Planar Dynamical Systems with Pure Lebesgue Diffraction Spectrum

Michael Baake · Tom Ward

Abstract We examine the diffraction properties of lattice dynamical systems of algebraic origin. It is well-known that diverse dynamical properties occur within this class. These include different orders of mixing (or higher-order correlations), the presence or absence of measure rigidity (restrictions on the set of possible shift-invariant ergodic measures to being those of algebraic origin), and different entropy ranks (which may be viewed as the maximal spatial dimension in which the system resembles an i.i.d. process). Despite these differences, it is shown that the resulting diffraction spectra are essentially indistinguishable, thus raising further difficulties for the inverse problem of structure determination from diffraction spectra. Some of them may be resolved on the level of higher-order correlation functions, which we also briefly compare.

Keywords Mathematical diffraction theory · Dynamical systems of algebraic origin · Pure Lebesgue spectrum

1 Introduction

The diffraction measure is a characteristic attribute of a translation bounded measure ω on Euclidean space (or on any locally compact Abelian group). It emerges as the Fourier transform $\widehat{\gamma}$ of the autocorrelation γ of ω, and has important applications in crystallography, because it describes the outcome of kinematic diffraction (from X-rays or neutron scattering, say [9]). 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

M. Baake (✉)
Fakultät für Mathematik, Universität Bielefeld, Postfach 100131, 33501 Bielefeld, Germany
e-mail: mbaake@math.uni-bielefeld.de

T. Ward
School of Mathematics, University of East Anglia, Norwich NR4 7TJ, UK
e-mail: t.ward@uea.ac.uk

point diffraction measure, meaning that $\widehat{\gamma}$ is a pure point measure, without any continuous component; see [6, 7, 12, 20] and references therein for details.

Clearly, reality is more complicated than that, in the sense that real world structures will (and do) show substantial continuous components in addition to the point part in their diffraction measure. Unfortunately, the methods around dynamical systems (in particular, the relations between dynamical and diffraction spectra) that are used to establish pure point spectra [5, 6, 20] and to explore some of the consequences [16] do not seem to extend to the treatment of systems with mixed spectrum [26], at least not in sufficient generality.

More recently, systems with continuous spectral components have been investigated also from a rigorous mathematical point of view (see [2] for a survey and references), with a number of unexpected results. In particular, the phenomenon of homometry (meaning the existence of different measures with the same autocorrelation) becomes more subtle. For example, on the basis of the autocorrelation alone, it is not possible to distinguish the Bernoulli comb (with completely positive entropy) from the deterministic Rudin–Shapiro comb (with zero entropy) [4, 13].

The purpose of this article is to show that, in higher dimensions, new phenomena emerge. In particular, one can have lattice systems of lower entropy rank that are again homometric to the Bernoulli system (of full entropy rank). Here, the entropy rank means the largest dimension for which the marginal of the invariant measure used has positive entropy. Paradigmatic is the Ledrappier shift, which will be one of our main examples, though we also discuss various extensions. We sum up with a sketch of a collection of systems with diverse dynamical properties that all have pure Lebesgue diffraction spectrum, which raises a number of interesting questions to follow up.

2 Ledrappier's Shift

Let x, y, z denote elements of $\mathbb{Z}^2$, and u, v, w elements of a subshift, which itself might be a group (for instance, w will often refer to a generic element in the Ledrappier system below). Let e_1 and e_2 denote the standard horizontal and vertical unit vectors in the Euclidean plane, and define

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

This defines a (closed) subshift, but also a closed Abelian subgroup (under pointwise multiplication) of the compact group $\{\pm 1\}^{\mathbb{Z}^2}$. The topology that $\mathbb{X}_{\mathrm{L}}$ inherits is the product topology, in which two points (or configurations) are close if they agree on a large neighbourhood of $0 \in \mathbb{Z}^2$. It is written multiplicatively here (in contrast to the additive notation in [15]) for reasons that will become clear shortly. We equip $\mathbb{X}_{\mathrm{L}}$ with its Haar measure μ_{L}, and denote the $\mathbb{Z}^2$ shift action by α, meaning that

$$\big(\alpha^z(w)\big)_x = w_{x+z}, \quad \text{for all } x, z \in \mathbb{Z}^2 \text{ and } w \in \mathbb{X}_{\mathrm{L}}.$$

This action is continuous (that is, for any $z \in \mathbb{Z}^2$, the map α^z is a homeomorphism) since, for any fixed $z \in \mathbb{Z}^2$, nearby configurations are shifted to nearby configurations by α^z. In this way, one obtains $(\mathbb{X}_{\mathrm{L}}, \mathbb{Z}^2)$ as a topological dynamical system.

Let us now take the measure μ_{L} into account (a remarkable feature of this system is that it has many invariant measures—see [10] for the details; we will only be interested in the

unique translation-invariant measure). The space $\mathbb{X}_L$ certainly contains some element v with value -1 at 0 (meaning that $v_0 = -1$). The group structure of $\mathbb{X}_L$ then implies that

$$\mu_L\{w \mid w_0 = 1\} = \mu_L\big(v \cdot \{w \mid w_0 = 1\}\big) = \mu_L\{w \mid w_0 = -1\},$$

since μ_L is the Haar measure, and hence invariant under multiplication by the element v. On the other hand, the whole group $\mathbb{X}_L$ is the disjoint union of the two cylinder sets $\{w \mid w_0 = 1\}$ and $\{w \mid w_0 = -1\}$, so that

$$\mu_L\{w \mid w_0 = 1\} = \mu_L\{w \mid w_0 = -1\} = \frac{1}{2}. \tag{2}$$

Similarly, one finds for the cylinder sets defined by the values ε at 0 and ε' at $x \neq 0$ that

$$\mu_L\big\{w \mid w_0 = \varepsilon, \, w_x = \varepsilon'\big\} = \frac{1}{4}, \tag{3}$$

for any choice of $\varepsilon, \varepsilon' \in \{\pm 1\}$. To see this, one observes that $\mathbb{X}_L$ certainly contains some element u that takes the values 1 at 0 and -1 at x, and another, v say, with the values at 0 and x interchanged. Using the group structure of $\mathbb{X}_L$ again, one can conclude that the four cylinder sets given by the choices for ε and ε' must have the same measure.

The shift action α preserves the Haar measure μ_L, and the $\mathbb{Z}^2$ measure-preserving dynamical system $(\mathbb{X}_L, \mu_L)$ was introduced by Ledrappier [15] to show that the (in general still open) Rokhlin problem, which asks if a mixing measure-preserving $\mathbb{Z}$-action must be mixing of all orders, has a negative answer for $\mathbb{Z}^2$. A discussion of this system in the context of Gibbs measures and extremality can be found in [25]. The system is easily shown to be mixing, and to have countable (dynamical) Lebesgue spectrum, but the following argument shows that it is *not* mixing of all orders. The relation (1) propagates to show that

$$w_x \, w_{x+2^n e_1} \, w_{x+2^n e_2} = 1$$

holds for all $n \geq 0$. Writing $A = \{w \mid w_0 = 1\}$, it follows that

$$\mu_L \left(A \cap \alpha^{(-2^n, 0)} A \cap \alpha^{(0, -2^n)} A \right) = \frac{1}{4}$$

for all $n \geq 0$, so that α is not mixing on triples of sets (or is not 3-mixing). Thus, as a two-dimensional system, there are correlations between arbitrarily distant triples of coordinates. In contrast to this, the one-dimensional subsystems (that is, the measure-preserving transformation α^z for any fixed $z \in \mathbb{Z}^2$) are all as chaotic as possible: each map α^z is measurably isomorphic to a Bernoulli shift (that is, to an i.i.d. process). This contrast between the properties of lower dimensional subsystems and the whole system is a characteristic feature of symbolic dynamics in higher dimensions.

3 Autocorrelation and Diffraction of Ergodic Subshifts

Since all initial measures that appear in this article are supported on the (planar) integer lattice, we formulate the main concepts and results for this (slightly simpler) case; for the general theory, we refer to [7, 12, 20]. Let $\mathbb{X} \subset \{\pm 1\}^{\mathbb{Z}^2}$ be a subshift (meaning a shift-invariant subset that is closed in the product topology) with an ergodic invariant probability

measure μ (more generally, we also consider any closed, shift-invariant subset of $(\mathbb{S}^1)^{\mathbb{Z}^2}$, where $\mathbb{S}^1 = \{z \in \mathbb{C} \mid |z| = 1\}$). Associate to each element $w \in \mathbb{X}$ a *Dirac comb* via

$$\omega = \omega_w := \sum_{x \in \mathbb{Z}^2} w_x \delta_x, \tag{4}$$

which is a translation bounded (and hence locally finite) measure on $\mathbb{Z}^2$. At the same time, it can be considered as a measure on $\mathbb{R}^2$ with support in $\mathbb{Z}^2$. We will use both pictures in parallel below, where measures (and their limits) are always looked at in the vague topology. We will formulate the diffraction spectrum starting from individual Dirac combs attached to elements of the shift space, rather than via the invariant measure on $\mathbb{X}$. This is motivated by the physical process of diffraction, which deals with a realisation of the process and not with the entire ensemble. For ergodic systems (such as those considered here), this makes (almost) no difference due to the ergodic theorem.

Let $C_N = [-N, N]^2$ be the closed, centred square of side length $2N$, and denote the restriction of ω to C_N by ω_N. The *natural autocorrelation measure*, or autocorrelation for short, is defined as the vague limit

$$\gamma = \gamma_\omega = \omega \circledast \widetilde{\omega} := \lim_{N \to \infty} \frac{\omega_N * \widetilde{\omega_N}}{\mathrm{vol}(C_N)}, \tag{5}$$

provided that the limit exists, where $\widetilde{\nu}$ is the 'flipped-over' measure defined by $\widetilde{\nu}(g) = \overline{\nu(\widetilde{g})}$ for arbitrary continuous functions g of compact support, and $\widetilde{g}(x) = \overline{g(-x)}$. Here and below, we use $\circledast$ for the volume weighted (or Eberlein) convolution.

When ω is a translation bounded measure, there is always at least one accumulation point, by [12, Proposition 2.2]. Much of what we say below remains valid for each such accumulation point individually. Here, we will only consider situations where the limit exists, at least almost surely in the probabilistic sense. If so, the autocorrelation is, by construction, a positive definite measure, and hence Fourier transformable [8, Sect. I.4]. The result, the *diffraction measure* $\widehat{\gamma}$, is a translation bounded, positive measure on $\mathbb{R}^2$ (by the Bochner-Schwartz theorem [8, Theorem 4.7]) with a unique Lebesgue decomposition

$$\widehat{\gamma} = (\widehat{\gamma})_{\mathrm{pp}} + (\widehat{\gamma})_{\mathrm{sc}} + (\widehat{\gamma})_{\mathrm{ac}} \tag{6}$$

into its pure point, singular continuous and absolutely continuous parts. The measure $\widehat{\gamma}$ describes the outcome of kinematic diffraction in crystallography and materials science [9, 12]. The pure point and absolutely continuous parts are often referred to as Bragg spectrum and diffuse scattering, respectively.

It is perhaps interesting to note that also singular continuous components show up quite frequently, see [28] for an overview, and indicate subtle aspects of long-range order that are far from being well understood. The mathematical paradigm in one spatial dimension is the classic Thue-Morse system, which was first analysed by Wiener and Mahler, see [3, 13] and references therein for details.

However, $\widehat{\gamma}$ is also an interesting mathematical object in its own right. It has only recently been properly appreciated in the mathematical community, due to its connection with dynamical systems theory; see [5, 6, 12, 20] and references therein for more.

Let us return to the autocorrelation γ of a measure ω that corresponds to a point $w \in \mathbb{X}_L$ as in (4). If it exists, a simple calculation shows that it must be a pure point measure of the form

$$\gamma = \sum_{z \in \mathbb{Z}^2} \eta(z) \delta_z, \tag{7}$$

where (with the cube C_n from above) the *autocorrelation coefficients* $\eta(z)$ are given by

$$\eta(z) = \lim_{N \to \infty} \frac{1}{|\mathbb{Z}^2 \cap C_N|} \sum_{x \in \mathbb{Z}^2 \cap C_N} \overline{w_x} w_{x+z}, \tag{8}$$

with $|A|$ denoting the cardinality of a (finite) set A. When one considers η as a function on $\mathbb{Z}^2$, it is again positive definite. There are several distinct ways to write $\eta(z)$ as a limit, which differ by 'boundary terms' that vanish in the limit as $N \to \infty$. We have chosen the most convenient for our purposes; see the detailed discussion in [12, 20] for more on this. For lattice systems, it is clear that the existence of the limit in (5) is equivalent to the (simultaneous) existence of the limits in (8) for all $z \in \mathbb{Z}^2$. We will use this equivalence many times below without further notice; see [16, Theorem 4] for a direct formulation in a more general setting.

A closer look at (8) reveals that $\eta(z)$ (which depends on w) can be seen as the orbit average of the function $h_z : \mathbb{X} \to \mathbb{C}$ defined by $h_z(w) = \overline{w_0} w_z$, which is continuous (and hence measurable) on $\mathbb{X}$. In the ergodic case, we thus have

$$\eta(z) = \mu(h_z) = \int_{\mathbb{X}} h_z(v) \, d\mu(v), \quad \text{for a.e. } w \in \mathbb{X}, \tag{9}$$

by an application of Birkhoff's ergodic theorem; see [27] or [14, Theorem 2.1.5] for a formulation of the case at hand (with $\mathbb{Z}^2$-action). Since $\mathbb{Z}^2$ is countable, we get the almost sure existence of all coefficients $\eta(z)$, and hence the almost sure existence of the autocorrelation γ in this case.

Before we continue, let us briefly explain how to treat Dirac combs for ergodic shifts with more general weights. When we use the (possibly complex) numbers $\phi_\pm$ instead of ± 1, the new Dirac comb attached to $w \in \mathbb{X}$ is

$$\omega_\phi = \frac{\phi_+ + \phi_-}{2} \delta_{\mathbb{Z}^2} + \frac{\phi_+ - \phi_-}{2} \omega,$$

with ω as in (4). Let us assume that the original weights are balanced, in the sense that the cylinder sets $\{w \mid w_0 = 1\}$ and $\{w \mid w_0 = -1\}$ have the same measure (as is the case for Ledrappier's shift). Ergodicity then tells us that, for almost all $w \in \mathbb{X}$,

$$\omega \circledast \delta_{\mathbb{Z}^2} = \delta_{\mathbb{Z}^2} \circledast \widetilde{\omega} = 0,$$

so that the new autocorrelation simply becomes

$$\gamma_\phi = \frac{|\phi_+ + \phi_-|^2}{4} \delta_{\mathbb{Z}^2} + \frac{|\phi_+ - \phi_-|^2}{4} \gamma,$$

where γ is the autocorrelation of ω. Recalling that Poisson's summation formula for lattice Dirac combs (compare [7] and references given there) gives the self-dual formula

$$\widehat{\delta_{\mathbb{Z}^2}} = \delta_{\mathbb{Z}^2}, \tag{10}$$

one finds the new diffraction measure as

$$\widehat{\gamma_\phi} = \frac{|\phi_+ + \phi_-|^2}{4} \delta_{\mathbb{Z}^2} + \frac{|\phi_+ - \phi_-|^2}{4} \widehat{\gamma}, \tag{11}$$

which is thus a mixture of a pure point measure with whatever $\widehat{\gamma}$ is. Note that the point measure $\delta_{\mathbb{Z}^2}$ is trivial (that is, carries no information about the system)—it only reflects the fact that the support of ω_ϕ is the integer lattice. This corresponds to the suspension of the dynamical system $(\mathbb{X}_L, \mathbb{Z}^2)$ into its continuous counterpart under the action of the group $\mathbb{R}^2$.

This observation is the reason why we prefer to work with balanced weights, and hence the motivation for our preference of the multiplicative formulation chosen above over the usual additive one. It is clear how to generalise this to other lattices and other types of shifts.

4 Diffraction of Bernoulli Combs

Here, we briefly summarise the known results on the autocorrelation and diffraction of multi-dimensional Bernoulli systems, which includes (fair) coin tossing as a special case. Let $(W_x)_{x \in \mathbb{Z}^2}$ be a family of i.i.d. random variables with values in $\mathbb{S}^1$, common law ν and representing random variable W. This defines a Bernoulli shift on $\mathbb{Z}^2$, which is known to be ergodic (in fact, mixing of all orders).

Consider now the Dirac comb $\sum_{x \in \mathbb{Z}^2} W_x \delta_x$, which is a random measure on $\mathbb{Z}^2$, or on $\mathbb{R}^2$ with support $\mathbb{Z}^2$. The autocorrelation coefficients are given by $\eta(0) = 1$ together with $\eta(z) = |\mathbb{E}_\nu(W)|^2$ (a.s.) for all $z \neq 0$. This result can also be derived by an application of the strong law of large numbers (SLLN), which permits a significant generalisation to non-lattice systems; see [2] and references therein for more. Also, the weaker notion of pairwise independence is then sufficient, due to Etemadi's version [11] of the SLLN. A systematic way to write the result is

$$\eta(z) = \left|\mathbb{E}_\nu(W)\right|^2 + \left(\mathbb{E}_\nu\left(|W|^2\right) - \left|\mathbb{E}_\nu(W)\right|^2\right)\delta_{z,0} \quad \text{(a.s.)}. \tag{12}$$

This formulation remains valid even if we allow for more general random variables. The following result is now straight-forward.

Theorem 1 *Let $(W_x)_{x \in \mathbb{Z}^2}$ be a family of i.i.d. random variables with values in $\mathbb{S}^1$ and common law ν. The associated random Dirac comb $\omega = \sum_{x \in \mathbb{Z}^2} W_x \delta_x$ almost surely has the autocorrelation and diffraction measures*

$$\gamma = \left|\mathbb{E}_\nu(W)\right|^2 \delta_{\mathbb{Z}^2} + \mathrm{cov}(W)\delta_0 \quad and \quad \widehat{\gamma} = \left|\mathbb{E}_\nu(W)\right|^2 \delta_{\mathbb{Z}^2} + \mathrm{cov}(W)\lambda,$$

where λ is Lebesgue measure and $\mathrm{cov}(W) := \mathbb{E}_\nu(|W|^2) - |\mathbb{E}_\nu(W)|^2$ the covariance of W.

Proof The structure of the (countably many) autocorrelation coefficients explained above gives the almost sure form of γ by a simple calculation. Its Fourier transform exists, and has the claimed form due to $\widehat{\delta_0} = \lambda$ and the Poisson summation formula for lattice Dirac combs (10) mentioned above. □

Theorem 1 has an interesting special case that includes the (fair) coin tossing sequence and makes use of the fact that $\mathbb{E}_\nu(|W|^2) = 1$ for random variables with values in $\mathbb{S}^1$.

Corollary 2 *Consider the situation of Theorem 1 under the additional assumption that $\mathbb{E}_\nu(W) = 0$. Then, the autocorrelation and diffraction measures simplify to*

$$\gamma = \delta_0 \quad and \quad \widehat{\gamma} = \lambda,$$

again almost surely as before. □

The underlying two-dimensional Bernoulli shift has positive entropy, for instance $\log(2)$ when W takes values ± 1 with equal probability. It has long been known, due to work by Rudin and Shapiro [17, 24], that one can also construct a deterministic sequence (with zero entropy) with the same autocorrelation and diffraction [13]. Though the original construction was for $\mathbb{Z}$, it has an immediate generalisation to $\mathbb{Z}^2$ (and to $\mathbb{Z}^d$ as well), see [13] for details. Moreover, one can modify the system (by 'Bernoullisation' [4]) to construct an isospectral transition from the deterministic case to the Bernoulli system with continuously varying entropy [4]. This does not yet explore the full scenario of $\mathbb{Z}^2$ shifts though. In particular, we now have the possibility of genuinely two-dimensional systems (by which we mean to exclude simple Cartesian products) with entropy of rank 1.

5 Autocorrelation and Diffraction of Ledrappier's Shift

Consider the measure dynamical system $(\mathbb{X}_L, \mathbb{Z}^2, \mu_L)$ as introduced in Sect. 2. To any $w \in \mathbb{X}_L$, we attach the Dirac comb as defined in (4) and consider its autocorrelation.

Lemma 3 *Let $w \in \mathbb{X}_L$ and ω as in* (4). *The corresponding autocorrelation coefficients satisfy $\eta_L(0) = 1$ and, μ_L-almost surely, $\eta_L(z) = 0$ for all $0 \neq z \in \mathbb{Z}^2$.*

Proof The identity $\eta_L(0) = 1$ clearly holds for all $w \in \mathbb{X}_L$. Let now $z \in \mathbb{Z}^2 \setminus \{0\}$ be fixed. Ledrappier's shift is ergodic (indeed, is mixing; see [15] or [21] for details), so that we can employ Birkhoff's theorem as outlined above. This gives, μ_L-almost surely,

$$\eta_L(z) = \mu_L(h_z) = \sum_{\varepsilon, \varepsilon' \in \{\pm 1\}} \varepsilon \varepsilon' \cdot \mu_L \{ w \in \mathbb{X}_L \mid w_0 = \varepsilon, w_{-z} = \varepsilon' \} = 0,$$

because all cylinder sets under the sum have equal measure $1/4$ by (3). Since there are countably many such coefficients, the claim follows. □

A simple calculation now gives the following result.

Theorem 4 *Let w be any element of the Ledrappier shift, in its multiplicative formulation used above, and let ω be the attached Dirac comb of* (4). *Then, μ_L-almost surely,*

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

are the corresponding autocorrelation and diffraction measures. □

This means that the Bernoulli shift and the Ledrappier shift are homometric, despite the fact that the latter has zero two-dimensional entropy with complete correlations between coordinates 0, $2^n e_1$ and $2^n e_2$ for any $n \geq 0$ as explained earlier. The Bernoulli shift has vanishing 3-point correlation here, and thus differs.

As mentioned above, there are *many* other invariant measures on $\mathbb{X}_L$ by [10], including ones with any given entropy for α^{e_1} (it is not entirely clear what further entropy or correlation conditions would constrain the possible invariant measures to be Haar measure; Schmidt [22] has partial results relating the absence of higher-order correlations to measure rigidity for systems like $\mathbb{X}_L$).

Also, μ_L can be viewed as an ergodic measure on the full shift that is concentrated on $\mathbb{X}_L$. As such, it is mutually singular with the Bernoulli (or i.i.d.) measure.

Remark 1 (Extension of Theorem 4) A similar argument applies to a whole class of systems which may be constructed as follows. Take any prime ideal $P \subset R_d = \mathbb{Z}[x_1^{\pm 1}, \ldots, x_d^{\pm 1}]$ with the following properties:

- P contains a prime p (this makes the system a closed subshift of finite type inside the full d-dimensional p-shift, and in particular disconnected);
- $P \cap \{x_1^{a_1} \cdots x_d^{a_d} - 1 \mid (a_1, \ldots, a_d) \in \mathbb{Z}^d\} = \{0\}$, so the corresponding system is mixing;
- the Krull dimension[1] of R_d/P is k with $1 \leq k \leq d$.

Then, a similar conclusion holds for generic points in the corresponding $\mathbb{Z}^d$-action. Later, we will also see an extension to connected examples (with continuous local degree of freedom).

6 Correlation Functions

So far, we have concentrated on the autocorrelation measure, because its knowledge immediately gives the diffraction measure via the Fourier transform. The coefficients $\eta(m)$ can be seen as volume averaged two-point correlations, and it is natural to also consider other correlation functions. To this end, we define the n-point correlation

$$\langle z_1, \ldots, z_n \rangle(w) := \lim_{N \to \infty} \frac{1}{|\mathbb{Z}^2 \cap C_N|} \sum_{x \in \mathbb{Z}^2 \cap C_N} w_{x+z_1} \cdots w_{x+z_n} \tag{13}$$

for any fixed $w \in \mathbb{X}$ and $n \in \mathbb{N}$, where all $z_i \in \mathbb{Z}^2$. We only consider situations where the limit exists, which is (a.s.) the case when $\mathbb{X}$ is an ergodic subshift. Then, the ergodic theorem implies that

$$\langle z_1, \ldots, z_n \rangle(w) = \int_{\mathbb{X}} v_{z_1} \cdots v_{z_n} \, d\mu(v) \tag{14}$$

holds for almost every w, which also explains why we simply write $\langle z_1, \ldots, z_n \rangle$ from now on. It is clear that the n-point correlations are translation invariant in the sense that

$$\langle z_1, \ldots, z_n \rangle = \langle x + z_1, \ldots, x + z_n \rangle$$

holds for all $x \in \mathbb{Z}^2$.

Remark 2 In this new notation, we find $\eta(z) = \langle 0, z \rangle$ for $z \in \mathbb{Z}^2$, both for the Bernoulli (B) and the Ledrappier (L) shift, because all weights are real. On the other hand, we find $\langle z_1, z_2 \rangle_B = 0$ for any $z_1 \neq z_2$, hence also $\langle 0, z_1, z_2 \rangle_B = 0$, while we earlier observed that $\langle 0, 2^n e_1, 2^n e_2 \rangle_L = 1$ for all $n \geq 0$, which expresses the difference between the two shifts on the level of three-point correlations.

Since we also want to consider $\mathbb{S}^1$ as the local degree of freedom, we need complex correlation functions as well. Here, we write z_i^* on the lefthand side of (13) to indicate the factor $\overline{w_{x+z_i}}$ on the right. The almost sure validity of (14) extends to this more general

---

[1]This is calculated as $(d+1)$ minus the number of independent generators of P. If the Krull dimension is d, the system is the full d-dimensional i.i.d. shift on p symbols, since $P = pR_d$ is then the only possibility; as k decreases, the entropy rank gets smaller until one gets down to examples like Ledrappier's shift with $k = 1$. There, each single element is measurably isomorphic to a finite-entropy i.i.d. process.

setting in an obvious way. Now, the relation between autocorrelation coefficients and 2-point correlations is given by

$$\eta(z) = \langle 0^*, z \rangle = \langle 0, -z^* \rangle,$$

where we have used the translation invariance. The following result is immediate.

Lemma 5 *Let* $(W_x)_{x \in \mathbb{Z}^2}$ *be an i.i.d. family of random variables, represented by* V *with values in* $\mathbb{S}^1$ *and law* ν. *Assume that* V *has zero mean,* $\mathbb{E}_\nu(V) = 0$. *When* $z_1, \ldots, z_n \in \mathbb{Z}^2$ *are distinct, one almost surely has*

$$\langle z_1, \ldots, z_n \rangle = 0.$$

This relation also holds for the complex correlations, as long as the z_i *are distinct.*

Proof The corresponding Bernoulli system is mixing, hence ergodic. Equation (14) results in a factorisation of the righthand side. One obtains n factors, each of which (due to the i.i.d. nature of the W_{z_i}) is an integral of the form

$$\int_{\mathbb{S}^1} v \, d\nu(v) = \mathbb{E}_\nu(V) = 0,$$

so that the entire correlation function also vanishes.

In the case of complex correlations, as long as the z_i are distinct, each factor is either of this form or its complex conjugate, with the same conclusion. □

It is clear how one can generalise this result to also include powers, where one then needs further assumptions on higher moments of the law ν. Let us state one version that will become relevant below. To do so, we need a slightly more general notation for the mixture of moments and correlations. We write $\langle \ldots, (z_i, m_i), \ldots \rangle$ for the correlation function where we take the ith factor as $W_{x+z_i}^{m_i}$ in the orbit average, with $m_i \in \mathbb{Z}$ arbitrary. Since we work on $\mathbb{S}^1$, this includes complex conjugation via $m_i = -1$.

Proposition 6 *Consider the full shift on* $\mathbb{X} = (\mathbb{S}^1)^{\mathbb{Z}^2}$, *with the invariant measure* μ *that is constructed from the uniform distribution on* $\mathbb{S}^1$ *via the Bernoulli (or i.i.d.) process. Then, the generalised correlations* $\langle (z_1, m_1), \ldots, (z_n, m_n) \rangle$ *with* $n \in \mathbb{N}$ *and distinct* $z_i \in \mathbb{Z}^2$ *almost surely exist. In particular, they all vanish, unless* $m_1 = \cdots = m_n = 0$, *when they are* 1.

Proof The Bernoulli measure μ is ergodic, so that the almost sure existence claim is clear. By the ergodic theorem together with the i.i.d. property, one finds

$$\langle (z_1, m_1), \ldots, (z_n, m_n) \rangle = \prod_{j=1}^n \int_{\mathbb{X}} w_{z_j}^{m_j} \, d\mu(w) = \prod_{j=1}^n \int_0^1 e^{2\pi i m_j y} \, dy,$$

where the last step is just one way to write down the uniform distribution at (any) one site. Our claim is now obvious. □

7 The (×2, ×3)-shift

A related example, with continuous site space $\mathbb{S}^1$, is the following. Define

$$\mathbb{X}_{\mathrm{F}} = \left\{ w \in (\mathbb{S}^1)^{\mathbb{Z}^2} \mid w_{z+e_1} = w_z^2, \, w_{z+e_2} = w_z^3 \text{ for all } z \in \mathbb{Z}^2 \right\}$$

(that is, the $(\times 2, \times 3)$-shift [18] written multiplicatively, with ergodic invariant measure μ_F). Then, we may consider the complex-valued Dirac comb

$$\omega = \omega_w = \sum_{x \in \mathbb{Z}^2} w_x \delta_x. \tag{15}$$

As before, using the ergodic theorem, we see that the autocorrelation coefficients $\eta(z) = \langle 0^*, z \rangle$ almost surely exist, and that their calculation reduces to computing an integral over $\mathbb{X}_F$.

Theorem 7 *Let w be any element of the $(\times 2, \times 3)$-shift, in its multiplicative formulation used above, and let ω be the attached Dirac comb of* (15). *Then, μ_F-almost surely,*

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

are the corresponding autocorrelation and diffraction measures.

Proof The almost sure existence of γ follows from that of the countably many coefficients $\eta(z)$ with $z \in \mathbb{Z}^2$. To show the main claim, we need to show the almost sure validity of $\eta(z) = \delta_{z,0}$. Since $\eta(-z) = \overline{\eta(z)}$ by the positive definiteness of η as a function on $\mathbb{Z}^2$, it suffices to consider $z = m e_1 + n e_2$ with $m \geq 0$ and $n \in \mathbb{Z}$.

Observe that we have

$$\eta(z) = \lim_{N \to \infty} \frac{1}{|\mathbb{Z}^2 \cap C_N|} \sum_{x \in \mathbb{Z}^2 \cap C_N} \overline{w_x} w_{x+z},$$

and consider the case with $n \geq 0$ first. The rule for the translation action on $\mathbb{X}_F$ implies that

$$w_{x+z} = (w_x)^{2^m 3^n},$$

so that $\eta(z)$ can be viewed (as $w_x \in \mathbb{S}^1$) as an orbit average of $(w_x)^{2^m 3^n - 1}$, with the almost sure limit

$$\int_{\mathbb{X}_F} (w_0)^{2^m 3^n - 1} \, \mathrm{d}\mu_F(w) = \int_0^1 \exp\left(2\pi i (2^m 3^n - 1) x\right) \mathrm{d}x = \begin{cases} 1, & \text{if } m = n = 0, \\ 0, & \text{otherwise,} \end{cases}$$

where $m = n = 0$ means $z = 0$. Here, the first equality uses the fact that the invariant measure μ_F reduces to the uniform distribution on $\mathbb{S}^1$ when marginalised on all sites but one.

Similarly, when $m \geq 0$ with $n < 0$, we set $y = x - |n| e_2$, so that $\overline{w_x} = (\overline{w_y})^{3^{|n|}}$ and $w_{x+z} = (w_y)^{2^m}$, whence $\eta(z)$ is now an orbit average of $(w_y)^{2^m - 3^{|n|}}$, hence almost surely given by the integral

$$\int_0^1 \exp\left(2\pi i (2^m - 3^{|n|}) x\right) \mathrm{d}x$$

which always vanishes, as $n < 0$ was assumed.

Putting the arguments together indeed (almost surely) results in $\eta(z) = \delta_{z,0}$, hence $\gamma = \delta_0$ and $\widehat{\gamma} = \lambda$ as claimed. □

Quite remarkably, the similarities between the Bernoulli shift $(\mathbb{S}^1)^{\mathbb{Z}^2}$ and the $(\times 2, \times 3)$-shift go a lot further.

Theorem 8 *Consider the* $(\times 2, \times 3)$*-shift in its multiplicative version as used above, with invariant measure* μ_F. *If* $z_1, \ldots, z_n$ *are* n *arbitrary points of the lattice* $\mathbb{Z}^2$, *we almost surely have* $\langle z_1, \ldots, z_n \rangle_F = 0$. *More generally, with* $z_j = k_j e_1 + \ell_j e_2$, *one almost surely obtains*

$$\big\langle (z_1, m_1), \ldots, (z_n, m_n) \big\rangle_F = \begin{cases} 1, & \text{if } \sum_{j=1}^n m_j 2^{k_j} 3^{\ell_j} = 0, \\ 0, & \text{otherwise,} \end{cases}$$

for the generalised correlation coefficients.

Proof To calculate the generalised correlation coefficients, we need a variant of the trick used in Theorem 7. Given $z_1, \ldots, z_n$ with coordinates as stated, define $y = k e_1 + \ell e_2$ with $k = \min_i k_i$ and $\ell = \min_i \ell_i$, so that y is the lower left corner of the smallest lattice square (with edges parallel to e_1 and e_2) that contains all the z_i. One can now check that

$$\big\langle (z_1, m_1), \ldots, (z_n, m_n) \big\rangle_F$$

$$= \lim_{N \to \infty} \frac{1}{|\mathbb{Z}^2 \cap C_N|} \sum_{x \in \mathbb{Z}^2 \cap C_N} \prod_{j=1}^n (w_{x+y})^{m_j 2^{k_j - k} 3^{\ell_j - \ell}}$$

$$= \int_{\mathbb{X}_F} (w_y)^{\sum_{j=1}^n m_j 2^{k_j - k} 3^{\ell_j - \ell}} \, \mathrm{d}\mu_F(w) = \int_0^1 e^{2\pi i \sum_{j=1}^n m_j (2^{k_j - k} 3^{\ell_j - \ell}) t} \, \mathrm{d}t,$$

where the second last step holds (almost surely) by the ergodic theorem, while the last results from the appropriate marginalisation of the measure μ_F, as before.

For the first claim, all $m_i = 1$, so that the exponent under the integral is of the form $2\pi i N t$ with N a positive integer, wherefore the integral vanishes. More generally, since $N = \sum_{j=1}^n m_j (2^{k_j - k} 3^{\ell_j - \ell})$ is always an integer by construction, the integral vanishes unless $N = 0$, where it is 1. This happens precisely when $\sum_{j=1}^n m_j 2^{k_j} 3^{\ell_j} = 0$. $\square$

Remark 3 In comparison, we have the somewhat surprising situation that the full two-dimensional Bernoulli shift $(\mathbb{S}^1)^{\mathbb{Z}^2}$ and the $(\times 2, \times 3)$-shift are more or less indistinguishable by correlation functions. There are differences though, such as the relation

$$\big\langle ((0, 1), -2), ((1, 1), 1) \big\rangle_F = 1,$$

which rests on the identity $-2 \cdot 2^0 3^1 + 1 \cdot 2^1 3^1 = 0$, whereas the corresponding correlations for functions determined by distinct single coordinates in the Bernoulli shift always vanish. The condition $\sum_{j=1}^n m_j 2^{k_j} 3^{\ell_j} = 0$ appearing in Theorem 8 corresponds to a correlation between the characters (that is, functions) defined by the pairs (z_i, m_i), where (z, m) defines the character that takes the value $\exp(2\pi i m w_z)$ on the point $w = (w_z) \in \mathbb{X}_F$. The deep S-unit theorem of Schlickewei [19] shows that this condition will only be achieved in an essential way (that is, without a shorter vanishing sum) finitely often, and this Diophantine result is equivalent to the system being mixing of all orders by [23].

Clearly, the $(\times 2, \times 3)$-shift is a nullset for the Bernoulli measure, but the support of the invariant measure is not something that is usually known at the beginning of the inference problem, so that this result is further 'bad news' for the inverse problem of structure determination.

Table 1 Basic information and comments on some of the systems discussed

	Rudin-Shapiro	Ledrappier	$(\times 2, \times 3)$	2-dim. i.i.d.
$\mathbb{Z}^2$ entropy	0	0	0	>0
entropy rank	0	1	1	2
mixing of all orders?	No	No	Yes	Yes
many inv. measures?	No	Yes	No	Yes
pure Lebesgue diffr.?	Yes	Yes	Yes	Yes

Remark 4 The way in which correlations between characters (or between trigonometric polynomials) on $\mathbb{X}_F$ vanish may be viewed as a form of multiple m-dependence in the sense of [1]. For a given collection of trigonometric polynomials, the determination of a minimal value of m is a rather subtle Diophantine problem, but as indicated in Remark 3, such an m will always exist.

Remark 5 In contrast to the Ledrappier shift from Sect. 2, the $(\times 2, \times 3)$-system has few invariant measures in the following sense. If m is an ergodic invariant probability measure that gives some $z \in \mathbb{Z}^2$ positive entropy, then m must be the Haar measure by a result of Rudolph [18].

The two systems $\mathbb{X}_L$ and $\mathbb{X}_F$ have interesting overall properties as follows; in particular, in terms of having invariant measures, $\mathbb{X}_L$ is closer to i.i.d. than $\mathbb{X}_F$, while $\mathbb{X}_F$ is closer in terms of mixing. Some of the properties are summarised in Table 1.

8 Further Remarks and Outlook

Above, we have concentrated on systems that are supported on $\mathbb{Z}^2$. When one lifts this restriction, one naturally enters the realm of point process theory. An interesting example there is provided by the classic Poisson process and its many siblings. Starting from a homogeneous and stationary Poisson process of (point) density 1, and turning it into a marked point process by adding weights ± 1 with equal probability to the points of any given realisation, produces a randomly weighted point set with (almost sure) autocorrelation δ_0 and diffraction λ; see [2] for a proof and further details and examples.

It is well-known that lattice dynamical systems of algebraic origin are spectrally indistinguishable (at least once they are mixing) in the sense that they all have countable Lebesgue dynamical spectrum. Above, we saw that they also have an absolutely continuous diffraction spectrum. While the connection between dynamical and diffraction spectra is well understood for the pure point case (see [5] and references therein), this is not so in general (as follows from [26] by way of counterexample). However, the existing body of examples seems to indicate that for systems with pure Lebesgue spectrum, perhaps under some mild additional condition, there is again a closer connection between these two types of spectra, and it would be nice to understand this better.

References

1. Aaronson, J., Gilat, D., Keane, M., de Valk, V.: An algebraic construction of a class of one-dependent processes. Ann. Probab. **17**, 128–143 (1989)
2. Baake, M., Birkner, M., Mooody, R.V.: Diffraction of stochastic point sets: Explicitly computable examples. Commun. Math. Phys. **293**, 611–660 (2009). arXiv:0803.1266
3. Baake, M., Grimm, U.: The singular continuous diffraction measure of the Thue-Morse chain. J. Phys. A: Math. Theor. **41**, 422001 (2008). arXiv:0809.0580
4. Baake, M., Grimm, U.: Kinematic diffraction is insufficient to distinguish order from disorder. Phys. Rev. B **79**, 020203(R) (2009) and **80**, 029903(E) (2009). arXiv:0810.5750
5. Baake, M., Lenz, D.: Dynamical systems on translation bounded measures: Pure point dynamical and diffraction spectra. Ergod. Theory Dyn. Syst. **24**, 1867–1893 (2004). math.DS/0302231
6. Baake, M., Lenz, D., Moody, R.V.: Characterization of model sets by dynamical systems. Ergod. Theory Dyn. Syst. **27**, 341–382 (2007). arXiv:math/0511648
7. Baake, M., Moody, R.V.: Weighted Dirac combs with pure point diffraction. J. Reine Angew. Math. (Crelle) **573**, 61–94 (2004). arXiv:math.MG/0203030
8. Berg, C., Forst, G.: Potential Theory on Locally Compact Abelian Groups. Springer, Berlin (1975)
9. Cowley, J.M.: Diffraction Physics, 3rd edn. North-Holland, Amsterdam (1995)
10. Einsiedler, M.: Invariant subsets and invariant measures for irreducible actions on zero-dimensional groups. Bull. Lond. Math. Soc. **36**, 321–331 (2004)
11. Etemadi, N.: An elementary proof of the strong law of large numbers. Z. Wahrsch. Verw. Geb. **55**, 119–122 (1981)
12. Hof, A.: On diffraction by aperiodic structures. Commun. Math. Phys. **169**, 25–43 (1995)
13. Höffe, M., Baake, M.: Surprises in diffuse scattering. Z. Kristallogr. **215**, 441–444 (2000). arXiv:math-ph/0004022
14. Keller, G.: Equilibrium States in Ergodic Theory. LMSST, vol. 42. Cambridge University Press, Cambridge (1998)
15. Ledrappier, F.: Un champ markovien peut être d'entropie nulle et mélangeant. C. R. Acad. Sci. Paris Sér. A-B **287**, A561–A563 (1978)
16. Lenz, D.: Continuity of eigenfunctions of uniquely ergodic dynamical systems and intensity of Bragg peaks. Commun. Math. Phys. **287**, 225–258 (2009). arXiv:math-ph/0608026
17. Rudin, W.: Some theorems on Fourier coefficients. Proc. AMS **10**, 855–859 (1959)
18. Rudolph, D.J.: $\times 2$ and $\times 3$ invariant measures and entropy. Ergod. Theory Dyn. Syst. **10**, 395–406 (1990)
19. Schlickewei, H.P.: S-unit equations over number fields. Invent. Math. **102**, 95–107 (1990)
20. Schlottmann, M.: Generalised model sets and dynamical systems. In: Baake, M., Moody, R.V. (eds.) Directions in Mathematical Quasicrystals. CRM Monograph Series, vol. 13, pp. 143–159. AMS, Providence (2000)
21. Schmidt, K.: Automorphisms of compact Abelian groups and affine varieties. Proc. Lond. Math. Soc. **61**(3), 480–496 (1990)
22. Schmidt, K.: Invariant measures for certain expansive $\mathbb{Z}^2$-actions. Isr. J. Math. **90**, 295–300 (1995)
23. Schmidt, K., Ward, T.: Mixing automorphisms of compact groups and a theorem of Schlickewei. Invent. Math. **111**, 69–76 (1993)
24. Shapiro, H.: Extremal Problems for Polynomials and Power Series. Masters Thesis, MIT, Boston (1951)
25. Slawny, J.: Ergodic properties of equilibrium states. Commun. Math. Phys. **80**, 477–483 (1981)
26. van Enter, A.C.D., Miękisz, J.: How should one define a (weak) crystal? J. Stat. Phys. **66**, 1147–1153 (1992)
27. Walters, P.: An Introduction to Ergodic Theory. Springer, New York (2000), reprint
28. Withers, R.L.: Disorder, structured diffuse scattering and the transmission electron microscope. Z. Kristallogr. **220**, 1027–1034 (2005)