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MATHEMATICAL DIFFRACTION THEORY OF DETERMINISTIC AND STOCHASTIC STRUCTURES: AN INFORMAL SUMMARY

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ABSTRACT. Mathematical diffraction theory is concerned with the determination of the diffraction image of a given structure and the corresponding inverse problem of structure determination. In recent years, the understanding of systems with continuous and mixed spectra has improved considerably. Moreover, the phenomenon of homometry shows various unexpected new facets. This is particularly so when systems with stochastic components are taken into account.

After a brief introduction and a summary of pure point spectra, we discuss classic deterministic examples with singular or absolutely continuous spectra. In particular, we present an isospectral family of structures with continuously varying entropy. We augment this with more recent results on the diffraction of dynamical systems of algebraic origin and various further systems of stochastic nature. A systematic approach is mentioned via the theory of stochastic processes.

CONTENTS

1. Introduction to diffraction theory

The distribution of matter in Euclidean d-space is described by a measure ω on $\mathbb{R}^d$, where we assume an infinite system that is homogeneous and in equilibrium. In most cases, ω will be translation bounded, which means that, for any compact set $K \subset \mathbb{R}^d$, we have

$$\sup_{t \in \mathbb{R}^d} |\omega|(t+K) \; < \; \infty \, .$$

Moreover, we assume an amenability property of ω, namely the existence of its *autocorrelation measure*

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

where B_R denotes the open ball of radius R around $0 \in \mathbb{R}^d$ and $\omega|_R$ the restriction of ω to B_R. Given a measure μ, its 'flipped-over' version $\widetilde{\mu}$ is defined via $\widetilde{\mu}(g) = \overline{\mu(\widetilde{g})}$ for $g \in C_{\mathsf{c}}(\mathbb{R}^d)$, the space of continuous (complex-valued) functions g of compact support, where $\widetilde{g}(x) = \overline{g(-x)}$. The volume-averaged (or Eberlein) convolution $\circledast$ is needed because ω itself is an unbounded measure, so the direct convolution is not defined. Note that different measures ω can share the same autocorrelation γ.

By construction, the measure γ is positive definite, which means $\gamma(g * \widetilde{g}) \geq 0$ for all $g \in C_{\mathsf{c}}(\mathbb{R}^d)$. As a consequence, γ is Fourier transformable by general results [22]. The Fourier transform $\widehat{\gamma}$ exists and is a positive measure, called the *diffraction measure* of ω. It describes the outcome of kinematic diffraction by ω in the sense that $\widehat{\gamma}$ quantifies how much scattering intensity reaches a given volume in d-space. By the Lebesgue decomposition theorem, relative to Lebesgue measure λ, there is a unique splitting

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

of $\widehat{\gamma}$ into its pure point part (the Bragg peaks, of which there are at most countably many), its absolutely continuous part (the diffuse scattering with locally integrable density relative to λ) and its singular continuous part (which is whatever remains). The last contribution, if present, is described by a measure that gives no weight to single points, but is still concentrated to a set of zero Lebesgue measure.

Systems with $\widehat{\gamma} = \widehat{\gamma}_{\mathsf{pp}}$ are called *pure point diffractive*. Important examples are perfect crystals and quasicrystals, such as the icosahedrally symmetric AlMnPd alloy that produces the diffraction image of Figure 1. Mathematical examples of all spectral types will be discussed below. For general background, we refer to [18], and to [8] in particular. The increasing need for a better understanding of diffuse scattering is evident from [48] and references therein.

It is clear that the diffraction measure is a unique attribute of the structure described by ω (under the mild assumption that γ exists, which is a realistic assumption from the physical point of view). In contrast, the inverse problem of determining ω

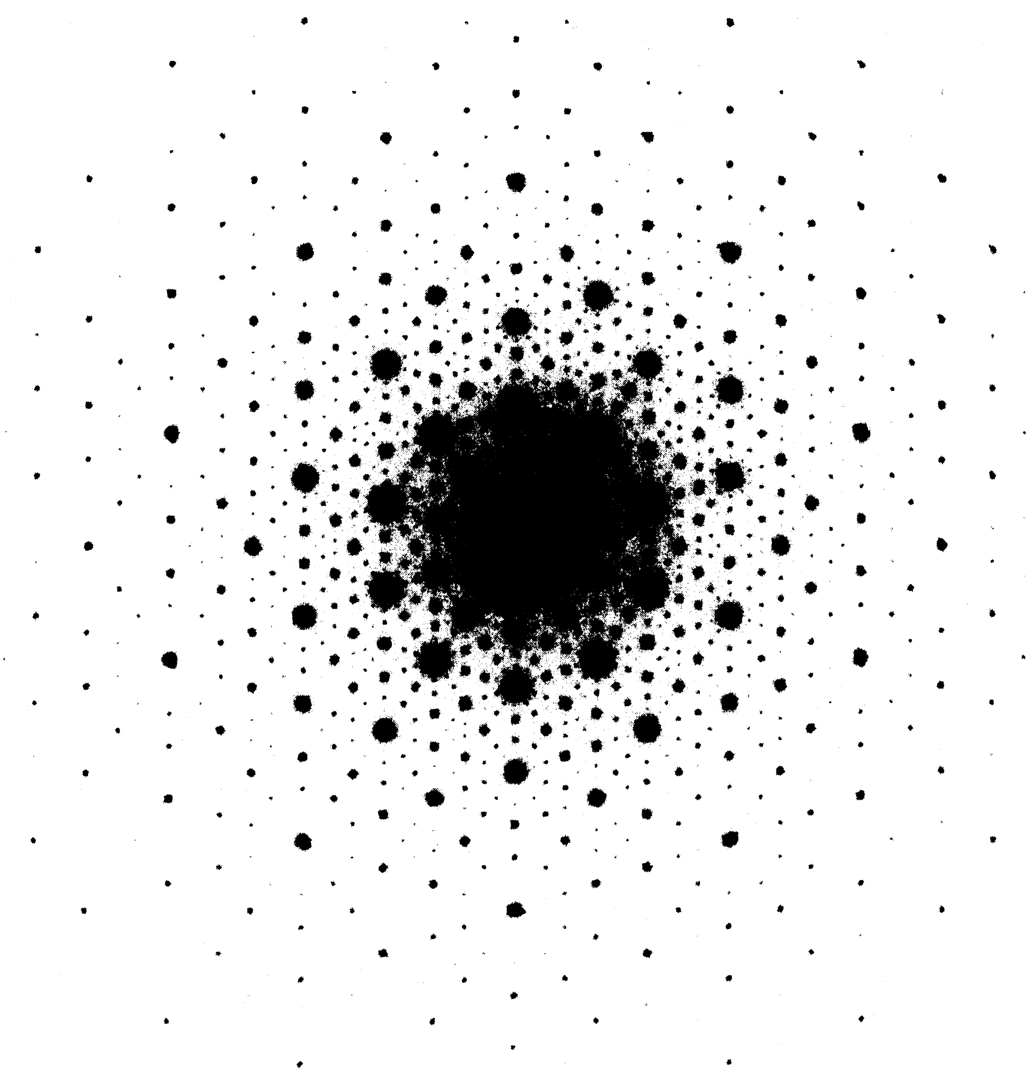

FIGURE 1. Experimental diffraction pattern of an icosahedral AlMnPd quasicrystal along the fivefold direction (courtesy C. Beeli).

from $\widehat{\gamma}$ is generally non-unique and a hard problem to solve, both mathematically and practically.

For simplicity, we will, whenever possible, explain the different scenarios with Dirac combs on $\mathbb{Z}$. This means that, given a bi-infinite sequence $w = (w_n)_{n\in\mathbb{Z}}$, we consider

$$\omega \;=\; w\,\delta_{\mathbb{Z}} \;:=\; \sum_{n\in\mathbb{Z}} w(n)\,\delta_n, \tag{1}$$

where δ_n is the normalised Dirac measure located at n. The weights $w(n) = w_n$ are assumed to be bounded, and we use the notations $w(n)$ and w_n interchangeably. A simple calculation shows that the corresponding autocorrelation (which will exist in all examples discussed here) is then of the form

$$\gamma = \sum_{m\in\mathbb{Z}} \eta(m)\, \delta_m, \tag{2}$$

with the autocorrelation coefficients

$$\eta(m) = \lim_{N\to\infty} \frac{1}{2N+1} \sum_{n=-N}^{N} w(n)\, \overline{w(n-m)}. \tag{3}$$

In line with our previous remark, we will assume that the limit exists for all $m \in \mathbb{Z}$, which is equivalent to the existence of γ in this case.

Let us now illustrate the possible spectral types by means of important and characteristic examples.

2. Pure point spectra

The Dirac comb of a general point set S is defined as $\delta_S := \sum_{x\in S} \delta_x$, with δ_x the normalised point measure at x. If $\varGamma \subset \mathbb{R}^d$ is a lattice (meaning a discrete co-compact subgroup of $\mathbb{R}^d$), the corresponding Dirac comb $\delta_\varGamma$ itself is Fourier transformable via the *Poisson summation formula* (PSF)

$$\widehat{\delta_\varGamma} = \mathrm{dens}(\varGamma)\, \delta_{\varGamma^*}\,, \tag{4}$$

where $\varGamma^*$ denotes the dual lattice of $\varGamma$ and $\mathrm{dens}(\varGamma)$ the density of $\varGamma$; see [19] and references therein for details.

2.1. **Crystallographic systems.** A perfect (infinite) crystal with $\varGamma$ as its lattice of periods can be described by the measure $\omega = \mu * \delta_\varGamma$, where μ is a suitable finite measure. A convenient (though not unique) choice for μ is the restriction of ω to a fundamental domain of $\varGamma$. A simple calculation leads to the autocorrelation

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

because $\widetilde{\delta_\varGamma} = \delta_\varGamma$ and $\delta_\varGamma \circledast \delta_\varGamma = \mathrm{dens}(\varGamma)\, \delta_\varGamma$. The Fourier transform of γ exists and reads

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

by an application of the convolution theorem together with the PSF (4). Note that $\big|\widehat{\mu}\big|^2$ is a uniformly continuous and bounded function that is evaluated only at points of the dual lattice $\varGamma^*$. Different admissible choices for the measure μ lead to different such functions that agree on all points of $\varGamma^*$. The measure $\widehat{\gamma}$ is a pure point measure, as one expects for lattice periodic measures ω.

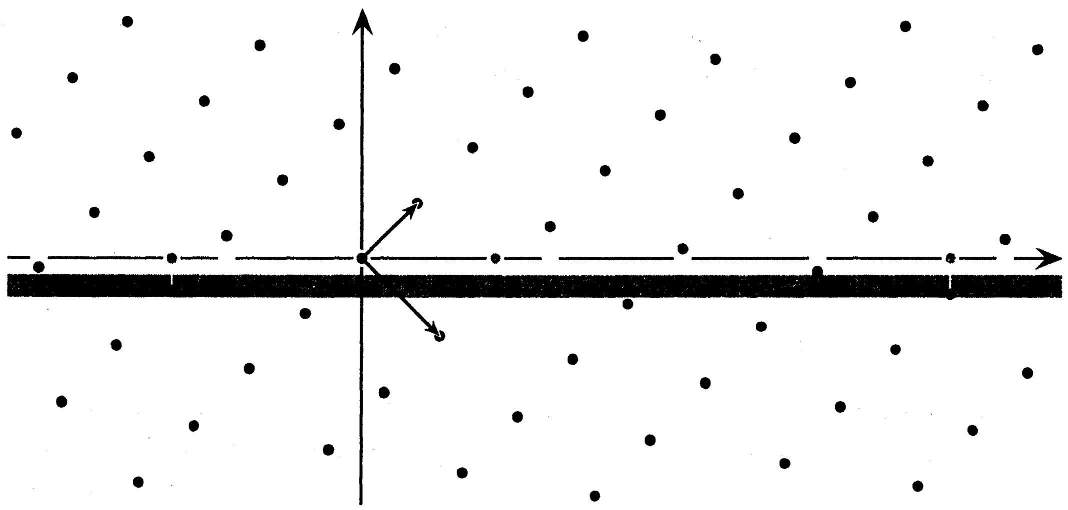

FIGURE 2. The silver mean point set $\varLambda$ of Equation (5) as a projection of a strip-shaped subset of the lattice $\varGamma = \{(x, x') \mid x \in \mathbb{Z}[\sqrt{2}\,]\}$. The shading marks the endpoints of a-type (light grey) and b-type (dark grey) intervals.

2.2. **Model sets.** Lattice periodic point sets form a special case of the larger class of regular model sets [39, 43], which also lead to pure point diffraction measures. One of the simplest non-periodic examples in one dimension emerges from the *silver mean* substitution rule

$$\varrho\colon \begin{array}{l} a \mapsto aba \\ b \mapsto a \end{array}$$

which has inflation multiplier $\sigma = 1 + \sqrt{2}$. The latter is known as the silver mean and is the Perron-Frobenius eigenvalue of the corresponding substitution matrix $\left(\begin{smallmatrix} 2 & 1 \\ 1 & 1 \end{smallmatrix}\right)$. Note that σ is a Pisot-Vijayaraghavan (PV) number.

The natural geometric realisation of this system, starting from a bi-infinite fixed point of ϱ with legal seed $a|a$, is built via two intervals of length ratio σ. If a represents an interval of length σ and b one of length 1, their left endpoints constitute the silver mean point set

$$\varLambda = \big\{x \in \mathbb{Z}[\sqrt{2}] \mid x' \in \big[-\tfrac{\sqrt{2}}{2}, \tfrac{\sqrt{2}}{2}\,\big]\big\}, \tag{5}$$

the proof of which is not entirely trivial; it is spelled out in detail in [13]. Here, $'$ denotes algebraic conjugation in the quadratic field $\mathbb{Q}(\sqrt{2}\,)$, as defined by $\sqrt{2} \mapsto -\sqrt{2}$. Equation (5) has a distinctive geometric meaning which is illustrated in Figure 2.

The algebraic aspects are encoded in a *cut and project scheme* (CPS), which we state for the general Euclidean case as follows:

$$
\begin{array}{ccccc}
\mathbb{R}^d & \xleftarrow{\;\pi\;} & \mathbb{R}^d \times \mathbb{R}^m & \xrightarrow{\;\pi_{\text{int}}\;} & \mathbb{R}^m \\
\cup & & \cup & & \cup \ \text{dense} \\
\pi(\mathcal{L}) & \xleftarrow{\;1-1\;} & \mathcal{L} & \longrightarrow & \pi_{\text{int}}(\mathcal{L}) \\
\| & & & & \| \\
L & & \xrightarrow{\qquad\quad\star\quad\qquad} & & L^\star
\end{array}
\tag{6}
$$

Here, $\mathcal{L}$ is a lattice in $\mathbb{R}^{d+m}$ with certain properties that are expressed via the images under the canonical projections π and π_{int}. In particular, $L = \pi(\mathcal{L})$ is a bijective image of $\mathcal{L}$, while $L^\star = \pi_{\text{int}}(\mathcal{L})$ is dense in internal space $\mathbb{R}^m$. Due to these properties, the $\star$-map $x \mapsto x^\star$ is well-defined on L; see [39] for more. In the silver mean example, we have a CPS with $d = m = 1$, $L = L^\star = \mathbb{Z}[\sqrt{2}\,]$, and the $\star$-map is given by algebraic conjugation, as mentioned above.

In general, a *model set* for a given CPS is a set of the form

$$
\varLambda = \{x \in L \mid x^\star \in W\}
\tag{7}
$$

where W is a relatively compact subset of $\mathbb{R}^m$; see Equation (5) for the silver mean case. A model set $\varLambda$ is *regular* when the boundary ∂W of the window W has zero Lebesgue measure. The entire setting generalises, without significant complications, to locally compact Abelian groups as internal spaces [39, 43]. We will refer to this freedom later on, where the internal space will be based on the 2-adic numbers.

Regular model sets are pure point diffractive [31, 43, 19]. This is a substantial theorem for which three different types of proofs are known. The most common one is based on the connection to dynamical systems theory [31, 43], another on a reformulation via almost periodic measures [19, 28]. An even simpler approach follows a suggestion by Lagarias and is based on the PSF for the embedding lattice together with Weyl's lemma on uniform distribution [13]. The theorem is also constructive in the sense that it provides an explicit and computable formula for the diffraction measure of $\delta_{\varLambda}$, namely

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

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

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

where 1_W is the characteristic function of the window W. This formula has several generalisations [43, 19], which we omit for simplicity.

Model sets are widely used to describe and analyse diffraction images such as that shown in Figure 1. Although real world quasicrystals will usually not be pure point

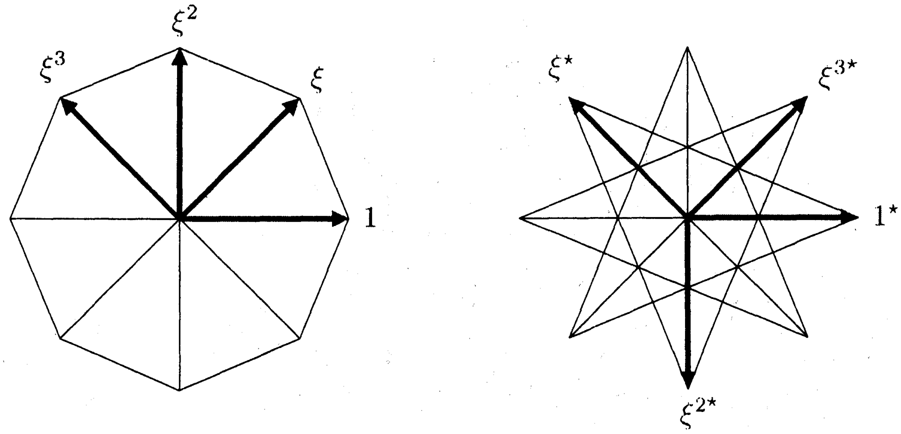

FIGURE 3. Action of the $\mathbb{Z}$-linear $\star$-map on the generating elements of the eightfold module $L = \mathbb{Z}[e^{2\pi\mathrm{i}/8}]$.

diffractive, their average structure is well captured by this approach. In this regard, quasicrystals behave pretty much like ordinary crystals.

Let us expand on the diffraction formula for the vertex set of the planar Ammann-Beenker (or octagonal) tiling [3]. This point set is a regular model set with $L = \mathbb{Z}[\xi]$, where $\xi = \exp(2\pi\mathrm{i}/8)$ is a primitive eighth root of unity. The $\star$-map (illustrated in Figure 3) is defined by $\xi \mapsto \xi^3$, which is an automorphism of the cyclotomic field $\mathbb{Q}(\xi)$, so that $L^\star = L$. The lattice $\mathcal{L} = \{(x, x^\star) \mid x \in \mathbb{Z}[\xi]\}$ is the Minkowski embedding of L, which is a scaled copy of $\mathbb{Z}^4$ in this case. The standard window is a regular octagon O of edge length 1, centred at the origin. The model set construction produces the point set

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

and its $\star$-image $\varLambda^\star_{\mathrm{AB}}$ of Figure 4. The corresponding tiling emerges by connecting all vertices of distance 1 in $\varLambda_{\mathrm{AB}}$.

The diffraction measure is calculated via the Fourier transform of the characteristic function 1_O. This leads to a dense (but countable) set of Bragg peaks whose intensities are locally summable. This means that, in any compact region, there are only finitely many peaks above any given positive threshold. A precise explicit calculation can easily be performed by one of the standard computer algebra packages. Figure 5 shows the result for a central patch of the Ammann-Beenker diffraction, with cutoff at 1/1000 of the central intensity. Here, a Bragg peak is represented by a small disk whose area is proportional to the intensity and whose centre is the position of the Bragg peak.

A related and very interesting question concerns the spectral type of systems that are defined by substitutions; see [41] for background. More recently, practically useful tests for pure pointedness of substitution systems have been developed, compare [2] and references given there, but the famous Pisot substitution conjecture and its

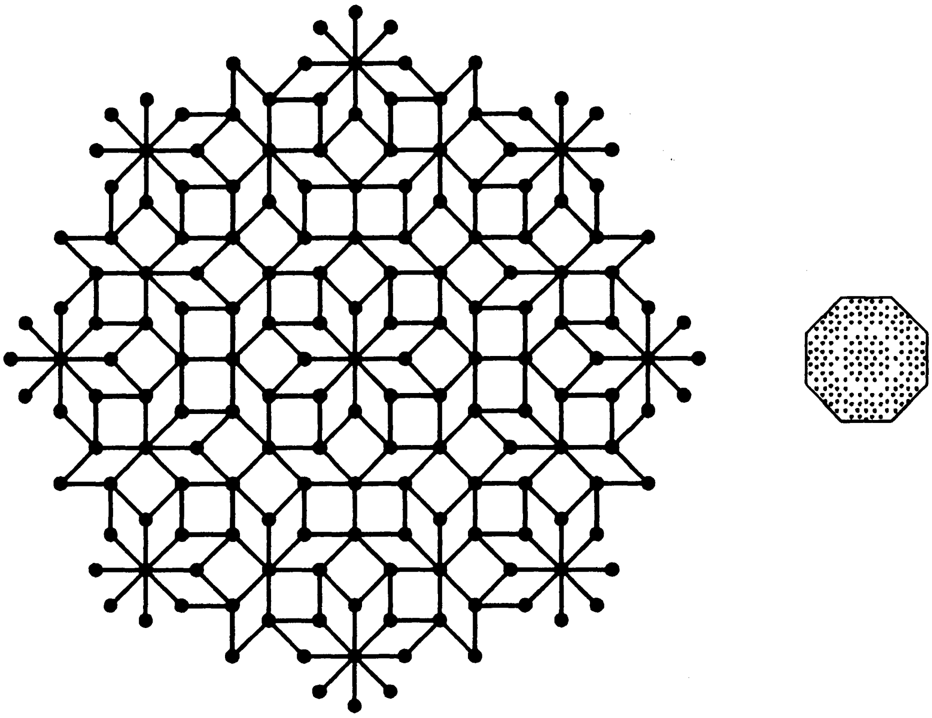

FIGURE 4. Patch of the Ammann-Beenker tiling and point set Λ_{AB} (left) and its lift to internal space (right).

higher dimensional generalisations still remain a mystery. We will not discuss this point of view in what follows, even though many of our examples will be defined by substitutions rules.

Let us close the paragraph with a brief general comment. A translation bounded measure ω also defines a dynamical system under the translation action of $\mathbb{R}^d$; see [43, 16, 17] for background. If ω is pure point diffractive, the corresponding dynamical spectrum is pure point as well (the converse also being true). This equivalence is well understood by now [36, 43, 16, 37], but does not extend to general systems with continuous spectral components [25, 7], as we will see later on.

2.3. **Homometry.** As mentioned previously, different measures may possess the same autocorrelation and hence the same diffraction. This phenomenon is called *homometry* [40]. Clearly, $\delta_t * \omega$ (with $t \in \mathbb{R}^d$) as well as $\widetilde{\omega}$ have the same diffraction as ω, but non-uniqueness is generally not exhausted by this. Let us illustrate how it appears already among pure point diffractive systems.

The simplest situation emerges for periodic Dirac combs on $\mathbb{Z}$ with rational weights. As an example, Grünbaum and Moore [30] constructed homometric Dirac combs of the form

$$\omega = \delta_{6\mathbb{Z}} * \sum_{j=0}^{5} c_j \, \delta_j \tag{8}$$

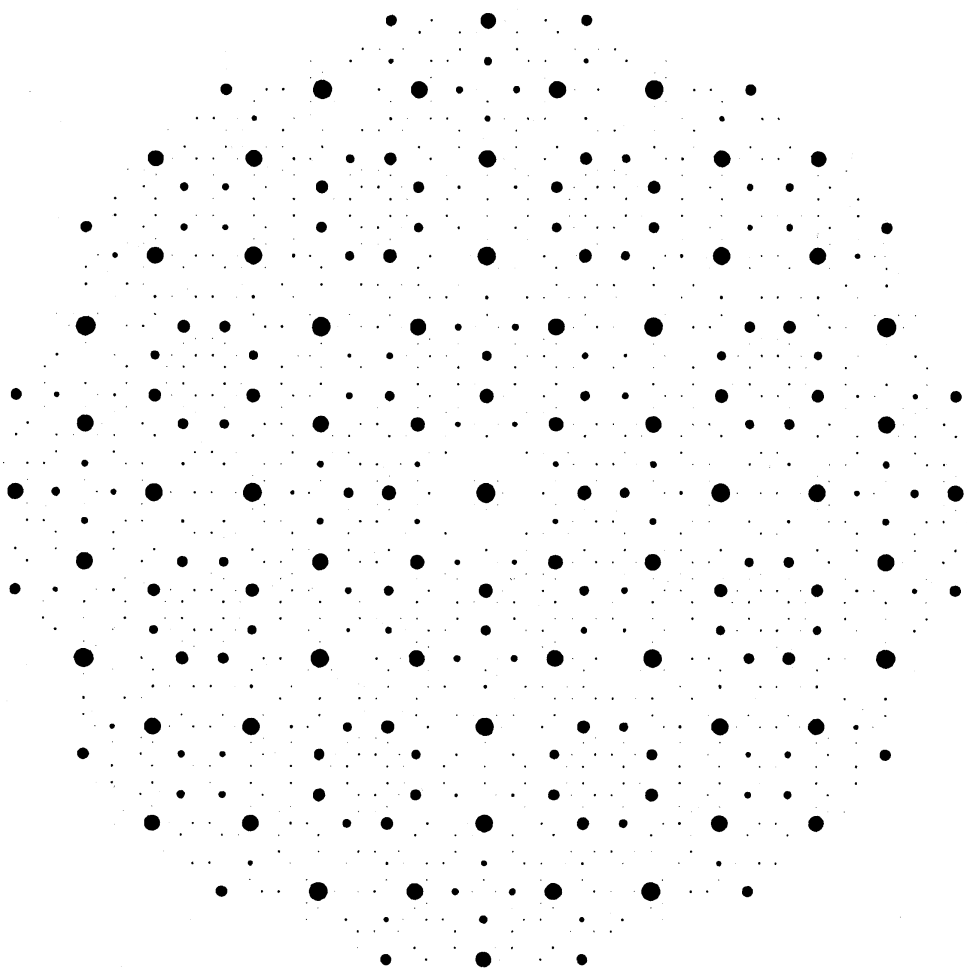

FIGURE 5. Computed diffraction image of the Ammann-Beenker point set Λ_{AB}; see text for details.

with integer weights c_j, which are thus 6-periodic. The two choices of Table 1 lead to the same autocorrelation. Even worse, these two cases have the same correlation functions up to 5th order, and differ only in higher orders. Nevertheless, the two Dirac combs are substantially different. Note that the diffraction measure, which is supported on $\mathbb{Z}/6$, shows systematic extinction (the intensity vanishes on all points

TABLE 1. Integer weights c_j for the two homometric Dirac combs built from Equation (8); see [30] for details.

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

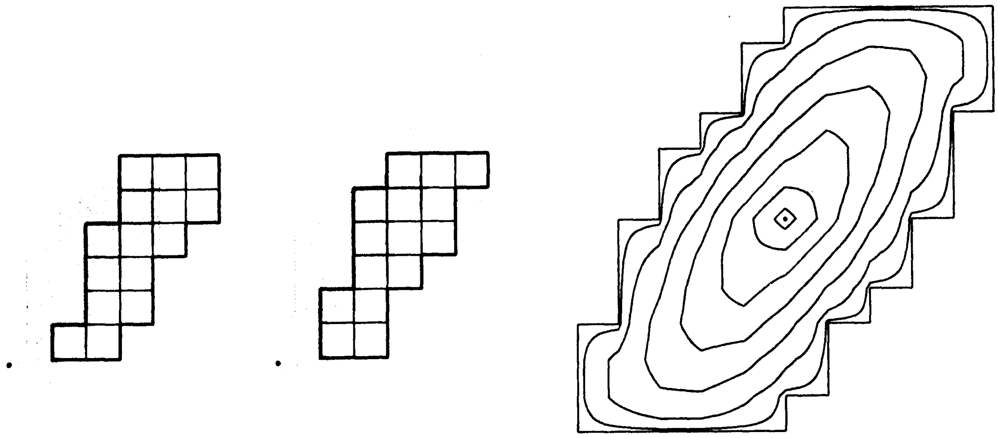

FIGURE 6. Two polyominoes (left) and their common covariogram (right). The small dots mark the origin, see text for further details.

of the form $k = \ell/6$ with $k \equiv 2$, 3 or 4 mod 6). Such extinctions are always an indication for non-trivial homometry of pure point diffractive systems.

Let us go one step beyond by showing a pair of homometric model sets. We use the CPS of the Ammann-Beenker tiling from above, but replace the octagonal window by one of the two polyominoes shown in Figure 6, where we follow [9]. The Dirac comb $\delta_\varLambda$ of the corresponding model set $\varLambda$ with window W has an autocorrelation of the form

$$\gamma_\varLambda \; = \sum_{z\in\varLambda-\varLambda} \eta(z)\,\delta_z\,, \tag{9}$$

where $\varLambda - \varLambda$ is locally finite because $\varLambda$ is a model set. The autocorrelation coefficients in (9) are given by

$$\eta(z) \; = \; \mathrm{dens}(\varLambda)\,\frac{\mathrm{vol}\big(W\cap(W-z^\star)\big)}{\mathrm{vol}(W)} \; = \; \mathrm{dens}(\mathcal{L})\,\mathrm{cvg}_W(z^\star)\,. \tag{10}$$

Here, cvg_W is the *covariogram* of W, defined by

$$\mathrm{cvg}_W(x) \; = \; \mathrm{vol}\big(W\cap(x+W)\big) \; = \; \big(1_W * 1_{-W}\big)(x)\,.$$

This function is symmetric under reflection in the origin, and one also has the relations $\mathrm{cvg}_{t+W} = \mathrm{cvg}_W$ for arbitrary $t\in\mathbb{R}^d$ as well as $\mathrm{cvg}_{(-W)} = \mathrm{cvg}_W$. The covariogram for our two polyominoes is illustrated as a contour plot in Figure 6. The polyominoes in the same figure are shown with a shifted overlay structure, which can be used by the reader to check the claimed homometry (for the displayed shift) on the basis of Equations (9) and (10).

The two model sets constructed this way differ on positions of positive density. Depending on the length scale of the windows, they may or may not be locally equivalent via a mutual local derivation (MLD) rule [4], but they are always homometric. Further details are discussed in [9, 29]. If one has access to correlation functions of

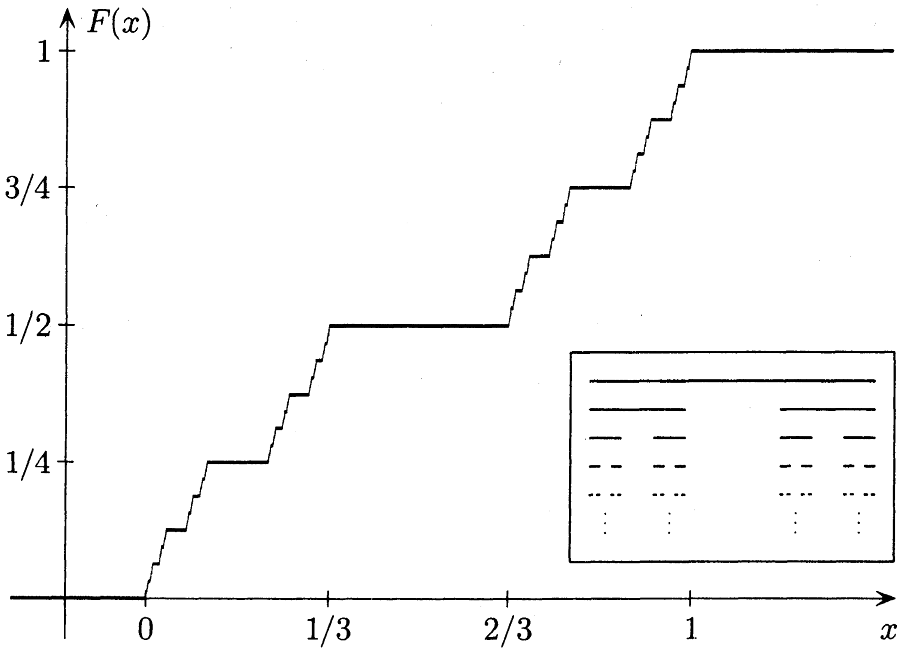

FIGURE 7. Illustration of the construction of the middle-thirds Cantor set $\mathcal{C}$ (inlay) and the distribution function F for the corresponding probability measure on $\mathcal{C}$.

higher order, a distinction is possible. A rather general result in this direction was recently derived in [24].

3. Singular continuous spectra

The probably best known singular continuous measure is the one that emerges from the middle-thirds Cantor set construction. Its distribution function F is shown in Figure 7, which is widely known as the Devil's staircase. This function is continuous and non-decreasing, but constant almost everywhere. More precisely, the underlying measure $\mu = \mathrm{d}F$ is concentrated on the Cantor set $\mathcal{C}$, which is an uncountable set of zero Lebesgue measure. The (positive) measure μ is singular continuous, with $\mu(\{x\}) = 0$ for all $x \in [0, 1]$ and $\mu(\mathcal{C}) = 1$.

3.1. **Thue-Morse sequence.** Let us now discuss a classic example from the theory of substitution systems that leads to a singular continuous diffraction measure with rather distinctive features in comparison with the Cantor measure. This example has a long history, which can be extracted from [47, 38, 33, 1]. We confine ourselves to a brief summary of the results, and refer to [10] and references therein for proofs and details.

The classic *Thue-Morse* (TM) sequence can be defined via the one-sided fixed point $v = v_0 v_1 v_2 \dots$ with $v_0 = 1$ of the primitive substitution rule

$$\varrho\colon \begin{array}{l} 1 \mapsto 1\bar{1} \\ \bar{1} \mapsto \bar{1}1 \end{array}$$

on the binary alphabet $\{1, \bar{1}\}$. It is the limit (in the obvious product topology) of the iteration sequence

$$1 \overset{\varrho}{\longmapsto} 1\bar{1} \overset{\varrho}{\longmapsto} 1\bar{1}\bar{1}1 \overset{\varrho}{\longmapsto} 1\bar{1}\bar{1}1\bar{1}11\bar{1} \overset{\varrho}{\longmapsto} \dots \longrightarrow v = \varrho(v) = v_0 v_1 v_2 v_3 \dots$$

and has a number of distinctive properties [1, 41], for instance

- $v_i = (-1)^{\text{sum of the binary digits of } i}$
- $v_{2i} = v_i$ and $v_{2i+1} = \bar{v}_i$
- $v = v_0 v_2 v_4 \dots$ and $\bar{v} = v_1 v_3 v_5 \dots$
- v is (strongly) cube-free.

A two-sided sequence w can be defined by

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

which is a fixed point of ϱ^2, because the seed $w_{-1}|w_0 = 1|1$ is a legal word (it occurs in $\varrho^3(1)$) and $w = \varrho^2(w)$. The (discrete) hull $\mathbb{X} = \mathbb{X}_{\mathrm{TM}}$ of the TM substitution is the closure of the orbit of w under the shift action, which is compact. The orbit of any of its members is dense in $\mathbb{X}$. We thus have a topological dynamical system $(\mathbb{X}, \mathbb{Z})$ that is minimal. When equipped with the standard Borel σ-algebra, the system admits a unique shift-invariant probability measure, so that the corresponding measure theoretic dynamical system is strictly ergodic [33, 41].

Any given $w \in \mathbb{X}$ is mapped to a signed Dirac comb (and hence to a translation bounded measure) ω via

$$\omega = \sum_{n \in \mathbb{Z}} w_n \, \delta_n \, .$$

We inherit unique ergodicity, and thus obtain an autocorrelation of the form (2) with coefficients $\eta(m)$ as in (3). Due to the nature of the fixed point w, an alternative way to express the coefficients is

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

for $m \geq 0$ together with $\eta(-m) = \eta(m)$. It is clear that $\eta(0) = 1$, and the scaling relations of v lead to the recursions

$$\eta(2m) = \eta(m) \quad \text{and} \quad \eta(2m+1) = -\frac{1}{2}\big(\eta(m) + \eta(m+1)\big) \tag{11}$$

which are valid for all $m \in \mathbb{Z}$. In particular, the second relation, used with $m = 0$, implies $\eta(1) = -\frac{1}{3}$, which can also be calculated directly.

Since ω is supported on $\mathbb{Z}$, the diffraction measure $\widehat{\gamma}$ is of the form $\widehat{\gamma} = \mu * \delta_{\mathbb{Z}}$ by an application of [5, Thm. 1], where

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

the latter due to the Herglotz-Bochner theorem. One can now analyse the spectral type of $\widehat{\gamma}$ via that of the finite measure μ, where we follow [33]. Defining $\Sigma(N) = \sum_{m=-N}^{N} \bigl(\eta(m)\bigr)^2$, a two-step calculation with the recursion (11) establishes the inequality $\Sigma(4N) \le \frac{3}{2}\Sigma(2N)$ for all $N \in \mathbb{N}$. This implies $\lim_{N\to\infty} \Sigma(N)/N = 0$, wherefore Wiener's criterion [47] tells us that μ is a continuous measure, so that $\widehat{\gamma}$ cannot have any pure point component.

Let us now define the distribution function F by $F(x) = \mu\bigl([0,x]\bigr)$ for $x \in [0,1]$, which is a continuous function that defines a Riemann-Stieltjes measure, so that $\mathrm{d}F = \mu$. The recursion relation for η now implies [33] the functional relations

$$\mathrm{d}F\bigl(\tfrac{x}{2}\bigr) \pm \mathrm{d}F\bigl(\tfrac{x+1}{2}\bigr) = \left\{ {1 \atop -\cos(\pi x)} \right\} \mathrm{d}F(x) \,,$$

which have to be satisfied by the ac and sc parts of F separately, because $\mu_{\mathsf{ac}} \perp \mu_{\mathsf{sc}}$ in the measure theoretic sense. Therefore, defining

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

we know that the coefficients $\eta_{\mathsf{ac}}(m)$ must satisfy the same recursions (11) as $\eta(m)$, possibly with a different initial condition $\eta_{\mathsf{ac}}(0)$. The Riemann-Lebesgue lemma states $\lim_{m\to\pm\infty} \eta_{\mathsf{ac}}(m) = 0$, with is only compatible with $\eta_{\mathsf{ac}}(0) = 0$, and hence $\eta_{\mathsf{ac}} \equiv 0$. This means $F_{\mathsf{ac}} = 0$ by the Fourier uniqueness theorem, wherefore μ and hence $\widehat{\gamma}$ (neither of which is the zero measure) are purely singular continuous. The resulting distribution function is illustrated in Figure 8. It was calculated by means of the quickly converging Volterra iteration

$$F_{n+1}(x) = \frac{1}{2} \int_0^{2x} \bigl(1 - \cos(\pi y)\bigr) F_n'(y) \, \mathrm{d}y \qquad \text{with} \qquad F_0(x) = x \,.$$

In contrast to the Devil's staircase, the TM function is *strictly* increasing, which means that there is no plateau (which would indicate a gap in the support of $\widehat{\gamma}$); see [10] and references therein for details and further properties of F.

Despite the above result, the TM sequence is closely related to the period doubling sequence, via the (continuous) block map

$$\phi\colon \quad 1\bar{1}, \bar{1}1 \mapsto a \,, \quad 11, \bar{1}\bar{1} \mapsto b \,, \tag{12}$$

which defines an exact 2-to-1 surjection from the hull $\mathbb{X}_{\mathrm{TM}}$ to $\mathbb{X}_{\mathrm{pd}}$, where the latter is the hull of the period doubling substitution defined by

$$\varrho_{\mathrm{pd}}\colon \quad a \mapsto ab \,, \quad b \mapsto aa \,. \tag{13}$$

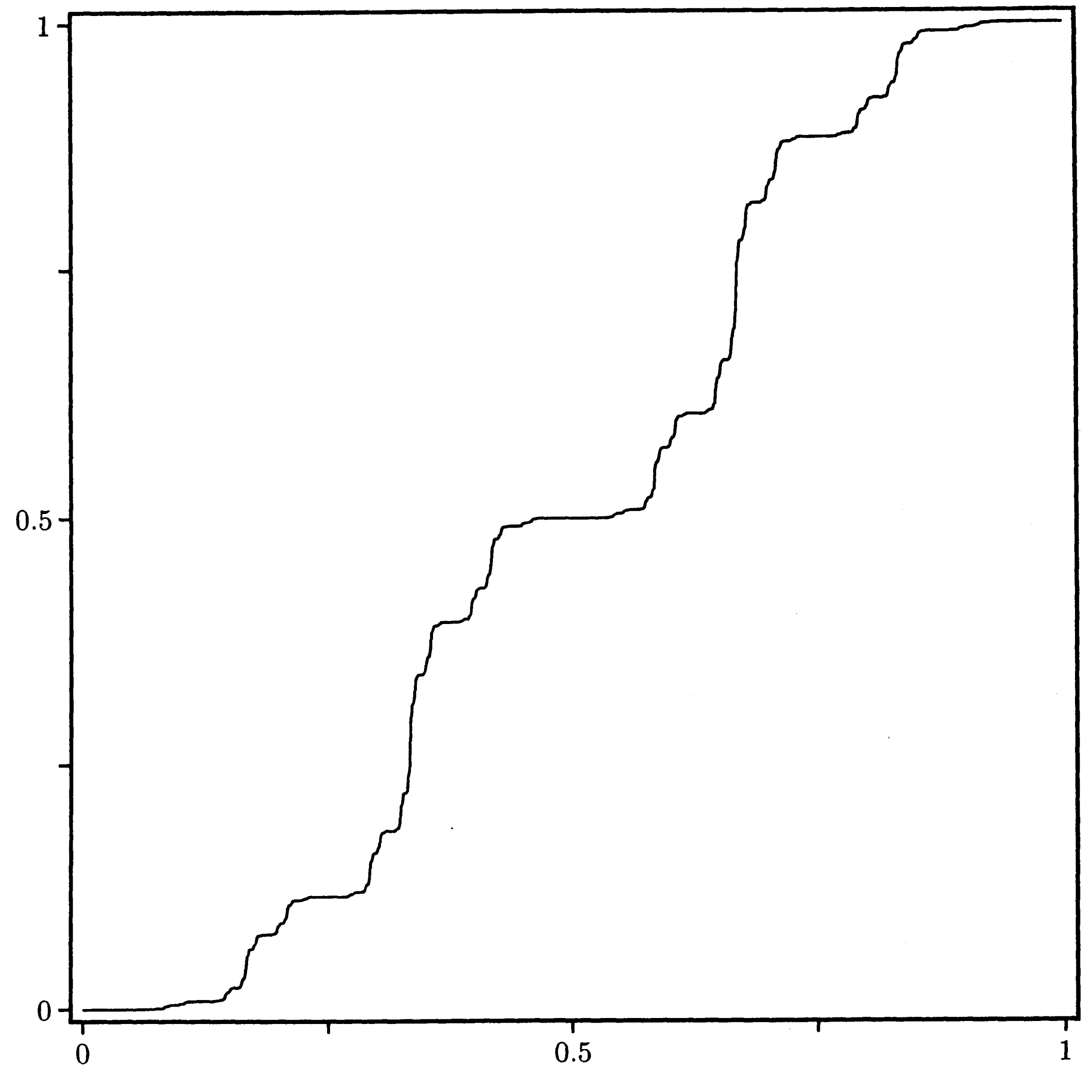

FIGURE 8. The strictly increasing distribution function F of the Thue-Morse diffraction measure on the unit interval.

Viewed as topological dynamical systems, this means that $(\mathbb{X}_{\mathrm{pd}}, \mathbb{Z})$ is a factor of $(\mathbb{X}_{\mathrm{TM}}, \mathbb{Z})$. Since both are strictly ergodic, this extends to the corresponding measure theoretic dynamical systems. The period doubling sequence can be described as a regular model set with a 2-adic internal space [20, 19] and is thus pure point diffractive. This pairing also explains a phenomenon observed in [25], as the missing part of the *dynamical* spectrum of the TM system is recovered via the *diffraction* measure of $\mathbb{X}_{\mathrm{pd}}$.

3.2. **Generalised Morse sequences.** The above example can be generalised to the family

$$\varrho : \begin{array}{l} 1 \mapsto 1^k \, \bar{1}^\ell \\ \bar{1} \mapsto \bar{1}^k \, 1^\ell \end{array}$$

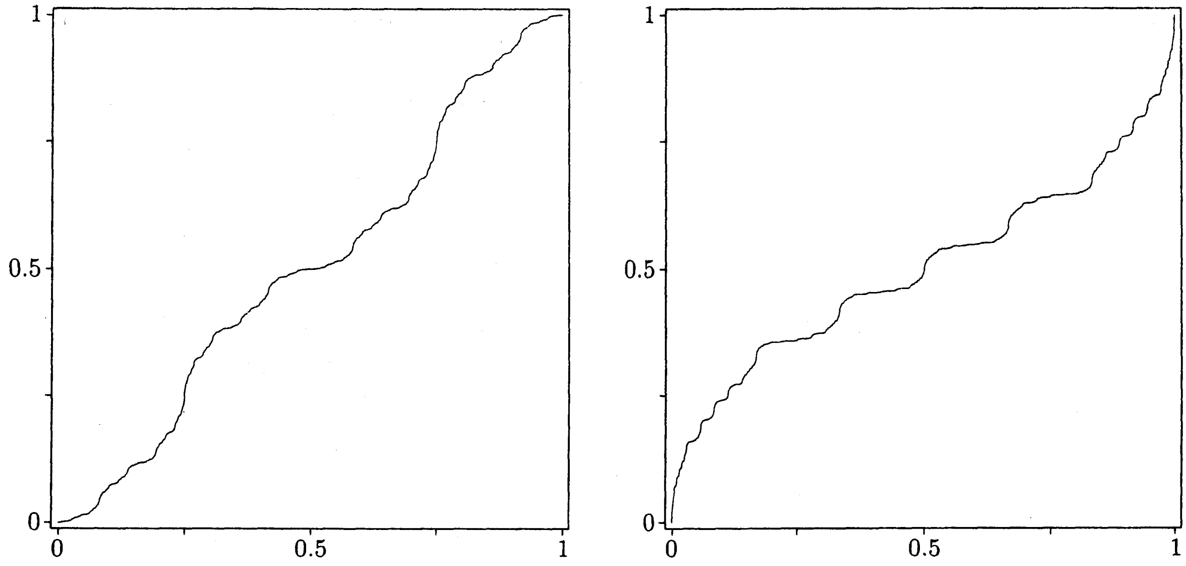

FIGURE 9. The continuous and strictly increasing distribution functions of for the generalised Morse sequences with parameters $(2,1)$ (left) and $(5,1)$ (right).

with $k, \ell \in \mathbb{N}$, inspired by [34]. They define a class of systems which we will refer to as the gTM systems. All display purely singular continuous diffraction, which follows from completely analogous arguments [12]. The entire analysis is based on the structure of the autocorrelation, which reads $\gamma = \eta\, \delta_{\mathbb{Z}}$ with $\eta(0) = 1$ and the recursion relations

$$\eta\big((k+\ell)m + r\big) = \frac{1}{k+\ell}\big(\alpha_{k,\ell,r}\, \eta(m) + \alpha_{k,\ell,k+\ell-r}\, \eta(m+1)\big),$$

with $\alpha_{k,\ell,r} = k + \ell - r - 2\min(k,\ell,r,k+\ell-r)$. They are valid for all $m \in \mathbb{Z}$ and $0 \le r < k+\ell$. In particular, one has $\eta\big((k+\ell)m\big) = \eta(m)$ for $m \in \mathbb{Z}$.

Given $k, \ell \in \mathbb{Z}$, the distribution function F is defined by $F(x) = \widehat{\gamma}([0,x])$ for $0 \le x < 1$, which extends to $x \in \mathbb{R}$ via $F(x+1) = 1 + F(x)$. It is also skew-symmetric ($F(-x) = -F(x)$) and thus satisfies $F(q) = q$ for all $q \in \frac{1}{2}\mathbb{Z}$. The continuous function F possesses the uniformly converging series expansion [12]

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

Two further examples are shown in Figure 9.

Another analogy with the TM system is that the block map ϕ of Equation (12) can still be used to induce a matching family of generalised period doubling sequences. They are defined by the primitive substitution rules

$$\varrho' : \begin{array}{l} a \mapsto b^{k-1} a b^{\ell-1} b \\ b \mapsto b^{k-1} a b^{\ell-1} a \end{array}$$

that are all pure point diffractive. The latter claim can most easily be seen from the letter coincidence (in the sense of Dekking [23]) at the kth position of the images. As before, this factor explores the pure point part of the dynamical spectrum of the gTM sequence.

4. Absolutely continuous spectra

The appearance of absolutely continuous diffraction spectra is usually seen as an indicator for randomness in the structure. Though this is perhaps generically true, there are also prominent deterministic sequences with such spectra, such as the Rudin-Shapiro sequence. In general, within the realm of random structures, one can only expect almost sure convergence results. In other words, most statements become measure theoretic in nature, though they are still completely rigorous.

4.1. **Coin tossing sequence.** The simplest example emerges from repeated coin tossing. Here, one obtains sequences $w \in \{\pm 1\}^{\mathbb{Z}}$ (for instance with 1 for 'head' and -1 for 'tail') which may be considered as the outcome of an eternal coin tosser. In more modern (and slightly more general) terminology, one considers a family $\bigl(W_n\bigr)_{n\in\mathbb{Z}}$ of independent and identically distributed (i.i.d.) random variables with values in $\{\pm 1\}$ and probabilities p (for 1) and $1-p$ (for -1). The ensemble of all possible realisations is $\mathbb{X}_{\mathrm{B}} = \{\pm 1\}^{\mathbb{Z}}$, which is equipped with a probability measure μ_{B} that emerges from the elementary probabilities via independence. This gives a measure theoretic dynamical system that is called the *Bernoulli shift* [46]. It has (metric) entropy $H(p) = -p\log(p) - (1-p)\log(1-p)$.

A random sequence W leads to a Dirac comb $\omega = W\delta_{\mathbb{Z}}$, which is now a translation bounded random measure with support $\mathbb{Z}$. Its autocorrelation, if it exists, is of the form $\gamma_{\mathrm{B}} = \eta_{\mathrm{B}}\,\delta_{\mathbb{Z}}$ with

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

Here, the convergence is almost sure by the strong law of large numbers (SLLN) [26], which means that this is the result for μ_{B}-almost all elements of $\{\pm 1\}^{\mathbb{Z}}$. Note that the use of the SLLN can also be replaced by an application of Birkhoff's ergodic theorem, because the Bernoulli shift is ergodic [46]. The corresponding diffraction measure reads

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

which follows from γ_{B} by an application of the PSF (4) together with $\widehat{\delta_0} = \lambda$. For the fair coin ($p = \frac{1}{2}$), this simplifies to $\widehat{\gamma_{\mathrm{B}}} = \lambda$, which is thus our first example of a purely absolutely continuous diffraction measure.

FIGURE 10. Illustration of the binary Rudin-Shapiro sequence.

4.2. **Rudin-Shapiro sequence.** Let us contrast the coin tossing sequence with a deterministic example that derives from [42, 45]. This sequence was originally constructed to show that the absence of pair correlations does not imply the presence of randomness. This has interesting consequences in diffraction theory, as pointed out in [32]. The modern formulation of the system is based on the substitution

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

Since $b|a$ is a legal seed (it occurs in $\varrho^2(b)$), one can construct a bi-infinite sequence u by the usual iteration procedure as

$$b|a \overset{\varrho^2}{\longmapsto} dbab|acab \overset{\varrho^2}{\longmapsto} \ldots \longrightarrow u = \varrho^2(u)\,,$$

where convergence is in the standard product topology. The hull (orbit closure) of u defines the *quaternary* Rudin-Shapiro system. Its reduction to a binary system is achieved by the mapping

$$\varphi: \quad a, c \mapsto 1\,, \quad b, d \mapsto \bar{1}\,,$$

and the orbit closure of $w := \varphi(u) = \ldots \bar{1}1\bar{1}\bar{1}|111\bar{1}\ldots$ defines the hull $\mathbb{X}_{\mathrm{RS}}$ of the *binary* Rudin-Shapiro system. The sequence w is illustrated in Figure 10. For the equivalent description as a weighted Dirac comb on $\mathbb{Z}$, we again use the identification of $\bar{1}$ with -1.

An alternative description of w uses the initial conditions $w(-1) = -1$, $w(0) = 1$ together with the recursion

$$w(4n + \ell) = \begin{cases} w(n), & \text{for } \ell \in \{0, 1\}, \\ (-1)^{n+\ell}\, w(n), & \text{for } \ell \in \{2, 3\}. \end{cases} \tag{14}$$

The autocorrelation of the corresponding weighted Dirac comb ω_{RS} exists and turns out to be $\gamma_{\mathrm{RS}} = \delta_0$. To prove this, one defines the coefficients

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

An application of Birkhoff's ergodic theorem to the quaternary Rudin-Shapiro system (which is strictly ergodic [41]) establishes the existence of all these limits. The recursion (14) for w now implies the recursion relations [12]

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

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

with initial conditions $\eta(0) = 1$ and $\vartheta(0) = 0$. This system has the unique solution $\vartheta \equiv 0$ together with $\eta(m) = \delta_{m,0}$, hence $\gamma_{\mathrm{RS}} = \delta_0$.

The diffraction measure for the binary Rudin-Shapiro system is thus given by $\widehat{\gamma}_{\mathrm{RS}} = \lambda$, which coincides with that of the coin tossing sequence for $p = \frac{1}{2}$; see also [32]. These two examples are thus homometric, despite the fact that one is deterministic (with entropy 0) while the other is stochastic (with entropy $\log(2)$); see [11, 12] for further details and discussions.

4.3. **Bernoullisation.** The homometry between the Dirac combs of the Rudin-Shapiro and the balanced coin tossing sequence raises the question how 'bad' the non-uniqueness of the inverse problem in this case really is. A partial answer (to the negative) can be given by means of the 'Bernoullisation' procedure which was introduced in [29, 11].

Starting from a uniquely ergodic sequence $S \in \{\pm 1\}^{\mathbb{Z}}$, its Dirac comb $\omega_S = S\,\delta_{\mathbb{Z}}$ possesses a unique autocorrelation γ_S. Let us now consider the random Dirac comb

$$\omega = \sum_{n\in\mathbb{Z}} S_n W_n\, \delta_n\,,$$

where $(W_n)_{n\in\mathbb{Z}}$ is once again an i.i.d. family of random variables with values in $\{\pm 1\}$ and probabilities p and $1-p$. Another application of the SLLN shows that ω almost surely has the autocorrelation

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

If S is the binary Rudin-Shapiro sequence, which is uniquely ergodic, a short calculation reveals that

$$\gamma_S \;=\; \gamma_{\mathrm{RS}} \;=\; \delta_0$$

in this case, *irrespective* of the value of the parameter $p \in [0,1]$. This way, we constructed a one-parameter family of homometric (or isospectral) structures whose entropy varies continuously between 0 and $\log(2)$. The conclusion is that kinematic diffraction alone cannot distinguish order from disorder here [11].

5. Further directions

After our brief discourse on the different spectral types of diffraction measures (by means of some paradigmatic examples), this section aims at indicating some more recent developments, which will again be explained informally by means of selected examples.

5.1. **Ledrappier's model.** Let us consider a prominent example of algebraic origin in the plane which is due to Ledrappier [35]. It is defined as

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

where e_1 and e_2 denote the standard Euclidean basis vectors in the plane. $\mathbb{X}_{\mathrm{L}}$ is a closed subset of the full shift $\{\pm 1\}^{\mathbb{Z}^2}$ and hence compact. It is also an Abelian group (under pointwise multiplication in our formulation, which follows [21]). As a dynamical system, it is thus equipped with the corresponding Haar measure μ_{L}, which is positive and normalised so that $\mu_{\mathrm{L}}(\mathbb{X}_{\mathrm{L}}) = 1$. Obviously, the system has no entropy, because the knowledge of a configuration along one horizontal line determines everything above it. However, it is clearly not deterministic. In fact, essentially along any given lattice direction, it looks like a one-dimensional Bernoulli system [35]. It is thus said to have rank 1 entropy, which means that the number of circular patches of a given size grows exponentially with its diameter, but not with its area.

Given an element $w \in \mathbb{X}_{\mathrm{L}}$, the corresponding Dirac comb

$$\omega = \sum_{x \in \mathbb{Z}^2} w_x \, \delta_x$$

possesses μ_{L}-almost surely the autocorrelation γ and the diffraction measure $\widehat{\gamma}$ given by [21]

$$\gamma = \delta_0 \quad \text{and} \quad \widehat{\gamma} = \lambda .$$

The system is thus homometric with the two-dimensional Bernoulli system with $p = \frac{1}{2}$ (coin tossing on $\mathbb{Z}^2$), and also with the direct product of two binary Rudin-Shapiro sequences. The similarity with the Bernoulli system goes a lot further, in the sense that also other correlation functions agree, although the systems differ for certain 3-point correlations; see [21] for details.

This system is meant to indicate that higher-dimensional symbolic dynamics is good for a surprise, as is well-known from [44]. It is thus clear that the inverse problem becomes more complicated. Another famous example is the $(\times 2, \times 3)$ dynamical system, which shares almost all correlation functions with a Bernoulli system with continuous degree of freedom [21].

5.2. **Random dimers on the integers.** Back to one dimension, let us briefly describe a system that was recently suggested by van Enter. First, consider $\mathbb{Z}$ as a close-packed arrangement of 'dimers' (pairs of neighbours), hence without gaps or overlaps. There are two possibilities to do so. Next, give each pair a random orientation by decorating it with either $(+,-)$ or $(-,+)$, with equal probability. Identifying $\pm$ with ± 1, this defines the closed (and hence compact) set

$$\mathbb{X} = \left\{ w \in \{\pm 1\}^{\mathbb{Z}} \mid M(w) \subset 2\mathbb{Z} \text{ or } M(w) \subset 2\mathbb{Z}+1 \right\},$$

where $M(w) := \{i \in \mathbb{Z} \mid w_i = w_{i+1}\}$. Note that $M(w)$ can be empty, which happens precisely for the two periodic sequences $\ldots+-|+-\ldots$ and $\ldots-+|-+\ldots$. One has an invariant measure on $\mathbb{X}$ that emerges from the stochastic process via the probability of the possible finite patches (which define the generating cylinder sets as usual).

Turning a configuration $w \in \mathbb{X}$ into a signed Dirac comb with weights $w_i \in \{\pm 1\}$ as before, another exercise with the SLLN shows that its autocorrelation almost surely exists. It is not difficult to derive [7] that $\gamma = \delta_0 - \frac{1}{2}(\delta_1 + \delta_{-1})$, so that the corresponding diffraction measure is

$$\widehat{\gamma_w} = \big(1 - \cos(2\pi k)\big)\lambda .$$

This is another example of a purely absolutely continuous diffraction measure. The Radon-Nikodym density relative to λ is written as a function of k. In contrast, the dynamical spectrum of this system contains eigenvalues, wherefore this is an analogue of the comparison between the Thue-Morse and period doubling systems [25], this time in the presence of absolutely continuous spectra.

This difference can be rectified by a block map that is very similar to the map ϕ encountered in (12). Defining $u_i = -w_i w_{i+1}$ for $i \in \mathbb{Z}$ maps w to a new sequence u, which almost surely has the diffraction

$$\widehat{\gamma_u} = \frac{1}{4}\delta_{\mathbb{Z}/2} + \frac{1}{2}\lambda$$

of mixed type. In particular, as in the Thue-Morse case, it displays the entire point part of the original dynamical spectrum.

5.3. **Renewal processes.** A large and interesting class of processes in one dimension can be described as a renewal process [6, 15]. Here, one starts from a probability measure μ on $\mathbb{R}_+$ (the positive real line) and considers a machine that moves at constant speed along the real line and drops a point on the line with a waiting time that is distributed according to μ. Whenever this happens, the internal clock is reset and the process resumes. Let us (for simplicity) assume that both the velocity of the machine and the expectation value of μ are 1, so that we end up with realisations that are, almost surely, point sets in $\mathbb{R}$ of density 1 (after we let the starting point of the machine move to $-\infty$).

Clearly, the resulting process is stationary and can thus be analysed by considering all realisations which contain the origin. Moreover, there is a clear (distributional) symmetry around the origin, so that we can determine the corresponding autocorrelation γ of almost all realisations from studying what happens to the right of 0.

Indeed, if we want to know the frequency per unit length of the occurrence of two points at distance x (or the corresponding density), we need to sum the contributions that x is the first point after 0, the second point, the third, and so on. In other words, we almost surely obtain the autocorrelation

$$\gamma = \delta_0 + \nu + \widetilde{\nu} \tag{15}$$

with $\nu = \mu + \mu * \mu + \mu * \mu * \mu + \ldots$, where the proper convergence of the sum of iterated convolutions follows from [6, Lemma 4]. Note that the point measure at 0 simply reflects that the almost sure density of the resulting point set is 1. Indeed, ν is a translation bounded positive measure, and satisfies the renewal relations (see [27, Ch. XI.9] or [6, Prop. 1] for a proof)

$$\nu = \mu + \mu * \nu \qquad \text{and} \qquad (1 - \widehat{\mu})\,\widehat{\nu} = \widehat{\mu}, \tag{16}$$

where $\widehat{\mu}$ is a uniformly continuous and bounded function on $\mathbb{R}$. Note that the second equation emerges from the first by Fourier transform, but has been rearranged to indicate why the set $S = \{k \mid \widehat{\mu}(k) = 1\}$ is important. In this setting, the measure γ of (15) is both positive and positive definite.

Based on the structure of the support of the underlying probability measure μ, one can determine the diffraction of the renewal process as follows. Let μ be a probability measure on $\mathbb{R}_+$ with mean 1, and assume that a moment of μ of order $1 + \varepsilon$ exists for some $\varepsilon > 0$ (we refer to [6] for details on this condition). Then, the point sets obtained from the stationary renewal process based on μ almost surely have a diffraction measure of the form

$$\widehat{\gamma} = \widehat{\gamma}_{\mathsf{pp}} + (1 - h)\,\lambda,$$

where h is a locally integrable function on $\mathbb{R}$ that is continuous except for at most countably many points (namely those of the set S). It is given by

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

Moreover, the pure point part reads

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

Proofs can be found in [6, 15].

The renewal process is a versatile method to produce interesting point sets on the line. These include random tilings with finitely many intervals (which are Delone sets) as well as the homogeneous Poisson process on the line (where μ is the exponential distribution with mean 1); see [6, Sec. 3] for explicit examples and applications.

5.4. **Random clusters and point processes.** Let us continue by considering the influence of randomness on the diffraction of point sets and certain structures derived from them in Euclidean spaces of arbitrary dimension. Here, we start from a single point set $\Lambda \subset \mathbb{R}^d$, which is then randomly modified by replacing each point by a (possibly complex) finite random cluster. This situation is still manageable (via the SLLN) when Λ is sufficiently 'nice', for instance if Λ is of finite local complexity and possesses an autocorrelation, which is then of the form $\gamma = \sum_{z\in\Lambda-\Lambda} \eta(z)\, \delta_z$. More generally, one can analyse this situation in the setting of stationary ergodic point processes [28, 6], which treats almost all of their realisations at once and permits a larger generality for the sets Λ, though the clusters will then be restricted to positive or signed measures.

Given such a point set Λ, its (deterministic) Dirac comb δ_Λ is turned into a random Dirac comb

$$\delta_\Lambda^{(\Omega)} = \sum_{x\in\Lambda} \Omega_x * \delta_x$$

by means of the i.i.d. family of random measure $(\Omega_x)_{x\in\Lambda}$ with common law Q and representing random variable Ω. Here, we assume that the expectation $\mathbb{E}_Q\big(|\Omega|\big)$ is a finite measure, and that $\mathbb{E}_Q\big((|\Omega|(\mathbb{R}^d))^2\big) < \infty$. Under some mild (but somewhat technical) conditions [6], one now obtains the autocorrelation

$$\begin{aligned}\gamma^{(\Omega)} &\overset{\text{(a.s.)}}{=} \big(\mathbb{E}_Q(\Omega) * \widetilde{\mathbb{E}_Q(\Omega)}\big) * \gamma \\ &\qquad + \operatorname{dens}(\Lambda)\,\big(\mathbb{E}_Q(\Omega * \widetilde{\Omega}) - \mathbb{E}_Q(\Omega) * \widetilde{\mathbb{E}_Q(\Omega)}\big) * \delta_0\end{aligned}$$

and hence the diffraction

$$\widehat{\gamma}^{(\Omega)} \overset{\text{(a.s.)}}{=} \big|\mathbb{E}_Q(\widehat{\Omega})\big|^2 \cdot \widehat{\gamma} + \operatorname{dens}(\Lambda)\,\big(\mathbb{E}_Q(|\widehat{\Omega}|^2) - |\mathbb{E}_Q(\widehat{\Omega})|^2\big) \cdot \lambda\,.$$

The diffraction of the modified structure emerges from the original one by a modulation of $\widehat{\gamma}$ and the addition of an absolutely continuous contribution, which in essence is the Fourier transform of the covariance of the representing random cluster Ω.

This approach comprises a wide range of models, including the random weight and the random displacement model as well as decorations by random clusters. The next level of generality replaces the deterministic set Λ by a general ergodic point process [28]. This way, both the underlying set (core process) and the modification (cluster process) are described in terms of stochastic processes. This point of view is a promising starting point for further investigations.

6. Concluding remarks

Our informal exposition was meant to demonstrate that mathematical diffraction theory provides useful tools for the analysis of deterministic and random systems, both for practical applications in crystallography and materials science and for theoretical questions in harmonic analysis and dynamical systems theory. While the majority of the crystallographic literature concentrates on the pure point case, we have shown that also continuous spectra are explicitly accessible in relevant cases, and certainly deserve more attention from this point of view. Merging methods from harmonic analysis and dynamical systems with well-established procedures from point process theory might be a good path to proceed.

The inverse problem of structure determination is already a formidable problem in the realm of pure point diffractive systems, due to the existence of non-trivially homometric structures. As we have shown above, the inverse problem becomes significantly more involved in the presence of disorder, including the potential insensitivity to quantities such as entropy. Although there is quite some knowledge about this problem in the point process community, it is fair to say that solutions to the inverse problem or satisfactory classifications of homometry classes are not in sight.

The setting is by no means restricted to lattice systems, which were mainly chosen for ease of presentation and concreteness of results. Also extensions to higher dimensions are possible, where one has to expect new phenomena (such as the lower rank entropy) that further complicate the picture. Although the general theory of point processes is highly developed, the treatment of stochastic systems with interaction becomes difficult as soon as concrete results are desired. This is already the case for equilibrium systems, as they require the full machinery of Gibbs measures. Their analysis from the point of view of mathematical diffraction theory is still in its infancy, although examples such as the Ising lattice gas show (see [14] and references therein) that explicit results are possible.

References

[1] J.-P. Allouche and J. Shallit. *Automatic Sequences: Theory, Applications, Generalizations* (Cambridge University Press, Cambridge, 2003).

[2] S. Akiyama and J.-Y. Lee, *Algorithm for determining pure pointedness of self-affine tilings*, preprint `arXiv:1003.2898`.

[3] R. Ammann, B. Grünbaum and G.C. Shephard, *Aperiodic tiles*, Discr. Comput. Geom. **8** (1992) 1–25.

[4] M. Baake, *A guide to mathematical quasicrystals*, in: *Quasicrystals – An Introduction to Structure, Physical Properties and Applications*, eds. J.-B. Suck, M. Schreiber and P. Häussler (Springer, Berlin, 2002) pp. 17–48; `arXiv:math-ph/9901014`.

[5] M. Baake, *Diffraction of weighted lattice subsets*, Can. Math. Bulletin **45** (2002) 483–498; `arXiv:math.MG/0106111`.

[6] M. Baake, M. Birkner and R.V. Moody, *Diffraction of stochastic point sets: Explicitly computable examples*, Commun. Math. Phys. **293** (2010) 611–660; `arXiv:0803.1266`.

[7] M. Baake and A.C.D. van Enter, in preparation.

[8] M. Baake and U. Grimm, *A guide to quasicrystal literature*, in: [18], pp. 371–373.

[9] M. Baake and U. Grimm, *Homometric model sets and window covariograms*, Z. Krist. **222** (2007) 54–58; `arXiv:math.MG/0610411`.

[10] M. Baake and U. Grimm, *The singular continuous diffraction measure of the Thue-Morse chain*, J. Phys. A.: Math. Theor. **41** (2008) 422001; `arXiv:0809.0580`.

[11] M. Baake and U. Grimm, *Kinematic diffraction is insufficient to distinguish order from disorder*, Phys. Rev. B **79** (2009) 020203(R) and **80** (2009) 029903(E); `arXiv:0810.5750`.

[12] M. Baake and U. Grimm, *Surprises in aperiodic diffraction*, J. Physics: Conf. Ser. **226** (2010) 012023; `arXiv:0909.5605`.

[13] M. Baake and U. Grimm, *Theory of Aperiodic Order: A Mathematical Invitation* (Cambridge University Press, in preparation).

[14] M. Baake and M. Höffe, *Diffraction of random tilings: some rigorous results*, J. Stat. Phys. **99** (2000) 219–261; `math-ph/9904005`.

[15] M. Baake and H. Kösters, *Random point sets and their diffraction*, Phil. Mag., in press; `arXiv:1007.3084`.

[16] M. Baake and D. Lenz, *Dynamical systems on translation bounded measures: Pure point dynamical and diffraction spectra*, Ergodic Th. & Dynam. Syst. **24** (2004) 1867–1893; `math.DS/0302231`.

[17] M. Baake, D. Lenz and R.V. Moody, *Characterization of model sets by dynamical systems*, Ergodic Th. & Dynam. Syst. **27** (2007) 341–382; `math.DS/0511648`.

[18] M. Baake and R.V. Moody (eds.), *Directions in Mathematical Quasicrystals*, CRM Monograph Series, vol. 13 (AMS, Providence, RI, 2000).

[19] M. Baake and R.V. Moody, *Weighted Dirac combs with pure point diffraction*, J. reine angew. Math. (Crelle) **573** (2004) 61–94; `arXiv:math.MG/0203030`.

[20] M. Baake, R.V. Moody and M. Schlottmann, *Limit-(quasi)periodic point sets as quasicrystals with p-adic internal spaces*, J. Phys. A: Math. Gen. **31** (1998) 5755–5765; `arXiv:math-ph/9901008`.

[21] M. Baake and T. Ward, *Planar dynamical systems with pure Lebesgue diffraction spectrum*, J. Stat. Phys. **140** (2010) 90–102; `arXiv:1003.1536`.

[22] C. Berg and G. Forst, *Potential Theory on Locally Compact Abelian Groups* (Springer, Berlin, 1975).

[23] F.M. Dekking, *The spectrum of dynamical systems arising from substitutions of constant length*, Z. Wahrscheinlichkeitsth. verw. Geb. **41** (1978) 221–239.

[24] X. Deng and 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`.

[25] A.C.D. van Enter and J. Miękisz, *How should one define a (weak) crystal?*, J. Stat. Phys. **66** (1992) 1147–1153.

[26] N. Etemadi, *An elementary proof of the strong law of large numbers*, Z. Wahrscheinlichkeitsth. verw. Gebiete **55** (1981) 119–122.

[27] W. Feller, *An Introduction to Probability Theory and Its Applications*, vol. II, 2nd ed. (Wiley, New York, 1971).

[28] J.-B. Gouéré, *Diffraction and Palm measure of point processes*, Comptes Rendus Acad. Sci. (Paris) **342** (2003) 141–146; `arXiv:math.PR/0208064`.

[29] U. Grimm and M. Baake, *Homometric point sets and inverse problems*, Z. Krist. **223** (2008) 777–781; `arXiv:0808.0094`.

[30] F.A. Grünbaum and C.C. Moore, *The use of higher-order invariants in the determination of generalized Patterson cyclotomic sets*, Acta Cryst. A **51** (1995) 310–323.

[31] A. Hof, *On diffraction by aperiodic structures*, Commun. Math. Phys. **169** (1995) 25–43.

[32] M. Höffe and M. Baake, *Surprises in diffuse scattering*, Z. Krist. **215** (2000) 441–444; `arXiv:math-ph/0004022`.

[33] 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 (Univ. of California Press, Berkeley, 1972) pp. 319–326.

[34] M. Keane, *Generalized Morse sequences*, Z. Wahrscheinlichkeitsth. verw. Gebiete **10** (1968) 335–353.

[35] F. Ledrappier, *Un champ markovien peut être d'entropie nulle et mélangeant*, C. R. Acad. Sci. Paris Sér. A-B, **287** (1978) A561–A563.

[36] J.-Y. Lee, R.Y. Moody and B. Solomyak, *Pure point dynamical and diffraction spectra*, Ann. Henri Poincaré **3** (2002) 1003–1018; `arXiv:0910.4809`

[37] D. Lenz and N. Strungaru, *Pure point spectrum for measure dynamical systems on locally compact Abelian groups*, J. Math. Pures Appl. **92** (2009) 323–341; `arXiv:0704.2498`.

[38] K. Mahler, *The spectrum of an array and its application to the study of the translation properties of a simple class of arithmetical functions. Part II: On the translation properties of a simple class of arithmetical functions*, J. Math. Massachusetts **6** (1927) 158–163.

[39] R.V. Moody, *Model sets: A survey*, in: *From Quasicrystals to More Complex Systems*, eds. F. Axel, F. Dénoyer and J.P. Gazeau (EDP Sciences, Les Ulis, and Springer, Berlin, 2000) pp. 145–166; `arXiv:math.MG/0002020`.

[40] A.L. Patterson, *Ambiguities in the X-ray analysis of crystal structures*, Phys. Rev. **65** (1944) 195–201.

[41] M. Queffélec, *Substitution Dynamical Systems — Spectral Analysis*, LNM 1294 (Springer, Berlin, 1987).

[42] W. Rudin, *Some theorems on Fourier coefficients*, Proc. AMS **10** (1959) 855–859.

[43] M. Schlottmann, *Generalised model sets and dynamical systems*, in: [18], pp. 143–159.

[44] K. Schmidt, *Dynamical Systems of Algebraic Origin* (Birkhäuser, Basel, 1995).

[45] H.S. Shapiro, *Extremal Problems for Polynomials and Power Series*, Masters Thesis (MIT, Boston, 1951).

[46] P. Walters, *An Introduction to Ergodic Theory*, reprint (Springer, New York, 2000).

[47] 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.

[48] R.L. Withers, *Disorder, structured diffuse scattering and the transmission electron microscope*, Z. Krist. **220** (2005) 1027–1034.

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