Renormalisation in Spectral Theory: Introduction and Diffraction

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Thue–Morse spectrum

(Wiener 1927, Mahler 1927, Kakutani 1972, Baake & G 2008)

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

Note that ϱ maps $a \in \{1, \bar{1}\}$ to $a\bar{a}$ (where $\bar{\bar{a}} = a$)

Iteration and fixed point:

$$\begin{aligned} 1 &\longmapsto 1\bar{1} \\ &\longmapsto 1\bar{1}\bar{1}1 \\ &\longmapsto 1\bar{1}\bar{1}1\bar{1}11\bar{1} \\ &\longmapsto 1\bar{1}\bar{1}1\bar{1}11\bar{1}\bar{1}11\bar{1}1\bar{1}\bar{1}1 \\ &\longmapsto \cdots \longrightarrow v = \varrho(v) = v_0 v_1 v_2 v_3 \ldots \end{aligned}$$

Starting from $\bar{1}$ results in the fixed point $\bar{v}$.

Thue–Morse spectrum

(Wiener 1927, Mahler 1927, Kakutani 1972, Baake & G 2008)

Fixed point $v = v_0 v_1 v_2 v_3 \ldots v_i \cdots = \varrho(v)$, so

$$\varrho(v) \;=\; \underbrace{\varrho(v_0)}_{v_0 v_1}\,\underbrace{\varrho(v_1)}_{v_2 v_3}\,\underbrace{\varrho(v_2)}_{v_4 v_5}\,\underbrace{\varrho(v_3)}_{v_6 v_7}\,\cdots\,\underbrace{\varrho(v_i)}_{v_{2i} v_{2i+1}}\,\cdots$$

which implies (noting that $\varrho(v_i) = v_i \overline{v_i}$)

$$\boxed{v_{2i} = v_i} \qquad \text{and} \qquad \boxed{v_{2i+1} = \overline{v_i}}$$

for all $i \geq 0$.

Given v_0, this determines v recursively.

Thue–Morse spectrum

(Wiener 1927, Mahler 1927, Kakutani 1972, Baake & G 2008)

Autocorrelation coefficients

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

Consider $\eta(2m)$ and split the sum into two parts:

$i = 2j$ even: $\quad v_i v_{i+2m} = v_{2j} v_{2j+2m} = v_j v_{j+m}$

$i = 2j+1$ odd: $\quad v_i v_{i+2m} = v_{2j+1} v_{2j+2m+1} = \overline{v_j}\,\overline{v_{j+m}} = v_j v_{j+m}$

This shows that

$$\eta(2m) = \eta(m)$$

for all $m \geq 0$.

Thue–Morse spectrum

(Wiener 1927, Mahler 1927, Kakutani 1972, Baake & G 2008)

Autocorrelation coefficients

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

Consider $\eta(2m+1)$ and split the sum into two parts:

$i = 2j$ even: $\quad v_i v_{i+2m+1} = v_{2j} v_{2j+2m+1} = v_j \overline{v_{j+m}} = -v_j v_{j+m}$

$i = 2j+1$ odd: $\quad v_i v_{i+2m+1} = v_{2j+1} v_{2j+2m+2} = \overline{v_j} v_{j+m+1}$

$$= -v_j v_{j+m+1}$$

This shows that

$$\eta(2m+1) = -\frac{1}{2}\Big(\eta(m) + \eta(m+1)\Big)$$

for all $m \geq 0$.

Thue–Morse spectrum

(Wiener 1927, Mahler 1927, Kakutani 1972, Baake & G 2008)

Autocorrelation coefficients

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

satisfy

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

for all $m \geq 0$. Given $\eta(0) = 1$, all coefficients $\eta(m)$ for $m > 0$ are uniquely determined. In particular,

$$\eta(1) \;=\; -\frac{1}{2}\Big(\eta(0) + \eta(1)\Big)$$

which implies $\eta(1) = -\frac{1}{3}$.

Thue–Morse spectrum

(Wiener 1927, Mahler 1927, Kakutani 1972, Baake & G 2008)

Autocorrelation coefficients

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

satisfy

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

for all $m \geq 0$.

Renormalisation relations

Equations contain a self-consistent part (here $m \in \{0, 1\}$) plus recursions (determining coefficients for $m > 1$).

Thue–Morse spectrum

(Wiener 1927, Mahler 1927, Kakutani 1972, Baake & G 2008)

Autocorrelation coefficients

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

Thue–Morse measure

η positive definite, Herglotz–Bochner theorem implies

$$\eta(m) \;=\; \int_0^1 \mathrm{e}^{2\pi\mathrm{i}my}\, \mathrm{d}\mu(y)$$

with positive measure μ on $[0,1)$.

Renormalisation relations for η

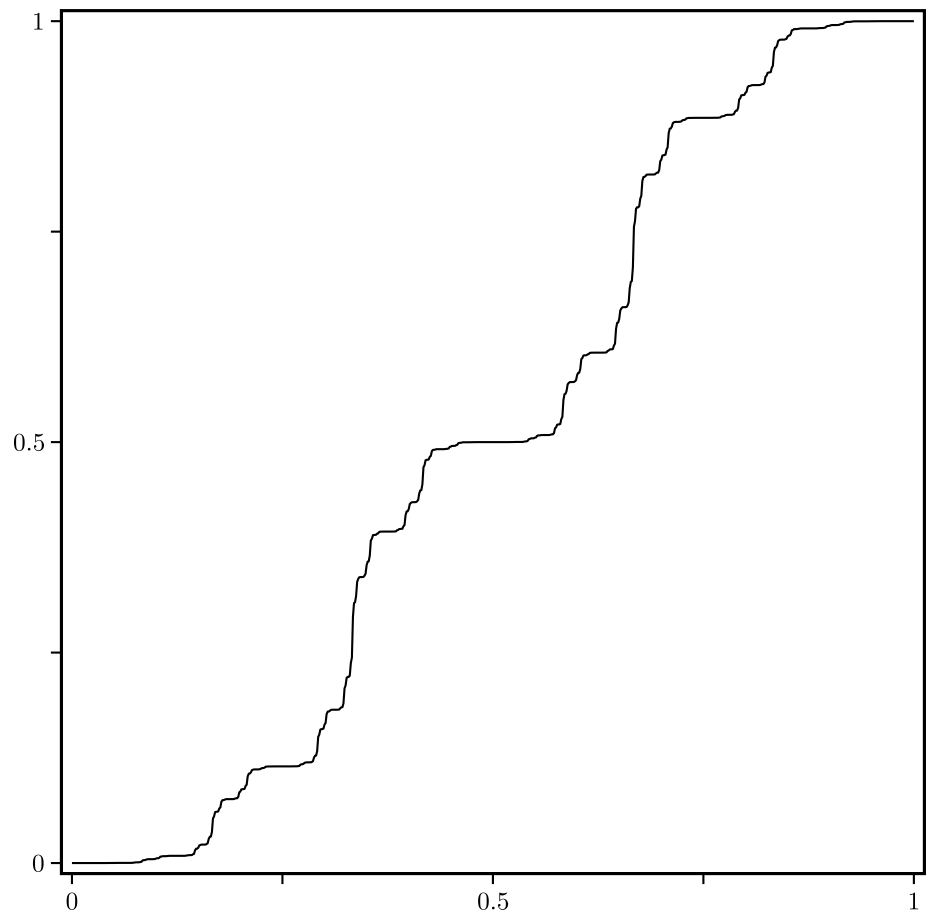
$\Longrightarrow$ μ **purely singular continuous** measure

$\Longrightarrow$ Riesz product $\prod_{\ell\geq 1}\bigl(1-\cos(2^{\ell}\pi y)\bigr)$

Thue–Morse spectrum

(Wiener 1927, Mahler 1927, Kakutani 1972, Baake & G 2008)

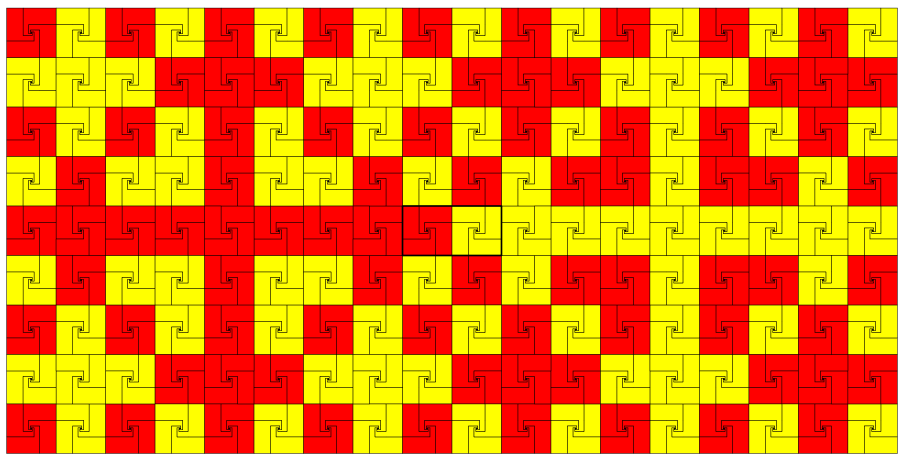
Thue–Morse measure



Plot of distribution function $F(x) = \int_0^x \mathrm{d}\mu(y) = x + \sum_{m \geq 1} \frac{\eta(m)}{mx} \sin(2\pi m x)$

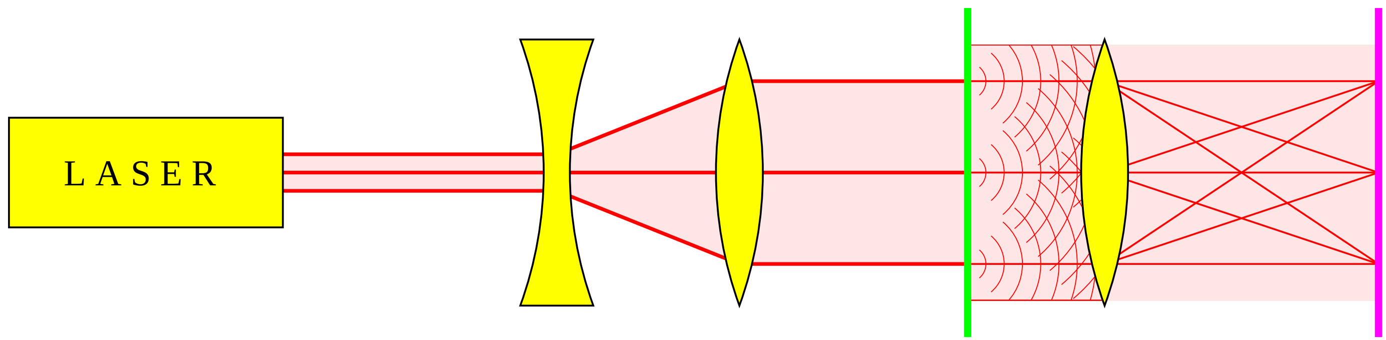
Renormalisation approach

This approach was generalised to show purely singular continuous spectrum for generalised Thue–Morse sequence (Baake, Gähler & G 2012) and higher-dimensional binary bijective block substitution tilings (Baake & G 2014), such as the 'squiral' tiling



More generally, rather than working with autocorrelation coefficients directly, renormalisation relations can be derived using the **pair correlation coefficients** (Baake & Gähler 2015).

Connection with diffraction



Wiener's diagram obstacle $f(x)$, with $\widetilde{f}(x) := \overline{f(-x)}$

$$\begin{array}{ccc} f & \xrightarrow{\;\;*\;\;} & f * \widetilde{f} \\ \mathcal{F}\big\downarrow & & \big\downarrow\mathcal{F} \\ \widehat{f} & \xrightarrow{\;|\cdot|^2\;} & |\widehat{f}\,|^2 \end{array}$$

Connection with diffraction

Structure translation bounded measure ω

assumed 'self-amenable' (Hof 1995)

(here, $\omega = \delta_{\varLambda} := \sum_{x \in \varLambda} \delta_x$ for point set $\varLambda \subset \mathbb{R}^d$)

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

Diffraction $\boxed{\widehat{\gamma} = \bigl(\widehat{\gamma}\bigr)_{\mathsf{pp}} + \bigl(\widehat{\gamma}\bigr)_{\mathsf{sc}} + \bigl(\widehat{\gamma}\bigr)_{\mathsf{ac}}}$ (relative to λ_{Leb})

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

Fibonacci inflation

Substitution rule and **substitution matrix**

$$\varrho\colon \quad \begin{matrix} \ell \mapsto \ell s \\ s \mapsto \ell \end{matrix} \qquad\qquad M = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}$$

One-sided **fixed point** $w = \varrho(w)$ by iteration of ϱ on $w^{(0)} = \ell$:

$$\ell \mapsto \ell s \mapsto \ell s \ell \mapsto \ell s \ell \ell s \mapsto \ell s \ell \ell s \ell s \ell \mapsto \cdots \mapsto w^{(n)} \xrightarrow{n\to\infty} w$$

Fibonacci numbers

$|w^{(n)}| = f_{n+2}$ with $\mathrm{card}_{\ell}(w^{(n)}) = f_{n+1}$ and $\mathrm{card}_{s}(w^{(n)}) = f_n$

where $f_0 = 0$, $f_1 = 1$ and $f_{n+1} = f_n + f_{n-1}$

Golden ratio

$$\lim_{n\to\pm\infty} \frac{f_{n+1}}{f_n} = \frac{1 \pm \sqrt{5}}{2} = \begin{cases} \tau \\ \tau' \end{cases}$$

Fibonacci inflation

Recursion: $w^{(n+1)} = w^{(n)} w^{(n-1)}$

Two-sided Fibonacci sequence

$$\ell|\ell \xmapsto{\varrho} \underline{\underline{\ell s}}|\ell s \xmapsto{\varrho} \ell \underline{s\ell}|\ell s \ell$$

$$\xmapsto{\varrho} \ell s \ell \underline{\underline{\ell s}}|\ell s \ell \ell s \xmapsto{\varrho} \ell s \ell \ell s \ell \underline{s \ell}|\ell s \ell \ell s \ell s \ell$$

$$\xmapsto{\varrho} \ell s \ell \ell s \ell s \ell \ell s \ell \underline{\underline{\ell s}}|\ell s \ell \ell s \ell s \ell \ell s \ell \ell s \xmapsto{\varrho} \cdots$$

limiting 2-cycle ▷ two fixed points under ϱ^2

Geometric realisation

as an inflation rule on one-dimensional tiles (intervals)

Displacement matrix

Inflation rule

Choose **natural tile lengths** according to left Perron–Frobenius eigenvector $(\tau, 1)$ of M

Displacement matrix

$$T = \begin{pmatrix} \{0\} & \{0\} \\ \{\tau\} & \varnothing \end{pmatrix}$$

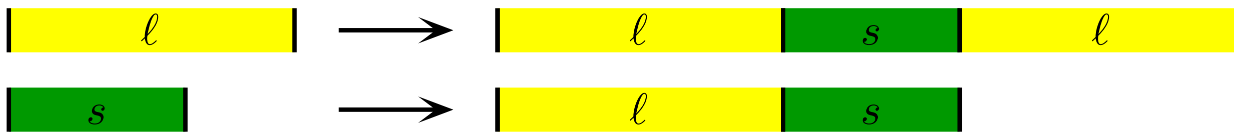
with $\mathrm{card}(T_{ab}) = M_{ab}$.

Consider **fixed-point tiling** obtained by an even number of inflations of the initial patch 

Control point sets $\varLambda_a \subset \mathbb{Z}[\tau]$: sets of left endpoints of intervals of type $a \in \{\ell, s\}$, and $\varLambda = \varLambda_\ell \cup \varLambda_s \subset \mathbb{Z}[\tau]$.

Displacement matrix

Squared inflation rule



Displacement matrix

$$T = \begin{pmatrix} \{0, \tau+1\} & \{0\} \\ \{\tau\} & \{\tau\} \end{pmatrix}$$

with $\mathrm{card}(T_{ab}) = M^2_{ab}$.

Fixed point equations for point sets $\varLambda_{\ell,s}$

$$\left.\begin{aligned} \varLambda_\ell &= \tau^2 \varLambda_\ell \cup \left(\tau^2 \varLambda_\ell + \tau^2\right) \cup \tau^2 \varLambda_s \\ \varLambda_s &= \left(\tau^2 \varLambda_\ell + \tau\right) \cup \left(\tau^2 \varLambda_s + \tau\right) \end{aligned}\right\} \qquad \varLambda_a = \bigcup_b \tau^2 \varLambda_b + T_{ab}$$

Pair correlations

Pair correlation coefficients

$$\nu_{ab}(z) \;:=\; \frac{\mathrm{dens}\bigl(\varLambda_a \cap (\varLambda_b - z)\bigr)}{\mathrm{dens}(\varLambda)}$$

satisfying $\nu_{ab}(z) > 0$ for $z \in \varLambda_b - \varLambda_a$ (and $\nu_{ab}(z) = 0$ otherwise)

Autocorrelation coefficients

$$\eta(z) \;:=\; \mathrm{dens}\bigl(\varLambda \cap (\varLambda - z)\bigr) \;=\; \mathrm{dens}(\varLambda) \sum_{a,b} \nu_{ab}(z)$$

Strategy

- derive renormalisation relations for $\nu_{ab}(z)$
- take the Fourier transform
- obtain conditions on spectral components

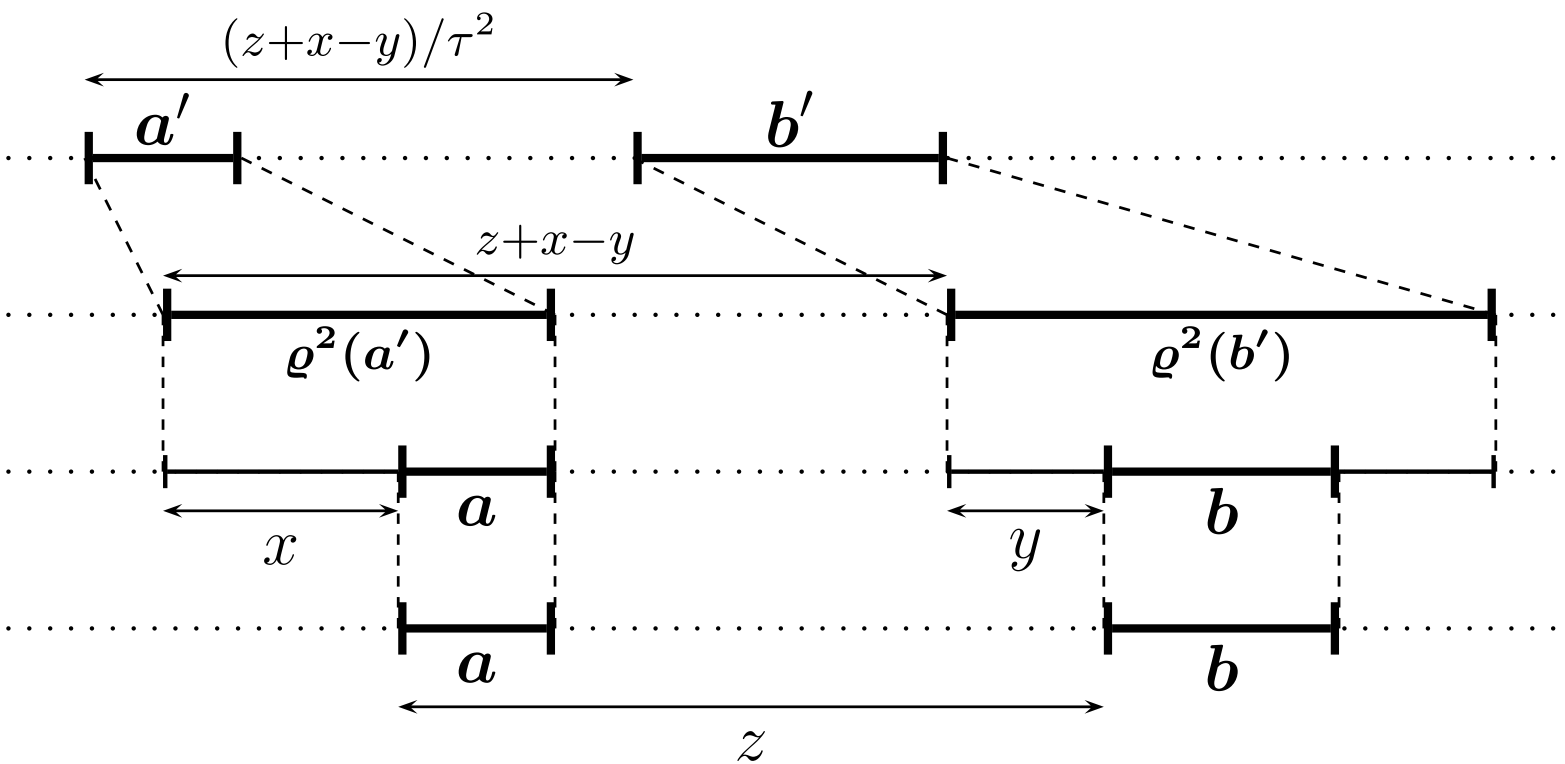
Pair correlations

From the fixed point equation we get

$$\begin{aligned}
\nu_{ab}(z) &= \frac{\mathrm{dens}\big(\varLambda_a \cap (\varLambda_b - z)\big)}{\mathrm{dens}(\varLambda)} \\
&= \frac{\mathrm{dens}\Big(\big(\bigcup_{a'} \tau^2 \varLambda_{a'} + T_{aa'}\big) \cap \big(\bigcup_{b'} \tau^2 \varLambda_{b'} + T_{bb'} - z\big)\Big)}{\mathrm{dens}(\varLambda)} \\
&= \sum_{a',b'} \sum_{x \in T_{aa'}} \sum_{y \in T_{bb'}} \frac{\mathrm{dens}\big((\tau^2 \varLambda_{a'} + x) \cap (\tau^2 \varLambda_{b'} + y - z)\big)}{\mathrm{dens}(\varLambda)} \\
&= \frac{1}{\tau^2} \sum_{a',b'} \sum_{x \in T_{aa'}} \sum_{y \in T_{bb'}} \frac{\mathrm{dens}\big((\varLambda_{a'} + \frac{x}{\tau^2}) \cap (\varLambda_{b'} + \frac{y-z}{\tau^2})\big)}{\mathrm{dens}(\varLambda)} \\
&= \frac{1}{\tau^2} \sum_{a',b'} \sum_{x \in T_{aa'}} \sum_{y \in T_{bb'}} \nu_{a'b'}\big(\tfrac{z+x-y}{\tau^2}\big)
\end{aligned}$$

Pair correlations

$$\nu_{ab}(z) = \frac{1}{\tau^2} \sum_{a',b'} \sum_{x \in T_{aa'}} \sum_{y \in T_{bb'}} \nu_{a'b'}\Big(\frac{z+x-y}{\tau^2}\Big)$$



Pair correlation measures

Define **pair correlation measures**

$$\Upsilon_{ab} := \sum_{z \in \varLambda_b - \varLambda_a} \nu_{ab}(z)\, \delta_z$$

The **autocorrelation measure** γ and the **diffraction measure** $\widehat{\gamma}$ are given by

$$\gamma = \sum_{z \in \varLambda - \varLambda} \eta(z)\, \delta_z = \mathrm{dens}(\varLambda) \sum_{a,b} \Upsilon_{ab}$$

$$\widehat{\gamma} = \mathrm{dens}(\varLambda) \sum_{a,b} \widehat{\Upsilon_{ab}}$$

Pair correlation measures

Define **pair correlation measures**

$$\Upsilon_{ab} := \sum_{z \in \varLambda_b - \varLambda_a} \nu_{ab}(z)\, \delta_z$$

and set $\widehat{\Upsilon} = \bigl(\widehat{\Upsilon_{\ell\ell}}, \widehat{\Upsilon_{\ell s}}, \widehat{\Upsilon_{s\ell}}, \widehat{\Upsilon_{ss}}\bigr)$. Then (with $\lambda = \tau^2$)

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

with $f(x) = \lambda x$ and $\boldsymbol{A}(k) = B(k) \otimes \overline{B(k)}$

$B(.)$ is the **Fourier matrix**

$$B(k) = \widecheck{\delta_T}(k) = \widehat{\delta_T}(-k)$$

Fourier matrix

For the Fibonacci inflation

$$T = \begin{pmatrix} \{0, \tau+1\} & \{0\} \\ \{\tau\} & \{\tau\} \end{pmatrix} \quad \Longrightarrow \quad B(k) = \begin{pmatrix} 1 + \mathrm{e}^{2\pi\mathrm{i}(\tau+1)k} & 1 \\ \mathrm{e}^{2\pi\mathrm{i}\tau k} & \mathrm{e}^{2\pi\mathrm{i}\tau k} \end{pmatrix}$$

For N-fold inflation, the Fourier matrix is ($\lambda = \tau^2$)

$$\begin{aligned} B^{(N)}(k) &= B(k)\, B^{(N-1)}(\lambda k) \\ &= B(k)\, B(\lambda k)\, B(\lambda^2 k) \cdots B(\lambda^{N-1} k) \end{aligned}$$

This cocycle, and in particular its Lyapunov exponents, provides information about the spectral components

$\longrightarrow\!\!\triangleright$ more on this in Neil's talk tomorrow

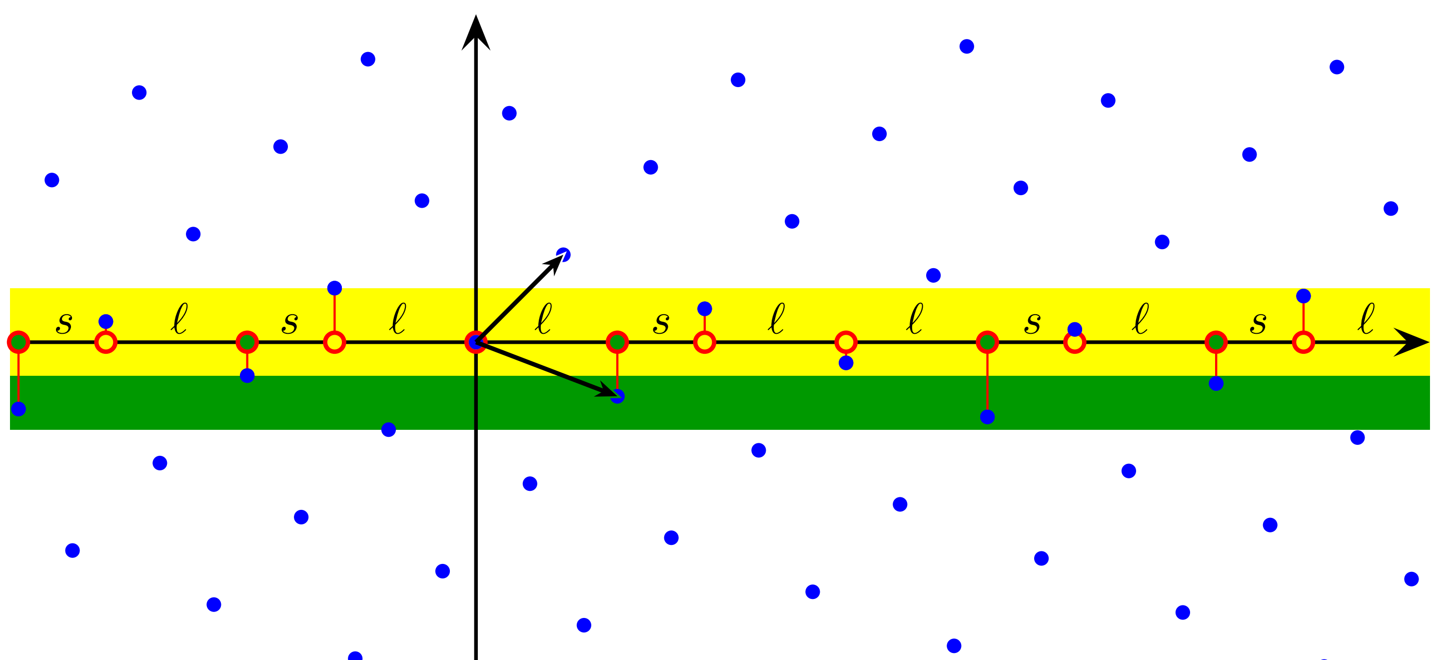
Fibonacci model set

Substitution $\ell \mapsto \ell s$, $s \mapsto \ell$ (inflation factor $\tau = \frac{1+\sqrt{5}}{2}$)

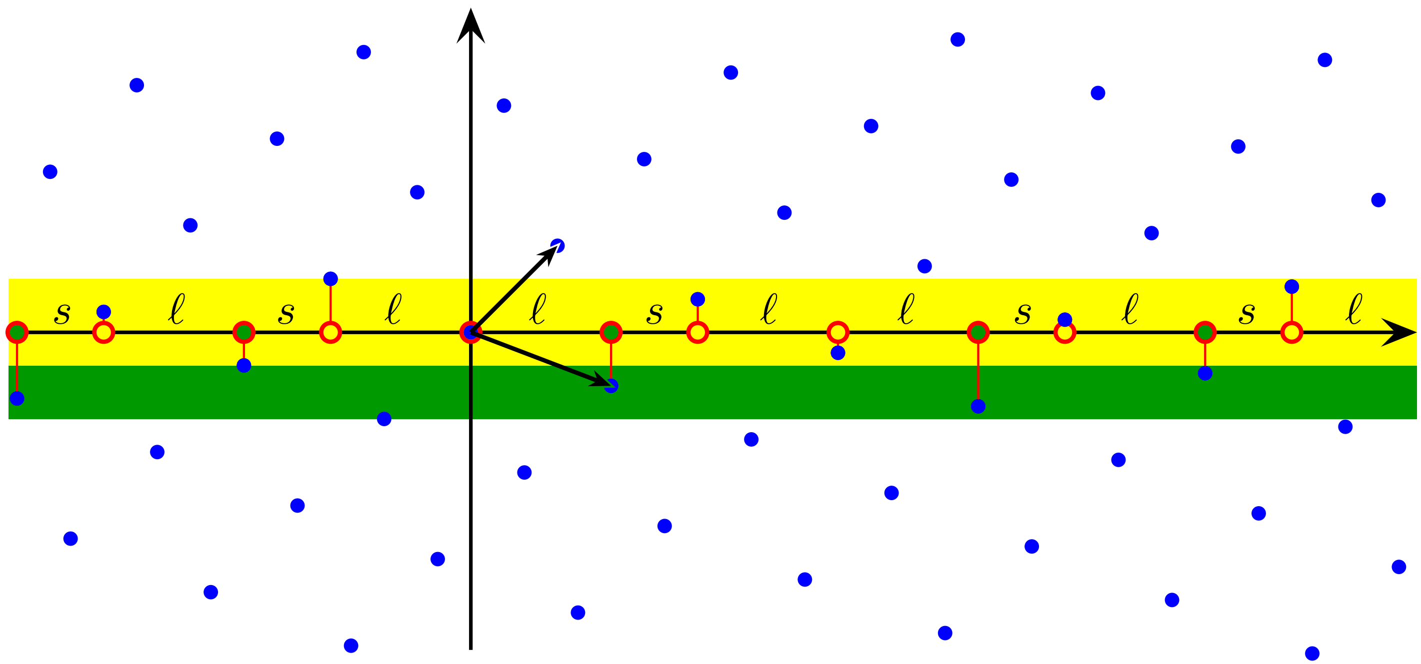
Point set $\varLambda = \big\{ x \in \mathbb{Z}[\tau] : x^{\star} \in W \big\}$ with $W = (-1, \tau - 1]$

$\star$-map $\sqrt{5} \mapsto -\sqrt{5}$ which means $\tau \mapsto \tau^{\star} = 1 - \tau$

Minkowski embedding $\mathcal{L} = \big\{ (x, x^{\star}) : x \in \mathbb{Z}[\tau] \big\}$ lattice



Diffraction of Fibonacci chain

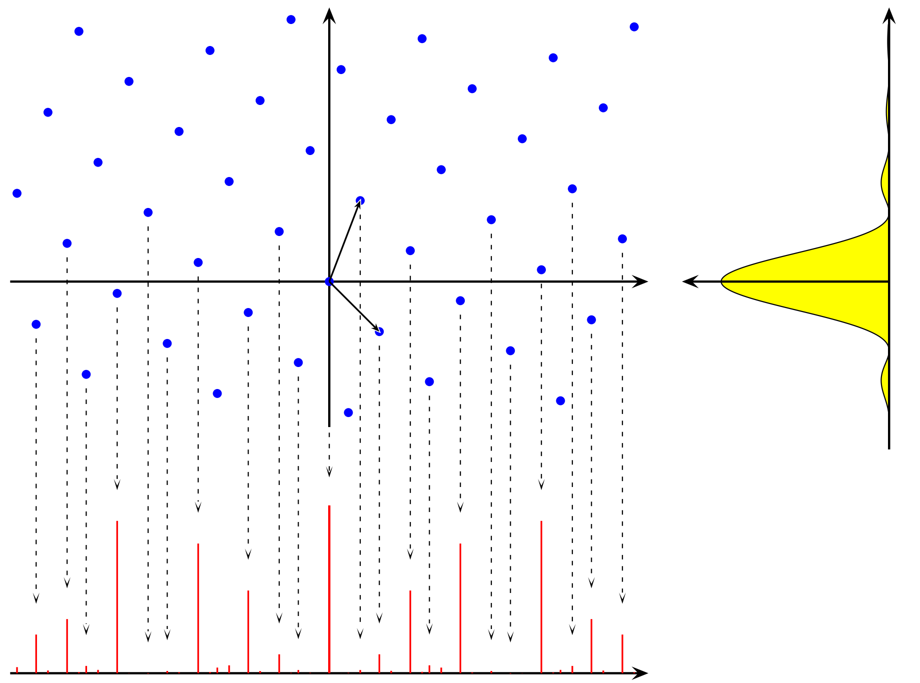


Basis matrices of $\mathcal{L}$ and $\mathcal{L}^*$: $\begin{pmatrix} \tau & 1 \\ 1-\tau & 1 \end{pmatrix}$ and $\frac{1}{\sqrt{5}}\begin{pmatrix} 1 & \tau-1 \\ -1 & \tau \end{pmatrix}$

Fourier module: $L^{\circledast} = L/\sqrt{5}$, Bragg peaks for $k \in L^{\circledast}$

Intensity: $I(k) = \left| \frac{\mathrm{dens}(\varLambda)}{\mathrm{vol}(W)} \, \widecheck{1_W}(k^\star) \right|^2 = \left(\frac{\tau}{\sqrt{5}} \, \mathrm{sinc}(\pi\tau k^\star) \right)^2$

Diffraction of Fibonacci chain

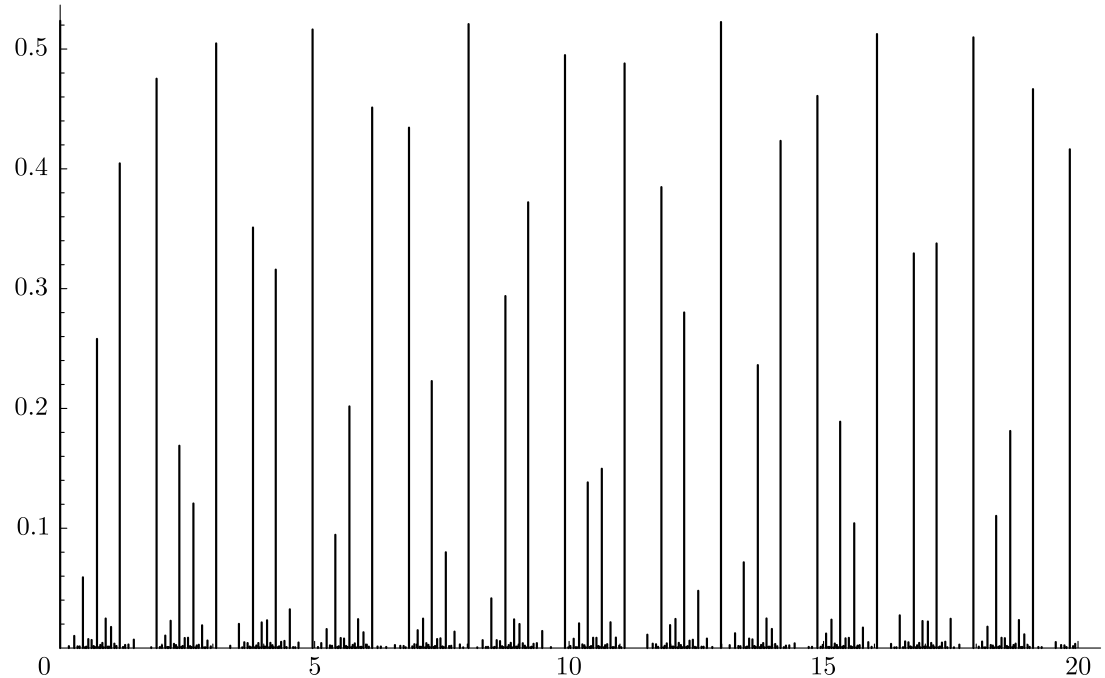


Basis matrices of $\mathcal{L}$ and $\mathcal{L}^*$: $\begin{pmatrix} \tau & 1 \\ 1-\tau & 1 \end{pmatrix}$ and $\frac{1}{\sqrt{5}}\begin{pmatrix} 1 & \tau-1 \\ -1 & \tau \end{pmatrix}$

Fourier module: $L^{\circledast} = L/\sqrt{5}$, Bragg peaks for $k \in L^{\circledast}$

Intensity: $I(k) = \left| \frac{\mathrm{dens}(\varLambda)}{\mathrm{vol}(W)} \, \widecheck{1_W}(k^\star) \right|^2 = \left(\frac{\tau}{\sqrt{5}} \, \mathrm{sinc}(\pi \tau k^\star) \right)^2$

Diffraction of Fibonacci chain



Basis matrices of $\mathcal{L}$ and $\mathcal{L}^*$: $\begin{pmatrix} \tau & 1 \\ 1-\tau & 1 \end{pmatrix}$ and $\frac{1}{\sqrt{5}}\begin{pmatrix} 1 & \tau-1 \\ -1 & \tau \end{pmatrix}$

Fourier module: $L^{\circledast} = L/\sqrt{5}$, Bragg peaks for $k \in L^{\circledast}$

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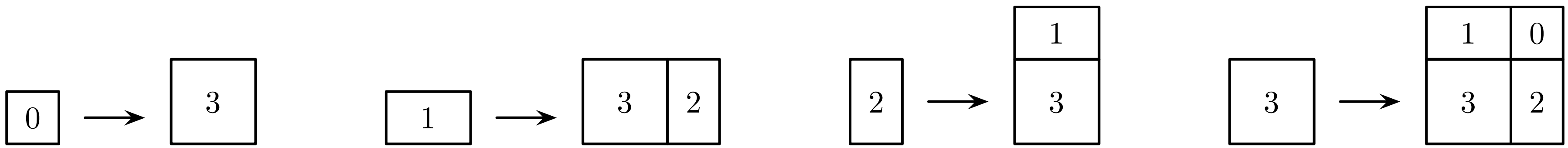
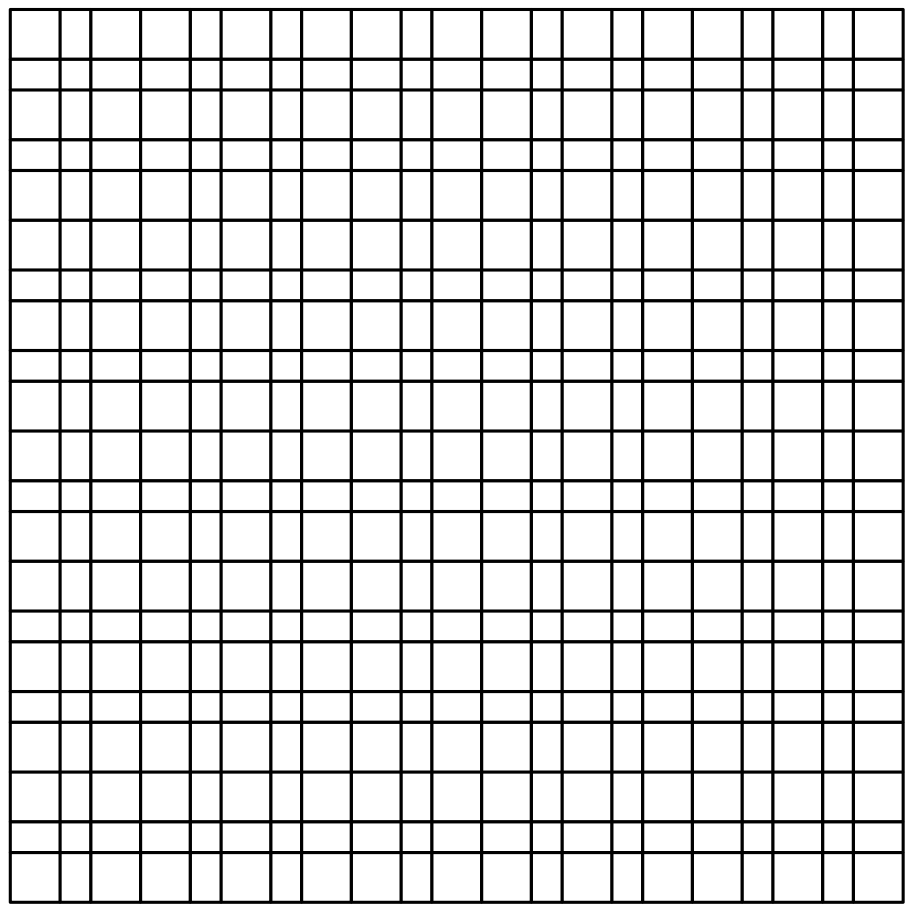
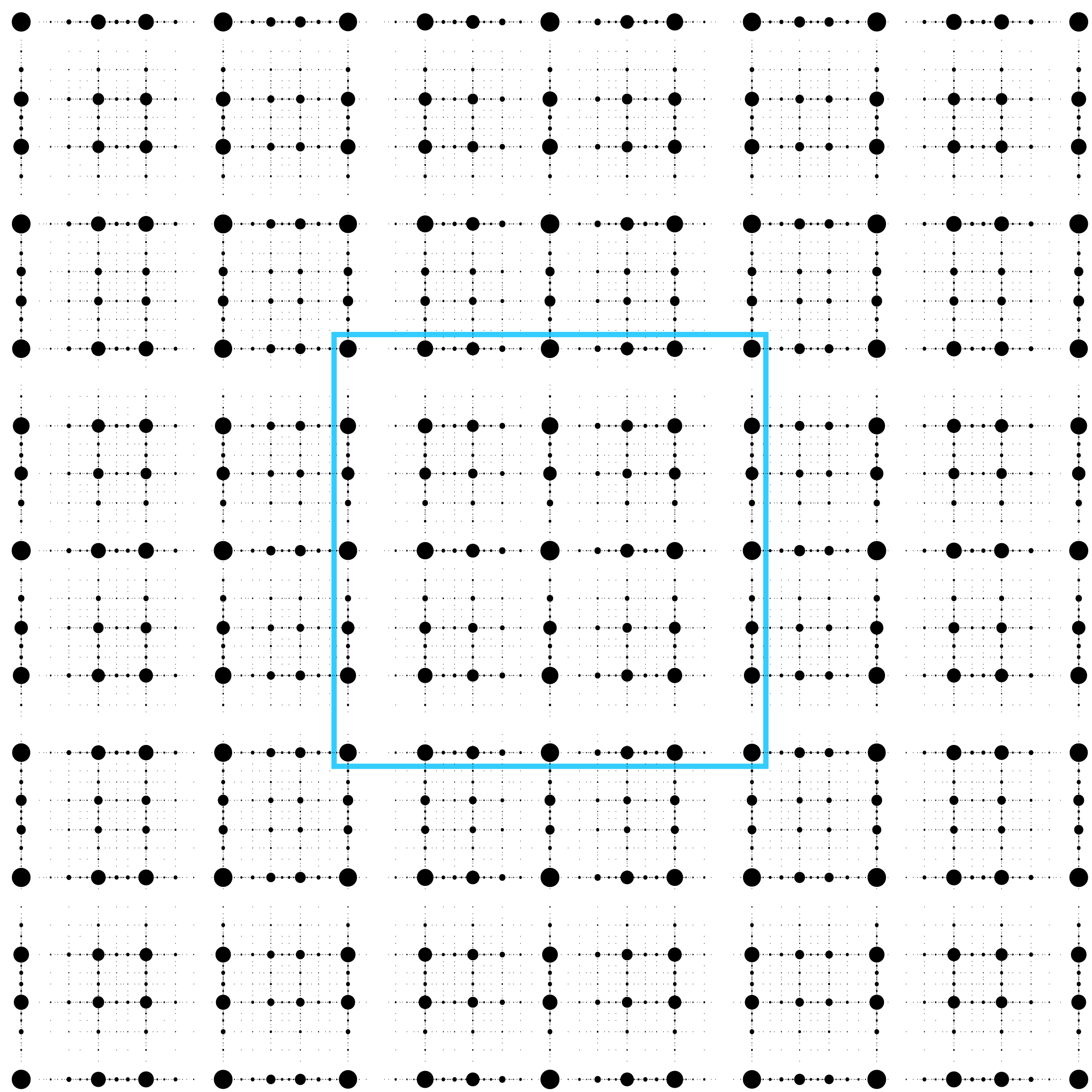
Square Fibonacci model set



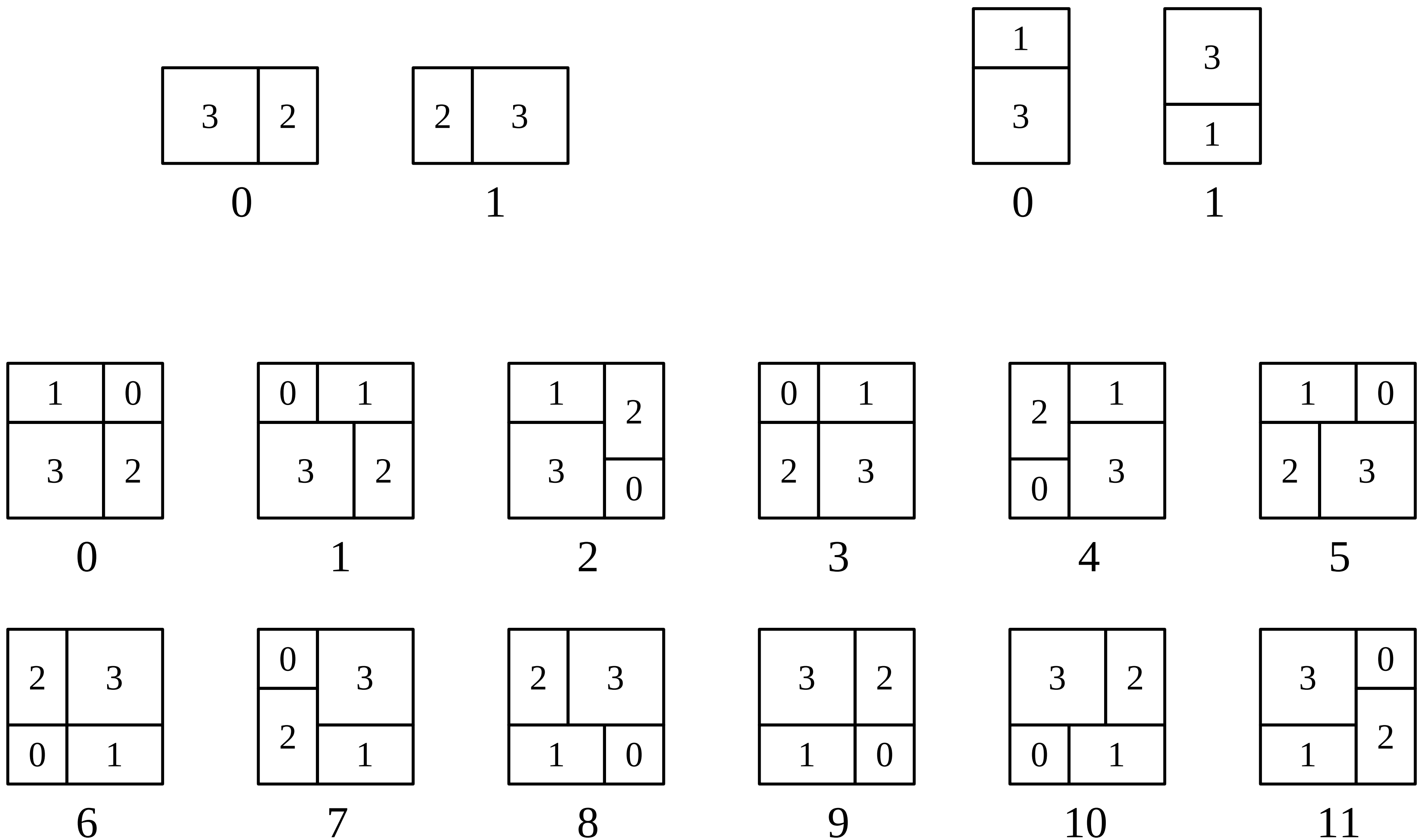


Square Fibonacci model set



Variations

(Baake, Frank & G 2021)



Variations

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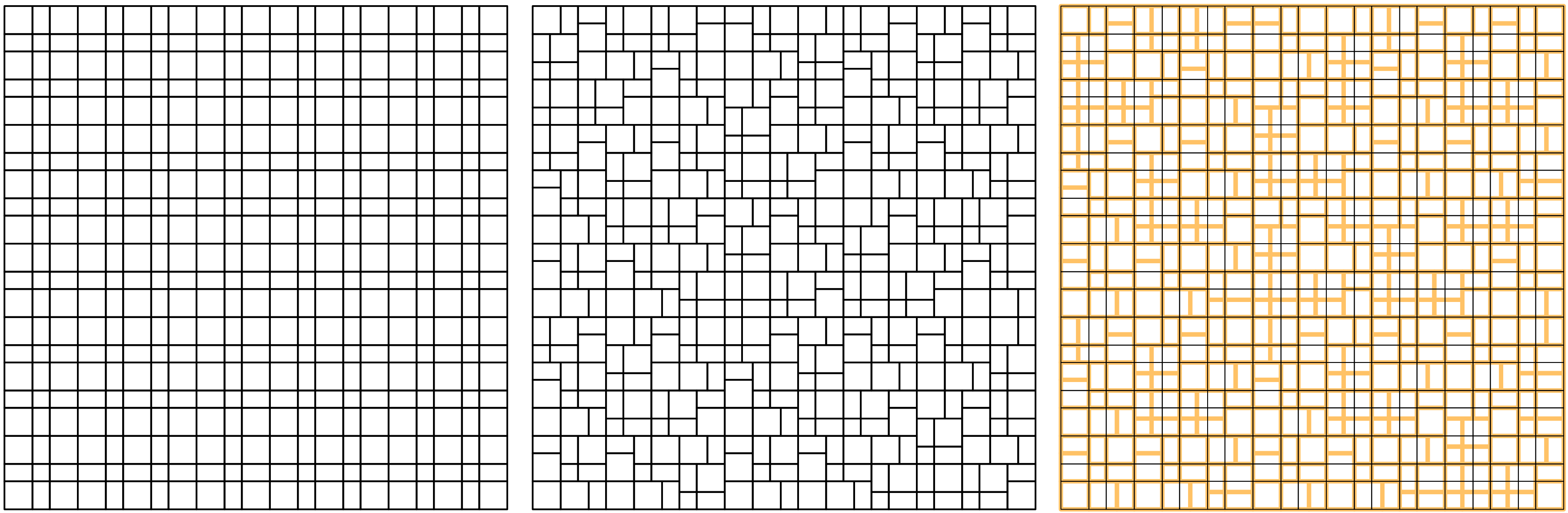

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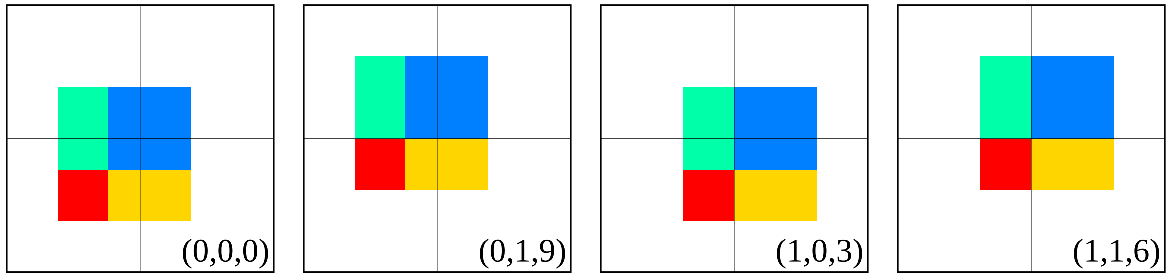

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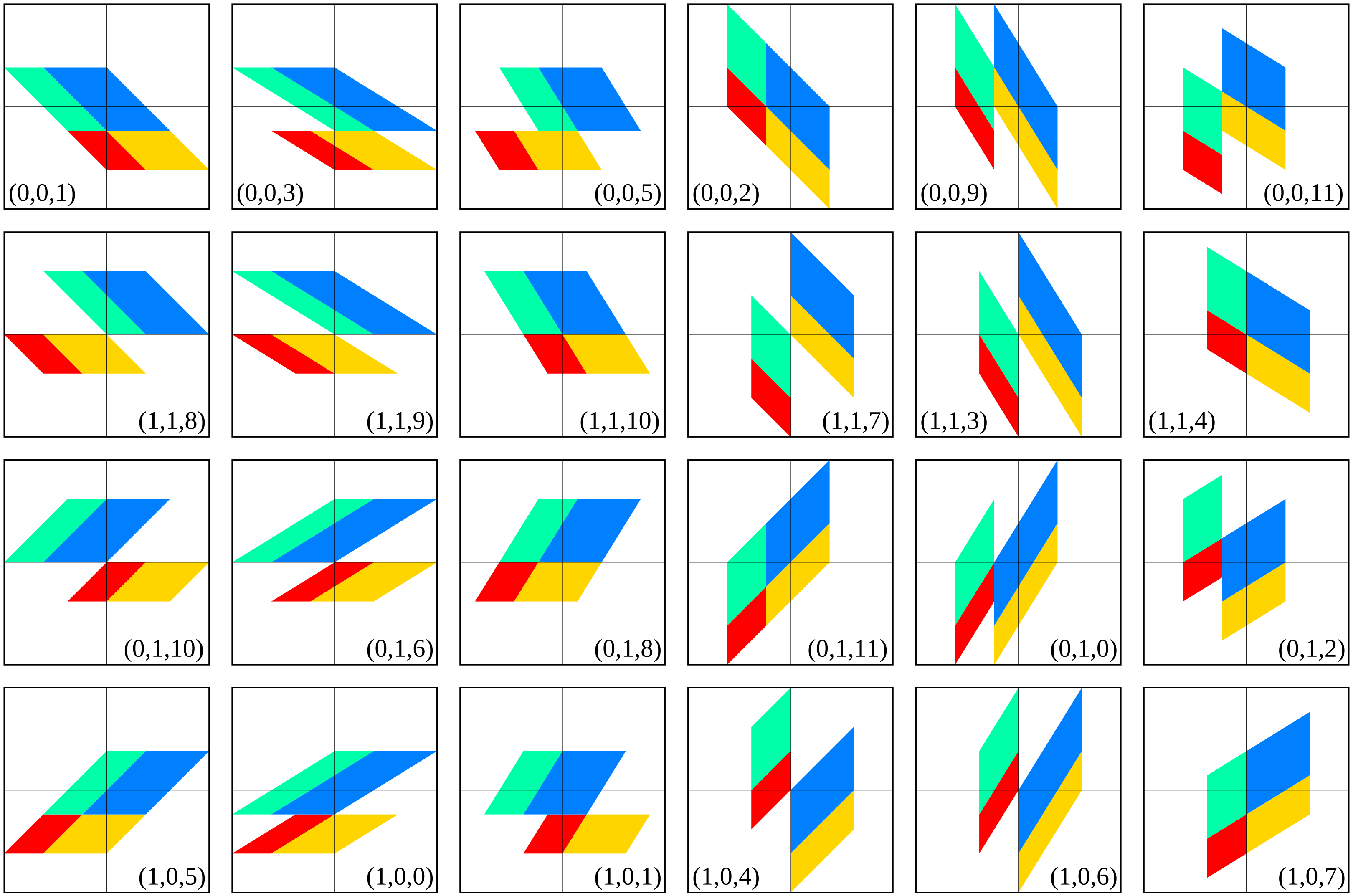

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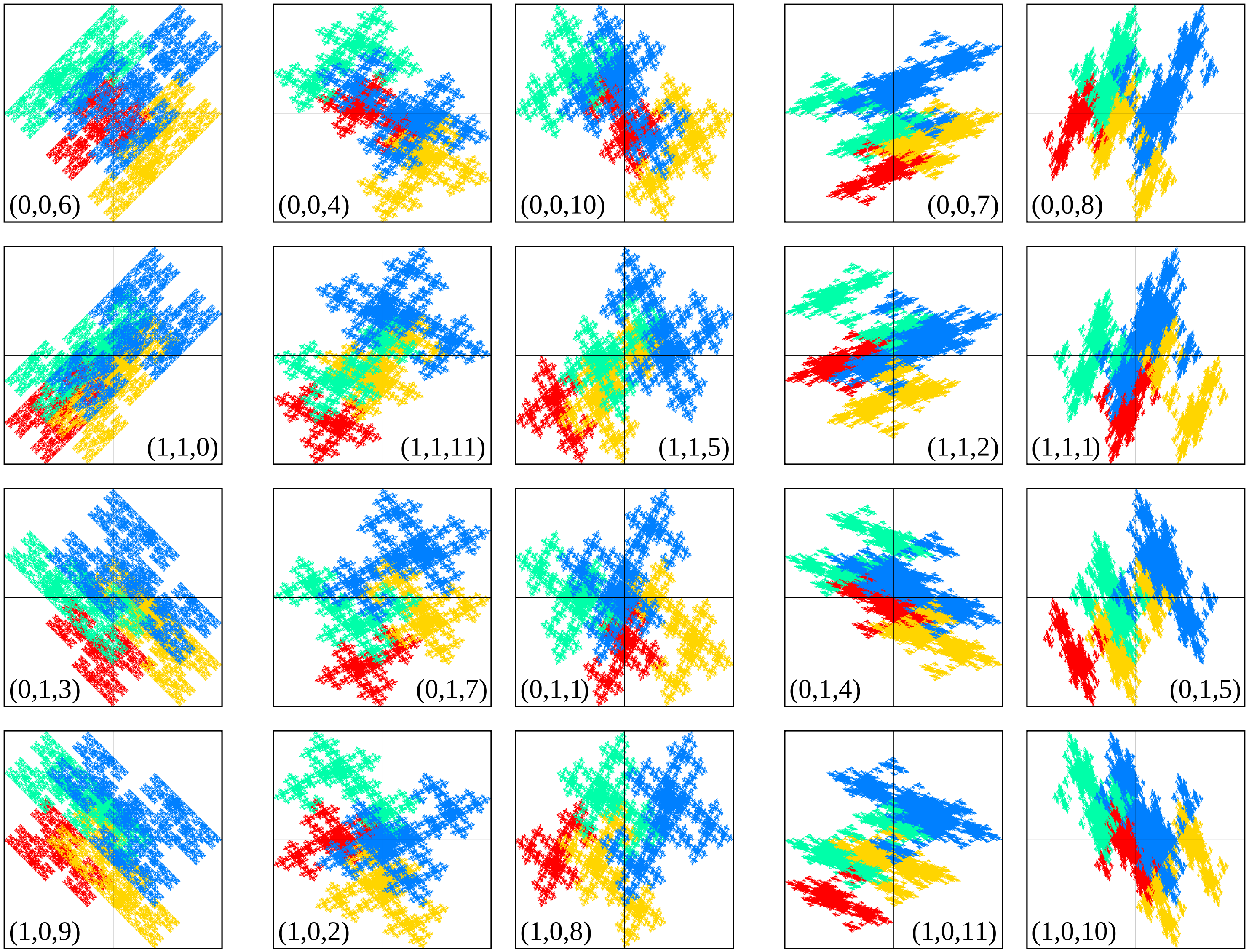


Diffraction for this case

Diffraction

- cut and project set, pure point diffractive
- general diffraction formula applies
- Fourier module stays the same
- but how to calculate $\widecheck{1_{W_i}}(y)$ for such windows?
- integration not feasible

Approach

- exploit substitution structure: renormalisation
- renormalisation in **internal** space
- infinite matrix product expression for $\widecheck{1_W}(y)$
- can be calculated efficiently

Internal Fourier matrix

Fibonacci square substitution and displacement matrix

$$\varrho^2 : \quad \begin{array}{l} \ell \mapsto \ell s \ell \\ s \mapsto \ell s \end{array} \qquad T = \begin{pmatrix} \{0, \tau+1\} & \{0\} \\ \{\tau\} & \{\tau\} \end{pmatrix}$$

Fixed-point equations ($\sigma = \tau^\star = 1 - \tau$)

$$\varLambda_a = \bigcup_b \tau^2 \varLambda_b + T_{ab} \quad \stackrel{\star}{\Longrightarrow} \quad W_a = \bigcup_b \sigma^2 W_b + T^\star_{ab}$$

implying relations for the (inverse) Fourier transforms of the characteristic functions

$$\widecheck{1_{W_a}}(y) = \sum_b \sum_{x \in T_{ab}} \widecheck{1_{\sigma^2 W_b + x^\star}}(y) = \sum_b \sum_{x \in T_{ab}} \sigma^2 \, \mathrm{e}^{2\pi \mathrm{i} x^\star y} \, \widecheck{1_{W_b}}(\sigma^2 y)$$

Internal Fourier matrix

$$\widecheck{1_{W_a}}(y) \;=\; \sum_b \sum_{x\in T_{ab}} \widecheck{1_{\sigma^2 W_b + x^\star}}(y) \;=\; \sum_b \sum_{x\in T_{ab}} \sigma^2\, \mathrm{e}^{2\pi\mathrm{i} x^\star y}\, \widecheck{1_{W_b}}(\sigma^2 y)$$

Defining $h = \bigl(\widecheck{1_{W_a}}, \widecheck{1_{W_b}}\bigr)^t$ this becomes a matrix equation

$$h(y) \;=\; \sigma^2\, \underline{B}(y)\, h(\sigma^2 y)$$

with **internal Fourier matrix**

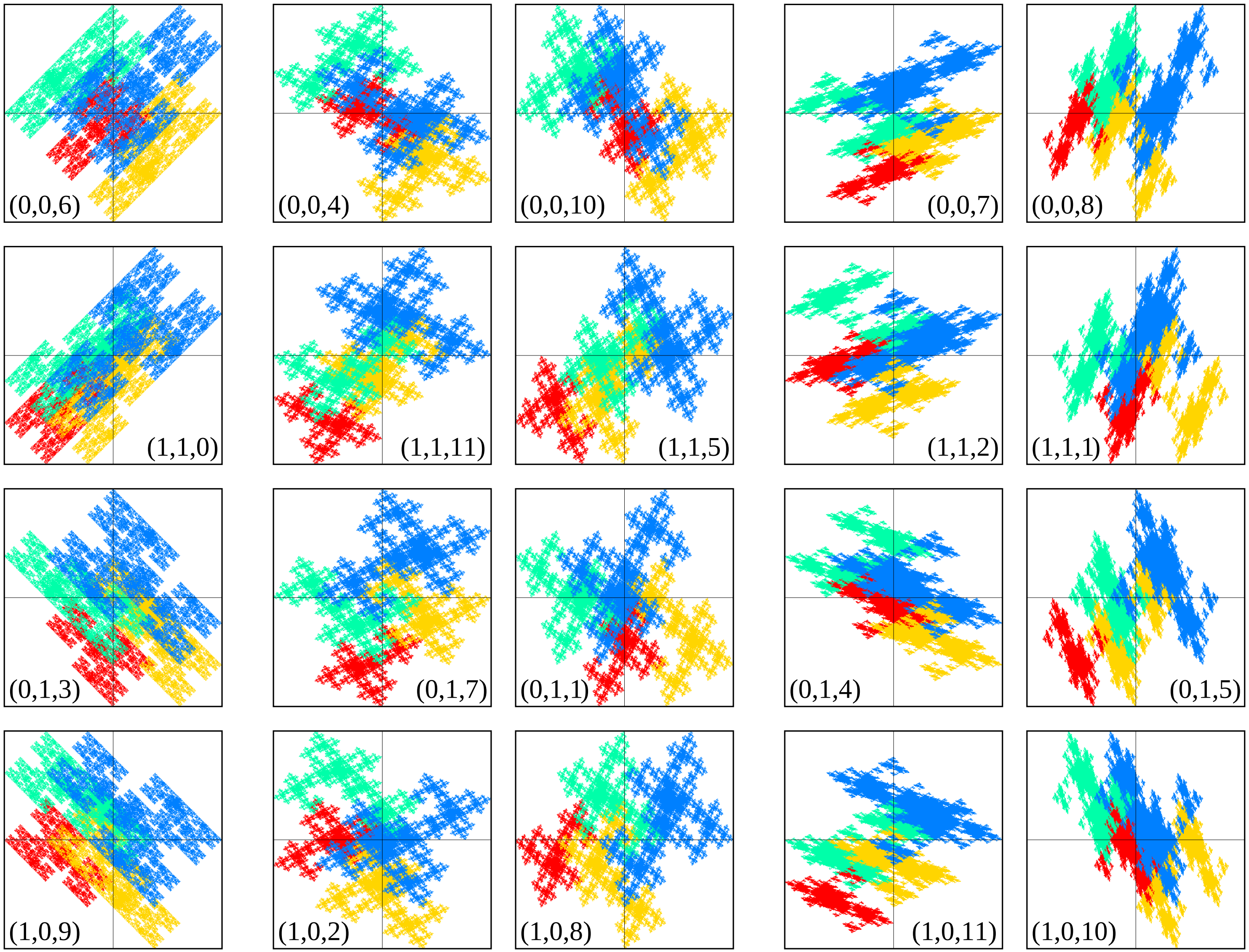
$$\underline{B}(y) \;=\; \widecheck{\delta_{T^\star}}(y) \;=\; \begin{pmatrix} 1+\mathrm{e}^{2\pi\mathrm{i}(\sigma+1)y} & 1 \\ \mathrm{e}^{2\pi\mathrm{i}\sigma y} & \mathrm{e}^{2\pi\mathrm{i}\sigma y} \end{pmatrix}$$

Internal cocycle

$$\underline{B}^{(N)}(y) \;=\; \underline{B}(y)\, \underline{B}(\sigma^2 y)\, \underline{B}(\sigma^4 y)\; \cdots\; \underline{B}(\sigma^{2(N-1)} y)$$

$h(y)$ encoded in $C(y) := \lim_{N\to\infty} \sigma^{2N} \underline{B}^{(N)}(y)$.

Variations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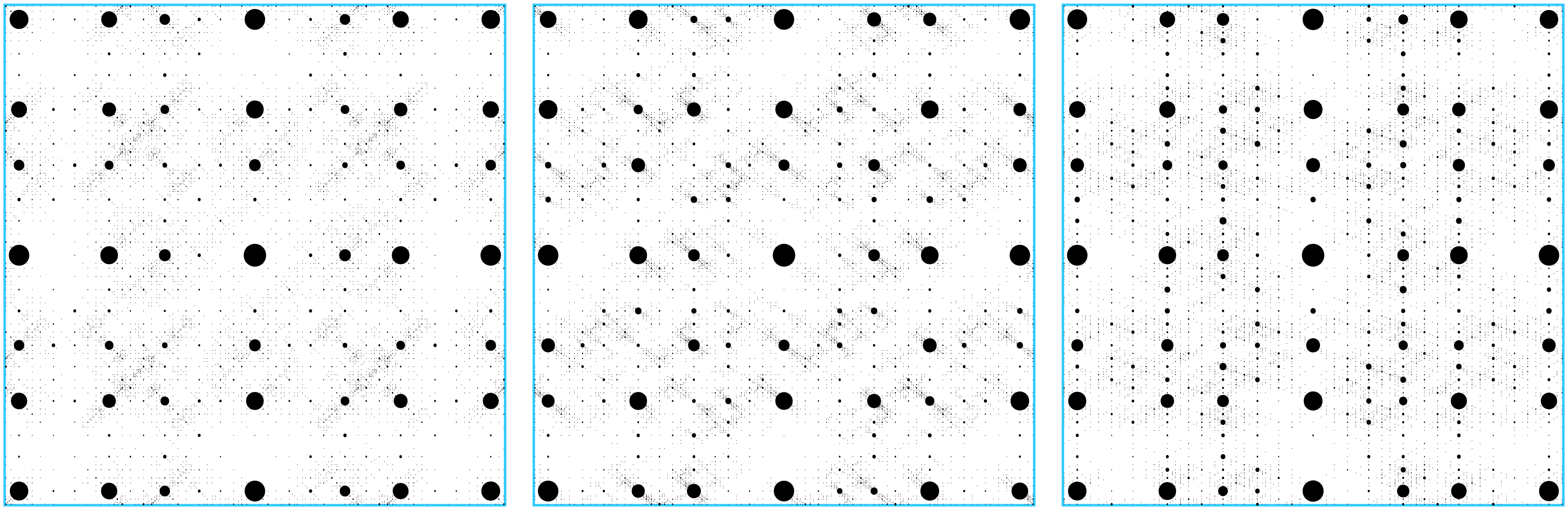
(0,0,4)
(0,0,10)
(0,0,7)
(0,0,8)
(1,1,0)
(1,1,11)
(1,1,5)
(1,1,2)
(1,1,1)
(0,1,3)
(0,1,7)
(0,1,1)
(0,1,4)
(0,1,5)
(1,0,9)
(1,0,2)
(1,0,8)
(1,0,11)
(1,0,10)

Variations



Summary

- substitution/inflation
- natural renormalisation structure
- pair correlation measures
- Fourier matrix cocycle
- information on spectral components
  - —▷ Neil's talk tomorrow
- model set —▷ internal Fourier matrix cocycle
  - —▷ diffraction for complex windows