

Surprises in aperiodic diffraction

Michael Baake¹ and Uwe Grimm²

¹ Fakultät für Mathematik, Universität Bielefeld, Postfach 100131, 33501 Bielefeld, Germany

² Department of Mathematics and Statistics, The Open University, Walton Hall, Milton

Keynes MK7 6AA, UK

E-mail: mbaake@math.uni-bielefeld.de and u.g.grimm@open.ac.uk

Abstract. Mathematical diffraction theory is concerned with 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. Here, we report on some of the recent results in an exemplary and informal fashion.

1. Introduction

The diffraction measure is a characteristic quantity of a translation bounded measure ω on Euclidean space (or on any locally compact Abelian group). It emerges as the Fourier transform $\hat{\gamma}$ of the autocorrelation measure γ of ω , and has important applications in crystallography, because it describes the outcome of kinematic diffraction (from X-rays or neutron scattering, say). In recent years, initiated by the discovery of quasicrystals (which are non-periodic but nevertheless show pure Bragg diffraction), a systematic study by many people has produced a reasonably satisfactory understanding of the class of measures with a pure point diffraction measure, meaning that $\hat{\gamma}$ is a pure point measure, without any continuous component.

Clearly, reality is more complicated than that, in the sense that real world structures will (and do) show lots of continuous components as well. Unfortunately, the methods around dynamical systems that are used to establish pure point spectra do not seem to extend to the treatment of systems with mixed spectrum, at least not in sufficient generality. Nevertheless, systems with continuous spectral components have recently been investigated also from a rigorous mathematical point of view, with a number of unexpected results. In particular, the phenomenon of homometry becomes more subtle, as we will see below.

In this informal exposition, we summarise some classic results that have recently resurfaced in the context of diffraction, with special emphasis on singular continuous and absolutely continuous spectra. For proofs (and the formal details) we refer to the original papers or to work in progress.

2. Mathematical setting and pure point spectra

Below, we mainly consider various (weighted) Dirac combs on the real line, with support on \mathbb{Z} (the set of integers), and their diffraction. Even in this simple and seemingly restricted setting, unexpected phenomena show up. If $\omega = \sum_{n \in \mathbb{Z}} w(n)\delta_n$, with δ_n the normalised point measure at n , the *natural autocorrelation* (if it exists) of ω is

$$\gamma = \omega \circledast \tilde{\omega} := \lim_{N \rightarrow \infty} \frac{\omega_N * \tilde{\omega}_N}{2N}, \quad (1)$$

which we view as a measure on \mathbb{R} . Here, $\omega_N = \omega|_{[-N, N]}$ is the restriction of ω to the closed interval $[-N, N]$, and $\tilde{\mu}$ is the ‘flipped over’ measure, defined by $\tilde{\mu}(g) = \overline{\mu(\tilde{g})}$ with g a continuous test function of compact support and $\tilde{g}(x) = \overline{g(-x)}$. Here, and in analogous situations below, the bar denotes complex conjugation. We will only consider situations where the limit in (1) exists, either always (in the deterministic cases) or almost surely (in the probabilistic cases). An explicit calculation shows that $\text{supp}(\omega) \subset \mathbb{Z}$ implies that γ must be of the form

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

with the autocorrelation coefficients

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

The existence of the limit in (1) is equivalent to the existence of the $\eta(m)$ for all $m \in \mathbb{Z}$.

By construction, γ is a positive definite measure, and hence Fourier transformable. The result is $\hat{\gamma}$, the *diffraction measure*, which is a positive, translation bounded measure on \mathbb{R} . It describes (kinematic) diffraction from the measure ω ; compare [12] for background and [18, 9] for the development of this approach to diffraction theory. One of the benefits of this approach is the unique decomposition

$$\hat{\gamma} = (\hat{\gamma})_{\text{pp}} + (\hat{\gamma})_{\text{sc}} + (\hat{\gamma})_{\text{ac}} \quad (4)$$

of the diffraction measure into its pure point, singular continuous and absolutely continuous parts, the latter splitting relative to Lebesgue measure λ , which is the natural reference measure for volume in Euclidean space.

The best known example is the lattice Dirac comb $\omega = \delta_{\mathbb{Z}} = \sum_{n \in \mathbb{Z}} \delta_n$, with autocorrelation $\gamma = \delta_{\mathbb{Z}}$ and diffraction $\hat{\gamma} = \delta_{\mathbb{Z}}$. Here, γ follows from an elementary calculation, while the formula for $\hat{\gamma}$ is a consequence of the *Poisson summation formula*

$$\widehat{\delta_{\Gamma}} = \text{dens}(\Gamma) \delta_{\Gamma^*} \quad (5)$$

for an arbitrary lattice Γ (in \mathbb{R}^d) of density $\text{dens}(\Gamma)$, with dual lattice Γ^* , the latter defined by $\Gamma^* := \{x \in \mathbb{R}^d \mid xy \in \mathbb{Z} \text{ for all } y \in \Gamma\}$; see [9] and references therein. The integer lattice is perhaps the simplest example for a system with pure point diffraction. More generally, if ω is any \mathbb{Z} -periodic measure, it can be written as $\omega = \mu * \delta_{\mathbb{Z}}$, with μ a finite measure. This leads to $\gamma = (\mu * \tilde{\mu}) * \delta_{\mathbb{Z}}$ and $\hat{\gamma} = |\widehat{\mu}|^2 \delta_{\mathbb{Z}}$, where $|\widehat{\mu}|^2$ is a continuous positive function on \mathbb{R} . Its values at integer points are the *intensities* of the Bragg peaks.

A similarly nice formula holds for regular model sets. Within a given cut and project scheme (CPS) $(\mathbb{R}^d, \mathbb{R}^m, \mathcal{L})$ with lattice $\mathcal{L} \subset \mathbb{R}^{d+m}$, consider $A = \{x \in L \mid x^* \in W\}$, where $L = \pi(\mathcal{L})$ is the projection of \mathcal{L} in \mathbb{R}^d , W is the (compact) window in \mathbb{R}^m (with boundary of measure 0), and \star denotes the star map of the CPS. By the general model set theorem [18, 27, 9], the diffraction $\hat{\gamma}$ of the Dirac comb δ_A is then the pure point measure

$$\hat{\gamma} = \sum_{k \in L^{\otimes}} |A(k)|^2 \delta_k, \quad (6)$$

where $L^{\otimes} = \pi(\mathcal{L}^*)$ is the projection of the dual lattice \mathcal{L}^* and the amplitude $A(k)$ is given by

$$A(k) = \frac{\text{dens}(A)}{\text{vol}(W)} \int_W e^{2\pi i k^* y} dy = \frac{\text{dens}(A)}{\text{vol}(W)} \widehat{1}_W(-k^*).$$

Table 1. Weights for the homometric pair from [17].

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

This formula has various generalisations, for instance to model sets with other internal spaces or to weighted model sets; see [27, 9] and references therein for more.

As an example, we consider the *period doubling sequence*, as defined by the substitution

$$\varrho = \varrho_{\text{pd}}: a \mapsto ab, b \mapsto aa. \quad (7)$$

A two-sided sequence can be obtained from a fixed point of ϱ^2 via the iteration

$$a|a \xrightarrow{\varrho^2} abaa|abaa \xrightarrow{\varrho^2} \dots \longrightarrow w = \varrho^2(w), \quad (8)$$

with convergence in the (obvious) product topology. Here and below, we write two-sided sequences as $w = \dots w_{-2}w_{-1}|w_0w_1 \dots$ and use $|$ to mark the origin. Note that $a|a$ in (8) is a legal seed, so that w is a fixed point of ϱ^2 in the strict sense.

We attach a Dirac comb to w by $\omega = \sum_{n \in \mathbb{Z}} h(w_n) \delta_n$, with $h(a) = h_+$ and $h(b) = h_-$. This turns out to define a (weighted) regular model set [10, 9], so that the diffraction is indeed a pure point measure. It is given by

$$\widehat{\gamma}_{\text{pd}} = \sum_{k \in L^{\otimes}} |h_+ A(k) + h_- B(k)|^2 \delta_k,$$

where $L^{\otimes} = \bigcup_{\ell \geq 1} \mathbb{Z}/2^\ell = \{\frac{m}{2^r} \mid (r = 0, m \in \mathbb{Z}) \text{ or } (r \geq 1, m \text{ odd})\}$ is the Fourier module of the period doubling sequence. The amplitudes read

$$A(k) = \frac{2}{3 \cdot (-2)^r} e^{2\pi i k} \quad \text{and} \quad B(k) = \delta_{r,0} - A(k),$$

where we implicitly refer to the parametrisation of L^{\otimes} . We state this formula here without further details; see [10, 9] for a proof.

Let us briefly mention the *homometry* problem. It refers to the possibility that distinct measures can still possess the same autocorrelation. An interesting example is constructed in [17], based on 6-periodic Dirac combs of the form $\delta_{6\mathbb{Z}} * \sum_{j=0}^5 c_j \delta_j$. In particular, the two choices of Table 1 lead to the same autocorrelation – and, in fact, even to identical correlation functions up to order 5. It is only the order 6 correlation that tells the two combs apart.

For model sets, there are further possibilities, because different windows can have the same covariogram. The latter (for a compact set K) is defined as $\text{cvg}_K(x) = \text{vol}(K \cap (x + K)) = (1_K * \widetilde{1_K})(x)$. This phenomenon results in identical autocorrelations and hence in homometric model sets. A simple planar example was constructed in [4]; see also [16, 14, 15]. We skip further details here and shift our attention to continuous spectra now.

3. Singular continuous spectra

The paradigm of a singular continuous measure is the distribution function for the classic middle-thirds Cantor measure, which is also called the Devil's staircase. Here, we show a class of structures that lead to somewhat similar functions, yet with significant differences.

The classic Thue-Morse (or Prouhet-Thue-Morse) sequence [1] can be defined via a fixed point of the substitution

$$\varrho = \varrho_{\text{TM}}: 1 \mapsto 1\bar{1}, \bar{1} \mapsto \bar{1}1 \quad (9)$$

on the binary alphabet $\{1, \bar{1}\}$. The one-sided fixed point starting with 1 reads

$$v = v_0 v_1 v_2 \dots = 1\bar{1}\bar{1}1\bar{1}1\bar{1}\bar{1} \dots, \quad (10)$$

while \bar{v} is the fixed point starting with $\bar{1}$. One can now define a two-sided sequence w by

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

It is easy to check that w defines a 2-cycle under ϱ , and hence a fixed point for ϱ^2 . Since the central seed $1|1$ is legal, an iteration of ϱ^2 applied to it converges to w in the product topology.

The sequence w defines a dynamical system (under the action of the group \mathbb{Z}). Its compact space is the (discrete) *hull*, obtained as the closure of the \mathbb{Z} -orbit of w ,

$$\mathbb{X}_{\text{TM}} = \overline{\{S^i w \mid i \in \mathbb{Z}\}},$$

where S denotes the shift operator and the closure is taken in the local (or product) topology, where two sequences are close when they agree on a large segment around the origin. Now, $(\mathbb{X}_{\text{TM}}, \mathbb{Z})$ is a strictly ergodic dynamical system (hence uniquely ergodic and minimal [25, 29]). Its unique invariant probability measure is given via the (absolute) frequencies of finite words (or patches) as the measures of the corresponding cylinder sets, which then generate the σ -algebra.

Here, we are interested in the diffraction of the (signed) Dirac comb $\omega_{\text{TM}} = \sum_{n \in \mathbb{Z}} w_n \delta_n$, where we interpret 1 and $\bar{1}$ as weights 1 and -1 . Its autocorrelation exists, as a consequence of unique ergodicity, and is actually the same measure for *all* sequences of \mathbb{X}_{TM} . We can now employ the special structure of our fixed point w to analyse it. The autocorrelation is of the general form (2), with coefficients $\eta(0) = 1$, $\eta(-m) = \eta(m)$ for all $m \in \mathbb{Z}$ and

$$\eta(m) = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=0}^{N-1} v_n v_{n+m} \quad (11)$$

for all $m \geq 0$. Here, the structure of w and its relation to v was used to derive (11) from (3). Observing that v satisfies $v_{2n} = v_n$ and $v_{2n+1} = \bar{v}_n$ for all $n \geq 0$, one can derive from (11) the recursions

$$\eta(2m) = \eta(m) \quad \text{and} \quad \eta(2m+1) = -\frac{1}{2}(\eta(m) + \eta(m+1)), \quad (12)$$

which actually hold for all $m \in \mathbb{Z}$. One finds $\eta(\pm 1) = -1/3$ from solving the recursion for $m = 0$ and $m = -1$ with $\eta(0) = 1$, while all other values are then recursively determined.

To analyse the diffraction measure $\hat{\gamma}$ of the TM sequence (following [23, 20]), one can start with its pure point part. Defining $\Sigma(N) = \sum_{n=-N}^N (\eta(n))^2$, one derives via the recursion (12) that $\Sigma(4N) \leq \frac{3}{2}\Sigma(2N)$, which implies $\frac{1}{N}\Sigma(N) \xrightarrow{N \rightarrow \infty} 0$. By Wiener's criterion [30], this means $(\hat{\gamma})_{\text{pp}} = 0$, so that $\hat{\gamma}$ is a continuous measure.

Defining the (continuous) distribution function F via $F(x) = \widehat{\gamma}([0, x])$, another consequence of (12) is the pair of functional relations

$$dF\left(\frac{x}{2}\right) \pm dF\left(\frac{x+1}{2}\right) = \left\{ \begin{array}{c} 1 \\ -\cos(\pi x) \end{array} \right\} dF(x).$$

Splitting F into its **sc** and **ac** parts (which is unique) now implies backwards that the recursion (12) holds separately for the two sets of autocorrelation coefficients, η_{sc} and η_{ac} , with yet unknown initial conditions at 0. An application of the Riemann-Lebesgue lemma, however, forces $\eta_{\text{ac}}(0) = 0$, and hence $\eta_{\text{ac}}(m) = 0$ for all $m \in \mathbb{Z}$, so that also $(\widehat{\gamma})_{\text{ac}} = 0$; compare [20]. This shows that $\widehat{\gamma}$, which is not the zero measure, is purely singular continuous. Figure 1 shows an image, where we have used the Volterra iteration

$$F_{n+1}(x) = \frac{1}{2} \int_0^{2x} (1 - \cos(\pi y)) F_n'(y) dy \quad \text{with} \quad F_0(x) = x$$

to calculate F with sufficient precision (note that $F(x+1) = F(x) + 1$, so that a display on $[0, 1]$ suffices). 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 [5] and references therein for details.

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

$$\varphi: \quad 1\bar{1}, \bar{1}1 \mapsto a, \quad 11, \bar{1}\bar{1} \mapsto b, \quad (13)$$

which defines an exact 2-to-1 surjection from the hull \mathbb{X}_{TM} to \mathbb{X}_{pd} .

The TM sequence is often considered as a rare and special example, which is misleading. To demonstrate the point (following [21]), consider the generalised Morse sequences defined by

$$\varrho = \varrho_{k,\ell}: \quad 1 \mapsto 1^k \bar{1}^\ell, \quad \bar{1} \mapsto \bar{1}^k 1^\ell \quad (14)$$

for arbitrary $k, \ell \in \mathbb{N}$. Here, the one-sided fixed point starting with $v_0 = 1$ satisfies

$$v_{m(k+\ell)+r} = \begin{cases} v_m, & \text{if } 0 \leq r < k, \\ \bar{v}_m, & \text{if } k \leq r < k + \ell, \end{cases} \quad (15)$$

for $m \geq 0$. A two-sided sequence can be constructed as above. Since each choice of k, ℓ leads to a strictly ergodic dynamical system, we know that all autocorrelation coefficients exist. Clearly (again with $\bar{1} \hat{=} -1$), we have $\eta(0) = 1$, while several possibilities exist to calculate $\eta(\pm 1) = \frac{k+\ell-3}{k+\ell+1}$. In general, we obtain the recursion

$$\eta((k+\ell)m+r) = \frac{1}{k+\ell} (\alpha_{k,\ell,r} \eta(m) + \alpha_{k,\ell,k+\ell-r} \eta(m+1)), \quad (16)$$

with $\alpha_{k,\ell,r} = k + \ell - r - 2 \min(k, \ell, r, k + \ell - r)$, which holds for all $m \in \mathbb{Z}$ and $0 \leq r \leq k + \ell - 1$.

The recursion can once again be used to show the absence of pure point components (by Wiener's criterion) as well as that of absolutely continuous components (by the Riemann-Lebesgue lemma), thus establishing that each sequence in this family leads to a signed Dirac comb with purely singular continuous diffraction. The distribution function satisfies

$$F(x) = \widehat{\gamma}([0, x]) = x + \sum_{m \geq 1} \frac{\eta(m)}{m\pi} \sin(2\pi mx),$$

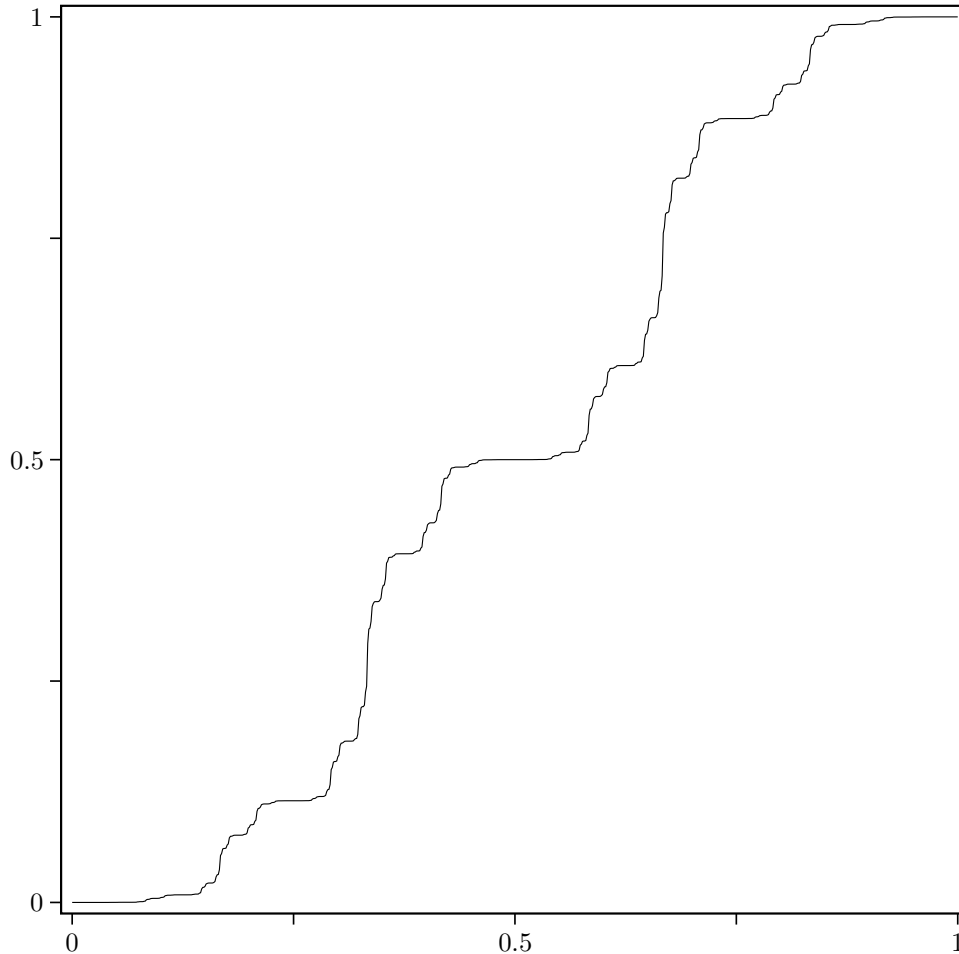


Figure 1. The distribution function of the TM measure on $[0, 1]$.

which is a uniformly converging series. Moreover, the measure $\hat{\gamma}$ has a (vaguely convergent) representation as an infinite *Riesz product*: With $\theta(x) := 1 + \frac{2}{k+\ell} \sum_{r=1}^{k+\ell-1} \alpha_{k,\ell,r} \cos(2\pi r x)$, it is given by $\prod_{n \geq 0} \theta((k+\ell)^n x)$. The entire analysis is thus completely analogous to that of the original TM sequence and shows that the latter is a typical example in an infinite family. Further details (and proofs) will be given in [3].

Let us finally mention that the block map (13) applies to any member of this family, and always gives a 2-to-1 cover of the hull that belongs to the generalised period doubling substitution

$$\varrho': a \mapsto b^{k-1} a b^{\ell-1} b, b \mapsto b^{k-1} a b^{\ell-1} a.$$

Since we always have a coincidence in the sense of Dekking [13], they all define systems with pure point spectrum – another analogy to the classic case $k = \ell = 1$.

4. Absolutely continuous spectra

The simplest example in this category is the Bernoulli (or coin tossing) comb. Let $(W_n)_{n \in \mathbb{Z}}$ be a family of independent and identically distributed (i.i.d.) random variables. We assume that W represents this family and takes values 1 and -1 with probabilities p and $1 - p$. We then

consider the random measure

$$\omega_B = \sum_{n \in \mathbb{Z}} W_n \delta_n, \quad (17)$$

which (almost surely in the probabilistic sense) has a natural autocorrelation of the form (2), with coefficients $\eta_B(0) = 1$ and (a.s.) $\eta_B(m) = (2p - 1)^2$ for all $0 \neq m \in \mathbb{Z}$, so that we have

$$\gamma_B = (2p - 1)^2 \delta_{\mathbb{Z}} + 4p(1 - p) \delta_0 \quad (\text{a.s.}). \quad (18)$$

In particular, when $p = 1/2$, it gives $\gamma_B = \delta_0$. Eq. (18) can be proved either by an application of Birkhoff's ergodic theorem for \mathbb{Z} -action or by the strong law of large numbers (SLLN). We refer to [6] for details and further references. Let us also mention that (18) can be rewritten as $\gamma_B = \beta^2 \delta_{\mathbb{Z}} + (1 - \beta^2) \delta_0$, where β has the meaning of the drift velocity of a one-dimensional random walk on the line; compare [11, 8].

As a consequence, we obtain a diffraction measure of mixed type,

$$\widehat{\gamma}_B = (2p - 1)^2 \delta_{\mathbb{Z}} + 4p(1 - p) \lambda \quad (\text{a.s.}), \quad (19)$$

where λ denotes Lebesgue measure. The special case of a fair coin ($p = 1/2$) leads to $\widehat{\gamma}_B = \lambda$, which is purely absolutely continuous. More generally, when W takes the (possibly complex) values h_+ and h_- , each with probability $1/2$, one obtains

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

which is another simple example of a mixed spectrum with pure point and absolutely continuous components.

An interesting deterministic counterpart is the *Rudin-Shapiro sequence* [26, 28, 25, 1]. Its quaternary version is usually defined by the substitution

$$\varrho = \varrho_{\text{RS}}: a \mapsto ac, b \mapsto dc, c \mapsto ab, d \mapsto db.$$

A fixed point $u = \varrho^2(u)$ can be constructed from the legal seed $b|a$ via iteration of ϱ^2 . The *binary* version follows then as the reduction $w = \varphi(u)$ with the mapping φ given by $\varphi(a) = \varphi(c) = 1$ and $\varphi(b) = \varphi(d) = -1$. The two-sided sequence w satisfies $w_{-1} = -1$ and $w_0 = 1$ together with the recursion

$$w(4n + \ell) = \begin{cases} w(n), & \text{for } \ell \in \{0, 1\}, \\ (-1)^{n+\ell} w(n), & \text{for } \ell \in \{2, 3\}, \end{cases} \quad (20)$$

for all $n \in \mathbb{Z}$. The sequence w and its hull once again define a strictly ergodic dynamical system, so that the natural autocorrelation γ_{RS} exists and is the same for all members of the hull. It is of the general form (2). To calculate it, one needs a little trick. Define the coefficients

$$\left. \begin{array}{l} \eta(m) \\ \vartheta(m) \end{array} \right\} := \lim_{N \rightarrow \infty} \frac{1}{2N + 1} \sum_{n=-N}^N w(n) w(n + m) \left\{ \begin{array}{l} 1 \\ (-1)^n \end{array} \right. \quad (21)$$

for $m \in \mathbb{Z}$. Note that all these limits exist, by Birkhoff's ergodic theorem (this is immediately clear for $\eta(m)$, but also follows for $\vartheta(m)$ on the basis of the quaternary sequence u , which also gives rise to a strictly ergodic system); compare [24] for an alternative approach.

It is easy to check that $\eta(0) = 1$ and $\vartheta(0) = 0$, while a slightly more involved calculation reveals the following coupled system of recursions,

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

together with

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

These equations are valid for all $m \in \mathbb{Z}$. Extracting $\vartheta(1) = \vartheta(-1) = 0$ from the last two equations (with $m = 0$ resp. $m = -1$), one can then recursively conclude that $\vartheta(m) = 0$ for all $m \in \mathbb{Z}$ and $\eta(m) = 0$ for all $m \neq 0$. This shows

$$\gamma_{\text{RS}} = \delta_0 \quad \text{and} \quad \widehat{\gamma}_{\text{RS}} = \lambda. \quad (22)$$

In particular, the (deterministic) diffraction (22) of the binary RS sequence is the same as the (almost sure) diffraction of the coin tossing sequence (19) for $p = 1/2$, despite the fact that their entropies are different (0 versus $\log(2)$); see [19, 6] for further details.

The situation is actually ‘worse’ in the following sense. Let $S \in \{\pm 1\}^{\mathbb{Z}}$ be a two-sided sequence, assumed ergodic, with associated Dirac comb $\omega_S = \sum_{n \in \mathbb{Z}} S_n \delta_n$ and autocorrelation γ_S . The latter exists due to the ergodicity assumption. Let $(W_n)_{n \in \mathbb{Z}}$ be the above family of i.i.d. random variables with values in $\{\pm 1\}$. Consider now the new random Dirac comb

$$\omega = \sum_{n \in \mathbb{Z}} S_n W_n \delta_n, \quad (23)$$

which we call the *Bernoullisation* of the original sequence. It can be considered as a ‘randomisation via second thoughts’, since the action of the W_n is to either keep S_n (with probability p) or to change its sign (with probability $1 - p$). By another (slightly more complicated) application of the SLLN, one finds [6]

$$\gamma = (2p - 1)^2 \gamma_S + 4p(1 - p) \delta_0 \quad (\text{a.s.}) \quad (24)$$

together with the corresponding almost sure diffraction $\widehat{\gamma} = (2p - 1)^2 \widehat{\gamma}_S + 4p(1 - p) \lambda$. If S is the binary RS sequence from above, one finds $\gamma = \delta_0$ and $\widehat{\gamma} = \lambda$, *independently* of the parameter p . This proves that the entire family defined by (23) for the RS sequence is homometric, with the entropy varying continuously between 0 and $\log(2)$; compare [7] for the connection between diffraction and entropy in the pure point case.

5. Outlook

The diffraction measure is a useful tool, both for the understanding of experiments and for various theoretical questions. Beyond the well-studied case of pure point spectra, also continuous spectra are explicitly accessible and sometimes (as above) even computable. However, as was to be expected, various aspects are more involved, and this includes the inverse problem. The latter is increasing in complexity also with growing dimension. For instance, the Ledrappier system [22] in the plane has the same autocorrelation as the Bernoulli comb (both living on \mathbb{Z}^2), but has rank-1 entropy despite being genuinely two-dimensional.

Various generalisations exist to non-lattice systems, which are best formulated via the theory of point processes [2]. Here, the classic Poisson process (of mean point density 1) is another example (with random positions) that gives diffraction measure λ when the points are randomly weighted with 1 and -1 . It is clear that higher order correlations can tell these systems apart, but many questions are still open.

Finally, more realistic models of randomness have to include interactions. The theory of Gibbs measures is a necessary and useful tool here, but only first steps in this direction have been taken; see [2] and references therein. Our present day understanding is still rather limited.

Acknowledgments

It is a pleasure to thank Shelomo I. Ben-Abraham, Daniel Lenz, Robert V. Moody and Tom Ward for various discussions. This work was supported by the German Research Council (DFG), within the CRC 701, by EPSRC, via Grant EP/D058465, and by a Leverhulme Trust Visiting Professorship Grant.

References

- [1] Allouche J-P and Shallit J 2003 *Automatic Sequences: Theory, Applications, Generalizations* (Cambridge: Cambridge University Press)
- [2] Baake M, Birkner M and Moody R V 2008 Diffraction of stochastic point sets: Explicitly computable examples *Preprint* arXiv:0803.1266
- [3] Baake M, Blomenkamp T, Gähler F and Grimm U 2009 A family of generalised Morse sequences with purely singular continuous diffraction (*in preparation*)
- [4] Baake M and Grimm U 2007 Homometric model sets and window covariograms *Z. Krist.* **222** 54–58
- [5] Baake M and Grimm U 2008 The singular continuous diffraction measure of the Thue-Morse chain *J. Phys. A: Math. Theor.* **41** 422001
- [6] Baake M and Grimm U 2009 Kinematic diffraction is insufficient to distinguish order from disorder *Phys. Rev. B* **79** 020203(R) and **80** 029903(E)
- [7] Baake M, Lenz D and Richard C 2007 Pure point diffraction implies zero entropy for Delone sets with uniform cluster frequencies *Lett. Math. Phys.* **82** 61–77
- [8] Baake M and Löwe M 2004 Comment on: Curious properties of simple random walks *J. Stat. Phys.* **116** 1449–1451
- [9] Baake M and Moody R V 2004 Weighted Dirac combs with pure point diffraction *J. reine angew. Math. (Crelle)* **573** 61–94
- [10] Baake M, Moody R V and Schlottmann M 1998 Limit-(quasi)periodic point sets as quasicrystals with p -adic internal spaces *J. Phys. A: Math. Gen.* **31** 5755–5765
- [11] Ben-Abraham S I 1993 Curious properties of simple random walks *J. Stat. Phys.* **73** 441–445
- [12] Cowley J M 1995 *Diffraction Physics* 3rd edition (Amsterdam: North-Holland)
- [13] Dekking F M 1978 The spectrum of dynamical systems arising from substitutions of constant length *Z. Wahrscheinlichkeitsth. verw. Geb.* **41** 221–239
- [14] Deng X and Moody R V 2009 How model sets can be determined by their two-point and three-point correlations *J. Stat. Phys.* (in press) (*Preprint* arXiv:0901.4381)
- [15] Deng X and Moody R V 2009 Weighted model sets and their higher point-correlations *Preprint* arXiv:0904.4552
- [16] Grimm U and Baake M 2008 Homometric point sets and inverse problems *Z. Krist.* **223** 777–781
- [17] Grünbaum F A and Moore C C 1995 The use of higher-order invariants in the determination of generalized Patterson cyclotomic sets *Acta Cryst. A* **51** 310–323
- [18] Hof A 1995 On diffraction by aperiodic structures *Commun. Math. Phys.* **169** 25–43
- [19] Höffe M and Baake M 2000 Surprises in diffuse scattering *Z. Krist.* **215** 441–444
- [20] Kakutani S 1972 Strictly ergodic symbolic dynamical systems *Proc. 6th Berkeley Symposium on Math. Statistics and Probability* ed L M LeCam L M, J Neyman and E L Scott (Berkeley: Univ. of California Press) pp 319–326
- [21] Keane M 1968 Generalized Morse sequences *Z. Wahrscheinlichkeitsth. Verw. Geb.* **10** 335–353
- [22] Ledrappier F 1978 Un champ markovien peut être d'entropie nulle et mélangeant *C. R. Acad. Sci. Paris Sér. A-B* **287** A561–A563
- [23] Mahler K 1927 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** 158–163
- [24] Pytheas Fogg N 2002 *Substitutions in Dynamics, Arithmetics and Combinatorics* LNM 1794 (Berlin: Springer)
- [25] Queffélec M 1987 *Substitution Dynamical Systems – Spectral Analysis* LNM 1294 (Berlin: Springer)
- [26] Rudin W 1959 Some theorems on Fourier coefficients *Proc. AMS* **10** 855–859
- [27] Schlottmann M 2000 Generalised model sets and dynamical systems *Directions in Mathematical Quasicrystals* CRM Monograph Series vol. 13, ed M Baake and R V Moody (Rhode Island: AMS) pp 143–159
- [28] Shapiro H S 1951 *Extremal Problems for Polynomials and Power Series* Masters Thesis (Boston: MIT)
- [29] Walters P 2000 *An Introduction to Ergodic Theory* reprint (New York: Springer)
- [30] Wiener N 1927 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** 145–157