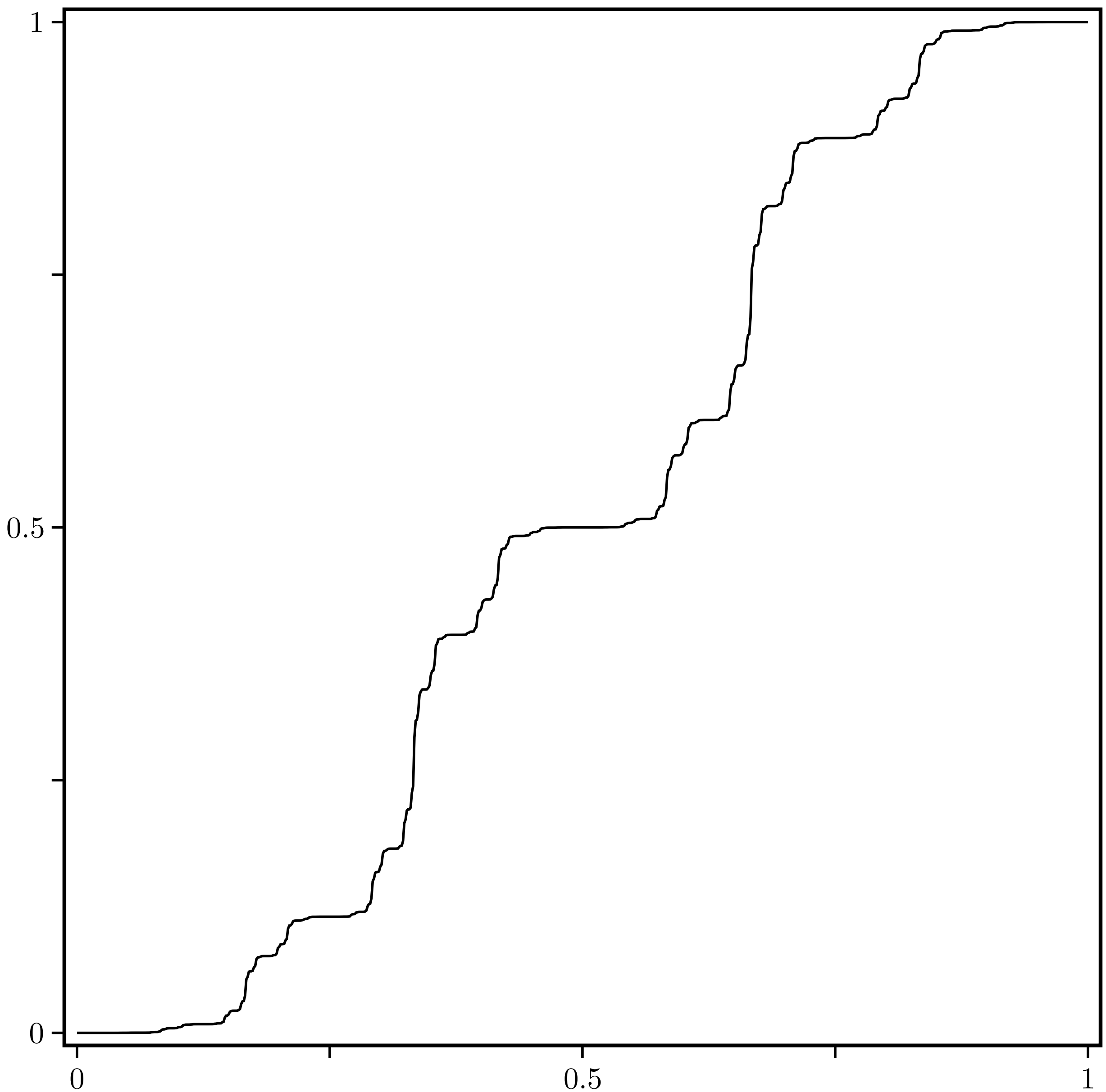
Riesz product:

$$\widehat{\gamma} \;=\; \prod_{n \geq 0} \bigl(1 - \cos(2^{n+1} \pi x)\bigr)$$

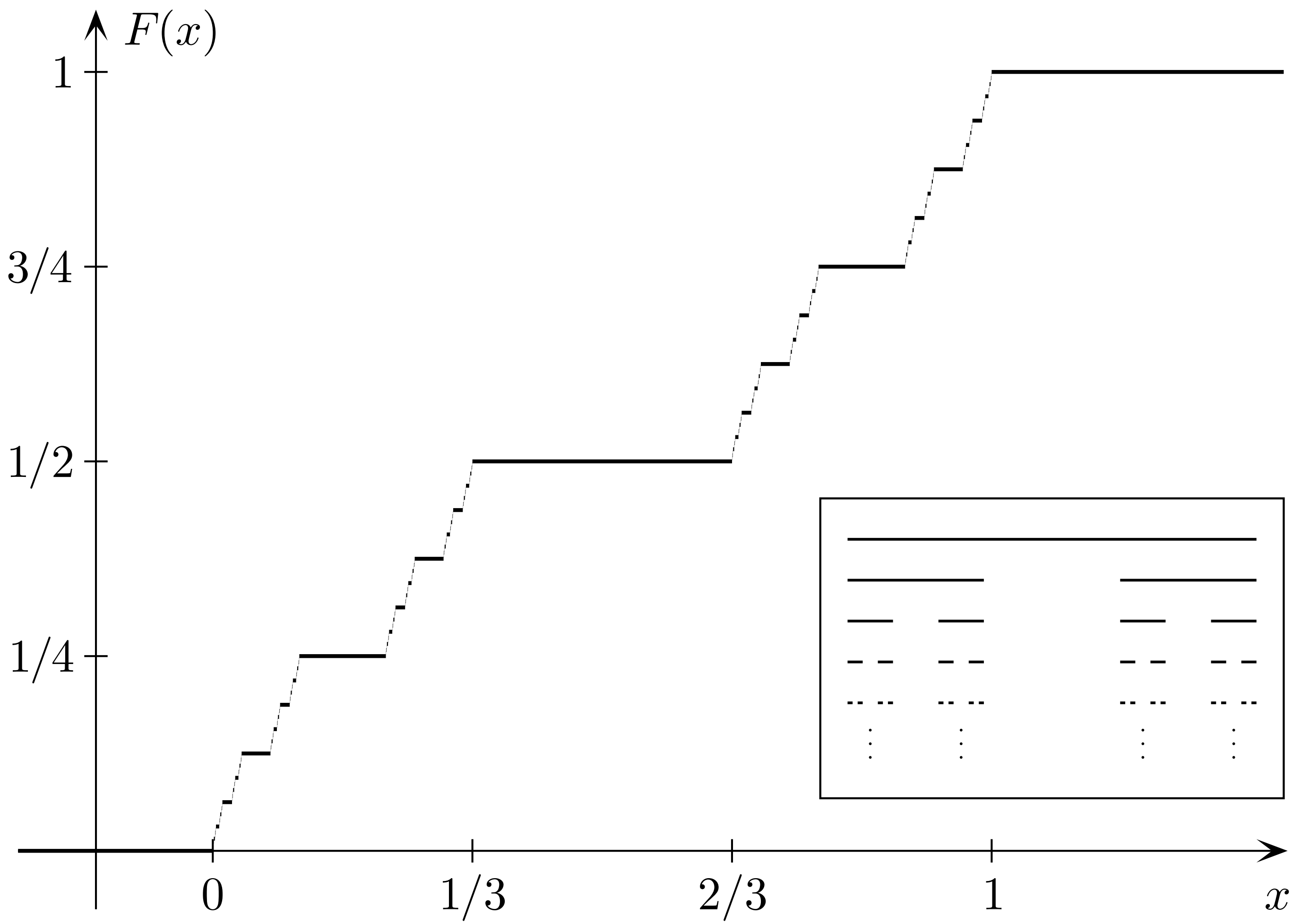
(vague convergence)

⟹ approach can be generalised to other sequences and higher-dimensional block substitutions

Thue–Morse measure



Comparison: Cantor measure



Pure point factor

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

$$\ldots\, 1\bar{1}\bar{1}1\bar{1}11\bar{1}\bar{1}11\bar{1}1\bar{1}\bar{1}1 \,|\, 1\bar{1}\bar{1}1\bar{1}11\bar{1}\bar{1}11\bar{1}1\bar{1}\bar{1}1 \,\ldots$$

$$\ldots\, abaaababab aaabab \,|\, abaaababab abaaabaa \,\ldots$$

- **period doubling:** $\varrho' : \begin{array}{l} a \mapsto ab \\ b \mapsto aa \end{array}$

  $\uparrow$

  coincidence $\Rightarrow$ model set

- global 2:1 factor of Thue–Morse
- recovers pure point part of dynamical spectrum

AC spectra: Coin tossing sequence

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

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

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

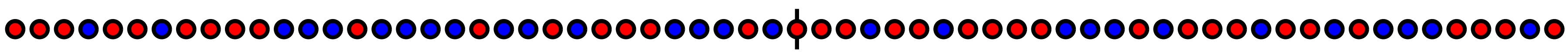
(strong law of large numbers)

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

‘Hidden’ order: Rudin–Shapiro

Binary Rudin–Shapiro sequence: $w(-1) = -1,\ w(0) = 1,$ and

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

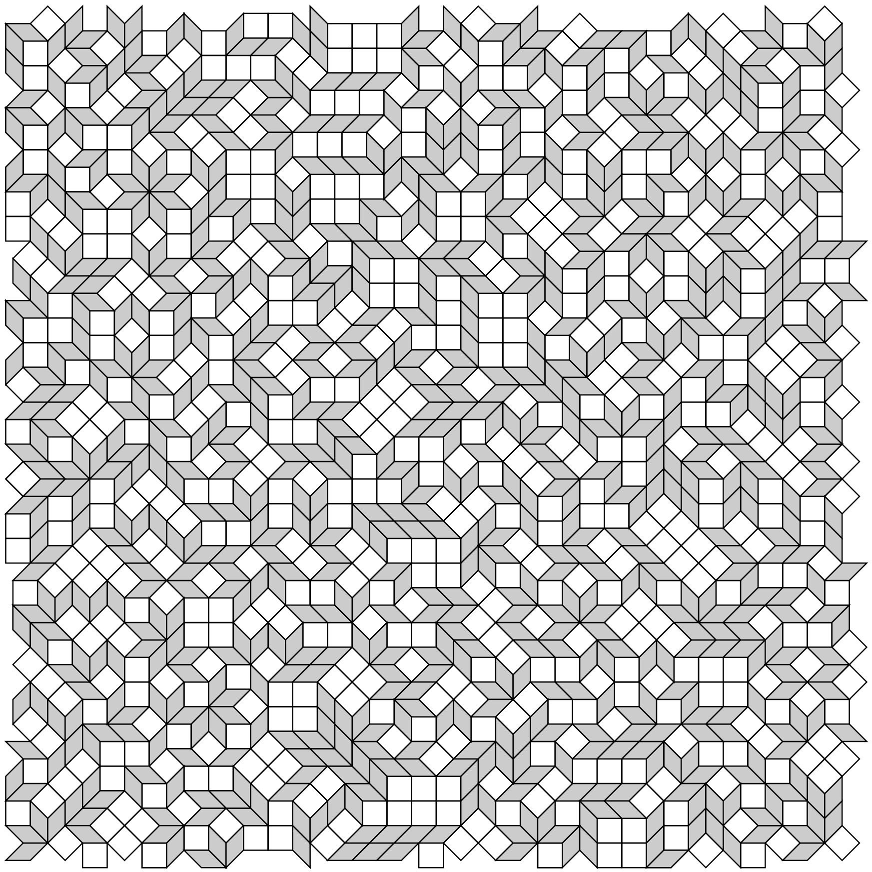


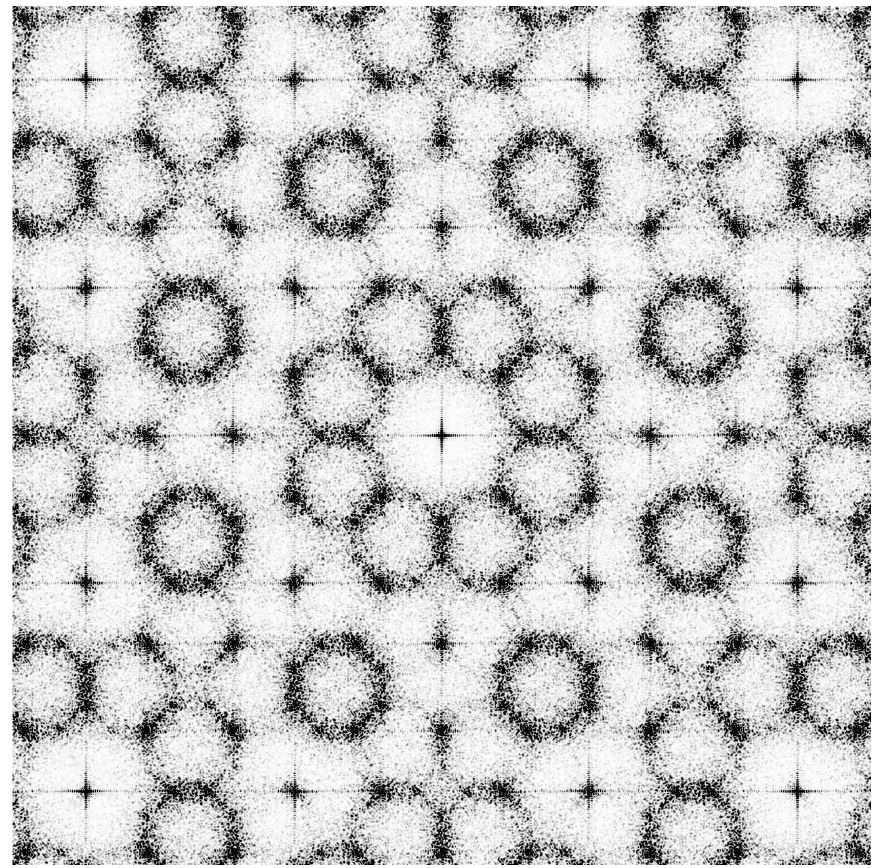
Autocorrelation and diffraction: $\boxed{\gamma_{\mathrm{RS}} = \delta_0}$ and $\boxed{\widehat{\gamma_{\mathrm{RS}}} = \lambda}$

- deterministic, but homometric with coin tossing
- all two-point correlations vanish
- featureless diffraction
- can be generalised (by ‘Bernoullisation’)
- family of homometric systems with varying entropy
- block map ψ induced pure point factor

Diffraction of random tilings

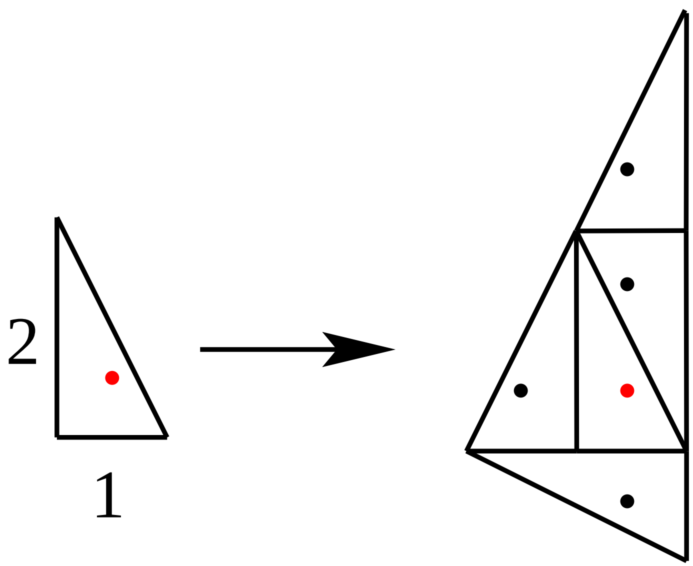
Patch of a square rhombus random tiling,
and diffraction from this finite patch:

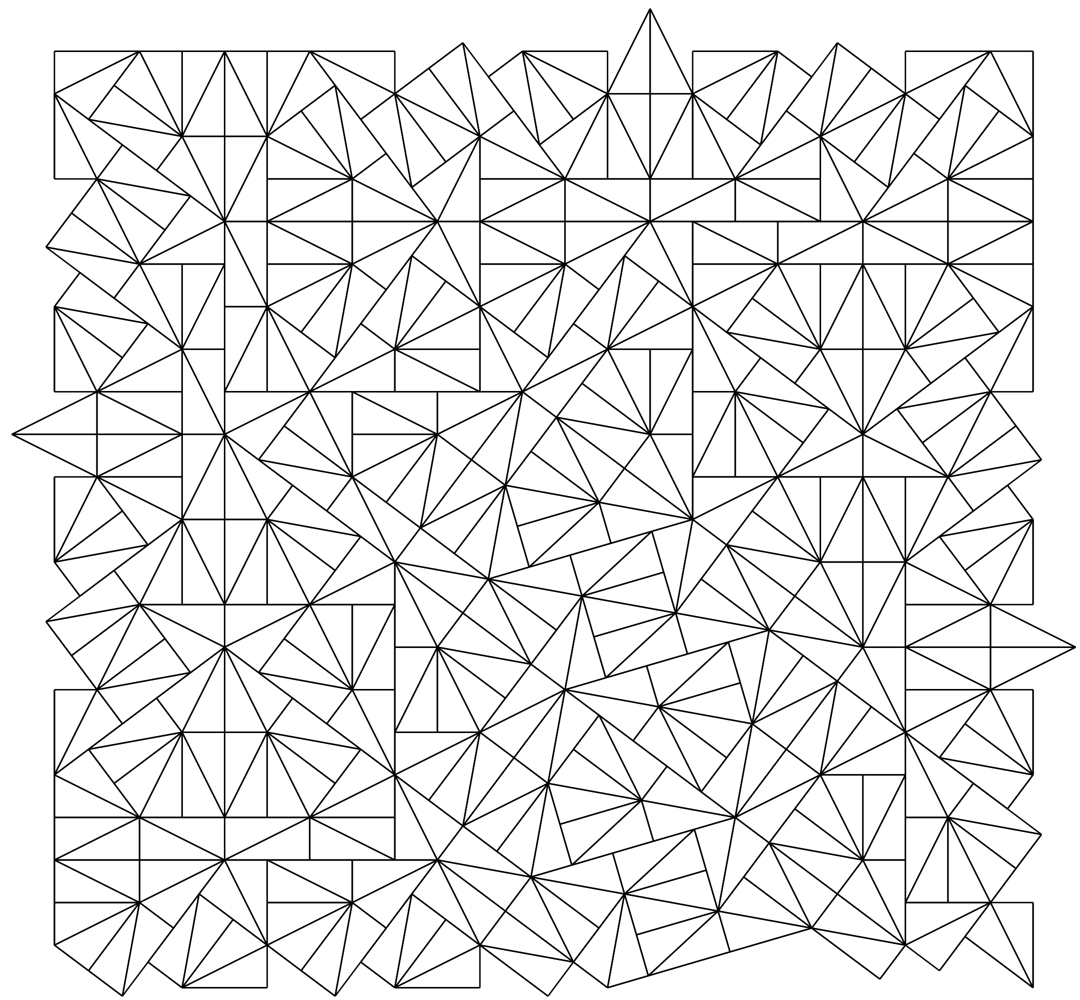




Expectation: mixed spectrum with trivial Bragg peak at 0,
and a mixture of singular and absolutely continuous parts

Pinwheel diffraction





Pinwheel diffraction

Autocorrelation is circularly symmetric,

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

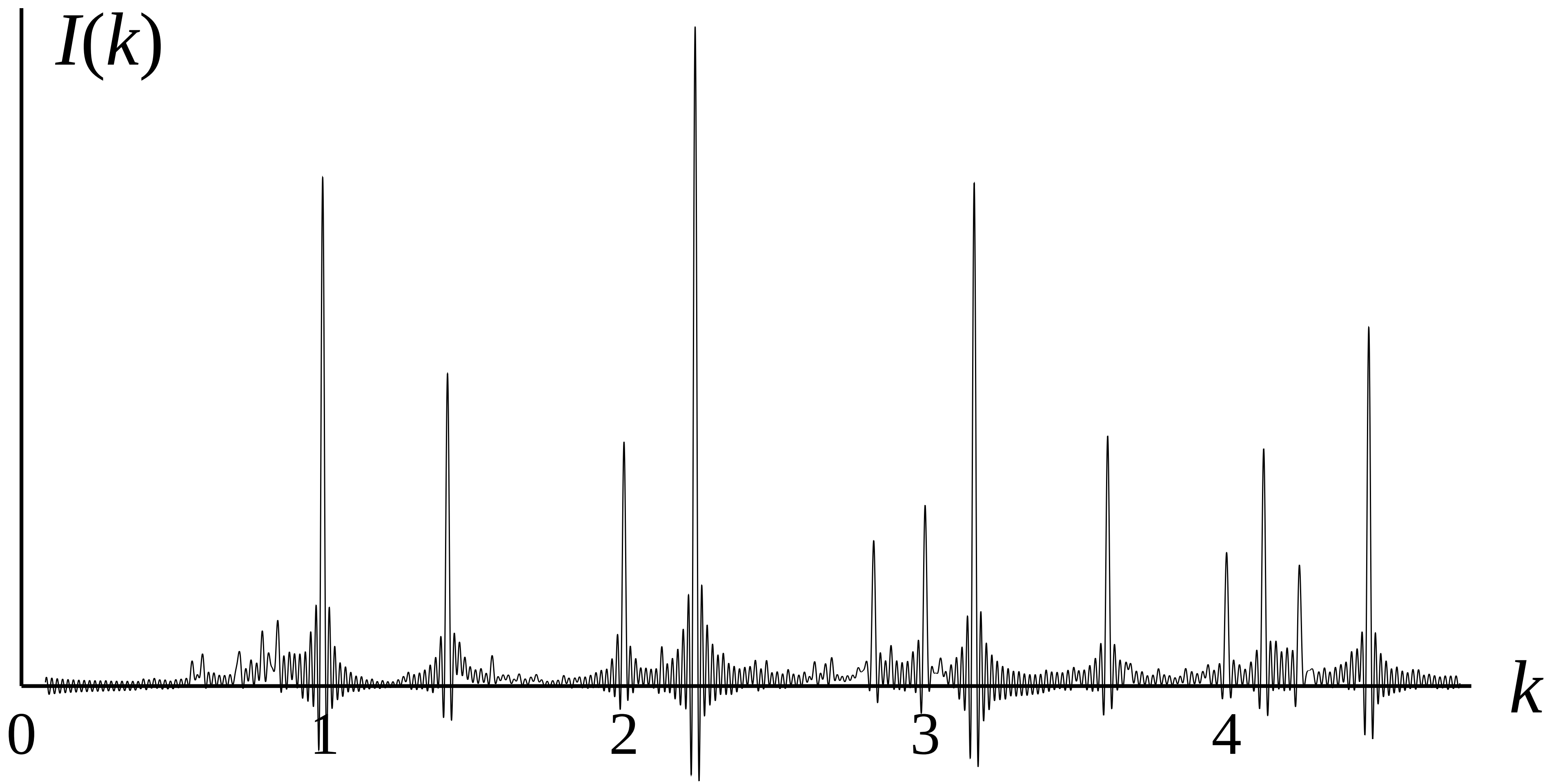
with μ_r the normalised uniform distribution on $r\mathbb{S}^1$

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 diffraction

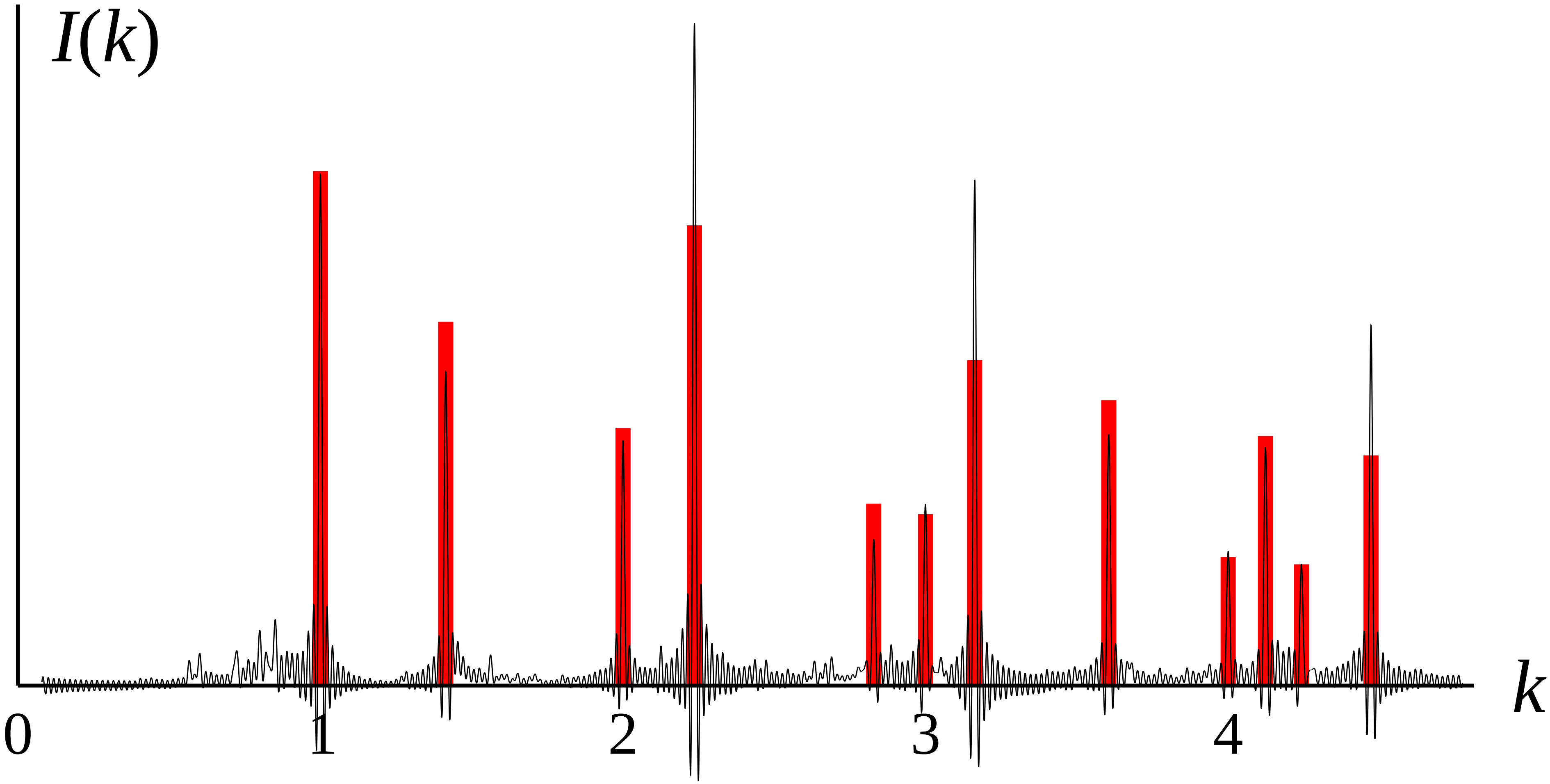
pinwheel radial intensity (numerical)



Pinwheel diffraction

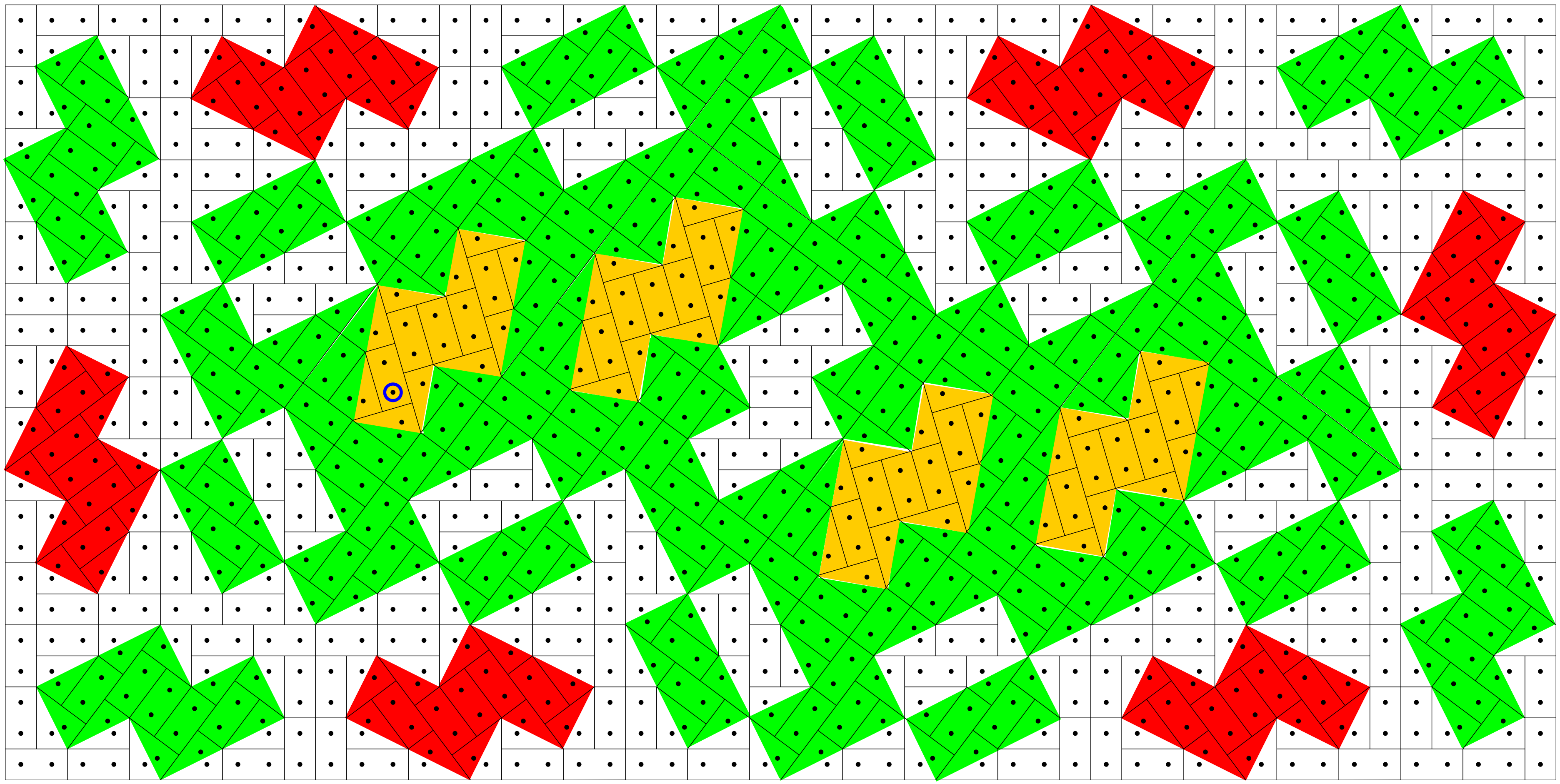
pinwheel radial intensity (numerical)

square lattice powder diffraction



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

Pinwheel diffraction



Summary

- cut and project sets well understood
- systems with continuous diffraction explicitly accessible
- ordered structures with continuous diffraction
- ‘hidden’ order in systems with continuous diffraction
- close relation between diffraction and dynamical spectra
- interesting structures beyond aperiodic crystals
- still many open questions

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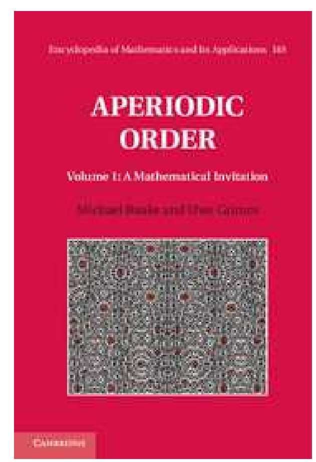
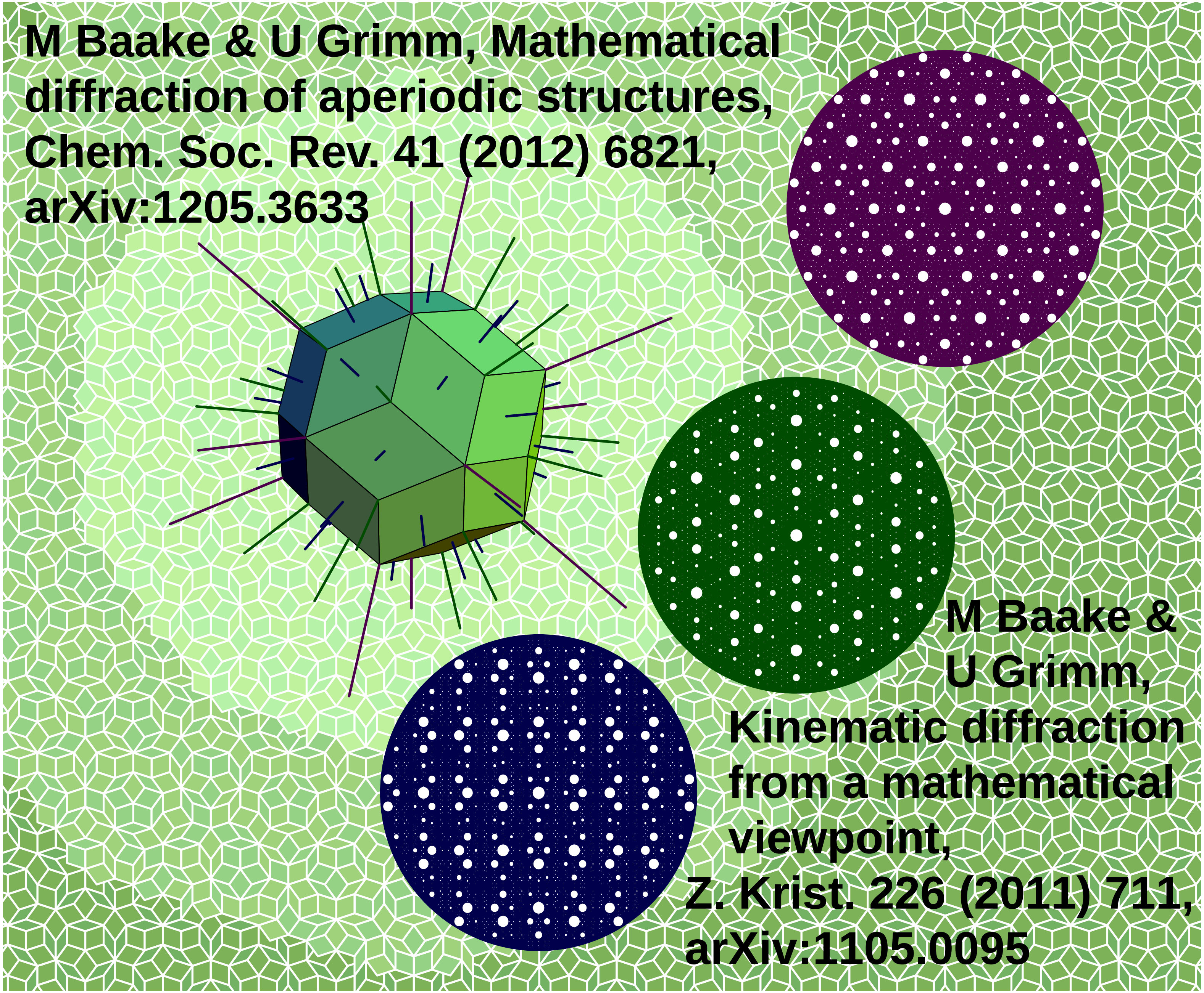


Review articles



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