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Diffractive point sets with entropy*

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Abstract. After a brief historical survey, this paper introduces the notion of entropic model sets (cut and project sets), and, more generally, the notion of diffractive point sets with entropy. Such sets may be thought of as generalizations of lattice gases. We show that taking the site occupation of a model set stochastically results, with probabilistic certainty, in well-defined diffractive properties augmented by a constant diffuse background. We discuss both the case of independent, but identically distributed (i.i.d.) random variables and that of independent, but different (i.e. site dependent) random variables. Several examples are shown.

1. Introduction

Diffraction is one of the most important ways of identifying long-range order in mathematical and physical structures. In this paper, we look at the effects on diffraction that occur in certain periodic and quasiperiodic point sets when the occupation of the point sites is taken stochastically rather than deterministically, with independence between the different sites. Under fairly mild assumptions, which are certainly valid for lattices and model sets, we show that the effect is simply one of scaling down the diffraction pattern by a constant factor and adding in a constant background. In the case of lattices, this type of phenomenon is well known [9, 39]. What is new here is that it remains true for a large class of non-periodic structures (theorems 1 and 2) and, in particular, for all regular model sets (also called cut-and-project sets).

The results are, on the one hand, a suitable reminder of the difficulty of interpreting the meaning of diffractivity, and, on the other hand, of the robustness of diffractivity under certain deformations and modifications of the underlying set.

It might be interesting to quickly review the history of aperiodic order and take a look at the reasons why stochastic forms of aperiodic structures seem to be a natural extension beyond the world of strict perfection. In the early 1980s, a new type of ordered state was found, both experimentally [31, 14] and theoretically [18, 19]. These discoveries, made independently of one another, created an enormous amount of scientific activity because the new ordered states, quickly dubbed quasicrystals, had properties previously thought to be incompatible with one another; namely, long-range orientational order, strong enough to produce sharp diffraction images, and at the same time non-crystallographic symmetries such as icosahedral [31, 19] or twelfefold symmetry [14].

* Dedicated to Hans-Ude Nissen on the occasion of his 65th birthday.

Since nothing has ever been discovered for the first time, one might expect precursors of this, and this is indeed correct. Clearly, Penrose's famous tiling of the plane with fivefold symmetry was important, particularly when coupled with de Bruijn's algebraic analysis that showed that it was also diffractive[†]. Ammann investigated this further and also found the matching icosahedral tiling made from two rhombohedra. However, this was not generally known in the physics community (a brief remark can be found in [23]), and has never been published by him. Even his planar results were published only much later [1], though some results are contained in [10].

In fact, the history goes back quite a bit before this. In the late 1930s of this century, Kowalewski [17] investigated the possibilities of filling Kepler's triacontahedron with the two rhombohedra mentioned above, but apparently did not realize the possibility of filling the entire space with them.

Kepler himself was very much interested in space fillings in his time, and his famous plate of planar tilings (resp. seeds of them) shows a considerable patch of a tiling with pentagons, decagons and rhombi, see the first plate in [10]. In modern terminology [7], this would be in the same MLD class as the famous Penrose tiling, in the sense that there is a derivation rule with a radius much smaller than the patch shown such that, on the size displayed, there is no way to tell the two tilings apart. This is probably not an accident because Kepler was well aware of the problems of space fillings, as were other people before him, such as Dürer who constructed a mechanism to create a fivefold twin made from pentagons and rhombi. Generally, the investigation of geometric form was well on the way. Dürer's polyhedron in his 'melancholia' has puzzled generations of scientists and art historians—with a really promising solution being found only very recently by Hans-Ude Nissen [26].

The development of the theory of incommensurate structures by the Nijmegen group and the new developments in the theory of quasicrystals showed that there is a lot more to the geometry and symmetry of the solid state than anticipated by ordinary school knowledge. Probably the most puzzling aspect in the beginning was the combination of perfect diffractivity (in the sense of a Bragg spectrum) with non-crystallographic symmetry. But again, the final explanation, in terms of the projection method [19], had a precursor, this time in pure mathematics.

Harald Bohr, the younger brother of Niels, developed the theory of quasi- and almost periodic functions in the 1920s. The basic idea was to describe non- but quasi-periodic functions as sections through periodic functions in higher dimensions. In this sense, the cut-and-project method owes a lot to his ideas. In the late 1960s, Yves Meyer studied the harmonic analysis of point sets in the context of algebraic numbers. In the process he rediscovered cut-and-project sets (here called *model sets*), though now in the much wider setting of locally compact Abelian groups, and introduced a very important class of ordered point sets, now called Meyer sets [24] (see later for one characterization of Meyer sets).

After this historically motivated introduction, let us come to the aim of this article. Although all the above mentioned connections might indicate that the (quasi-) crystalline world is perfect, in the sense that the alloys displaying such diffraction images are, reality tells us nowadays that this is not so [27, 16]. In fact, quite early on it was pointed out by Elser that, in order to explain the stability of such alloys, one might need an *entropic* side of the picture, an idea that led the Cornell group to develop the idea of a random tiling. From a more mathematical point of view, this is not fully satisfactory because quite a number of questions concerning the diffractivity, and even the well-definedness of some

[†] If not explicitly specified, the proper references are obvious by the names given, and can be found in [38].

of the ensembles, are still unanswered.

This is the point we want to consider and start to develop. However, we will not adopt the random tiling picture here, because it seems not yet fully in reach for a rigorous treatment (cf [29] and references therein for some recent developments). Instead, as an intermediate step, we shall rather consider a set-up of ideal *model sets*, or even more general diffractive point sets, that are coupled to stochastic processes to thin them out. This way, we can introduce some randomness into the picture, even with positive entropy density, without losing control of the diffractivity. This can be seen as a generalization of the diffraction theory of lattice gases which belongs to the standard body of literature, see [11, 9, 39] and references therein.

In doing so, we will actually arrive at results that exactly meet the expectation, but with the extra benefit of providing proofs for them, i.e. making a good deal of folklore rigorous in this way. It will turn out that there is a *natural* extension of the diffraction theory of lattices gases beyond lattices, *provided* one uses an approach that avoids techniques based upon translation invariance. Although the actual methods and results employed from probability theory and ergodic theory are pretty standard in mathematics, they are much less familiar to physicists.

Let us now briefly sketch how this paper is organized. We start with a section on the diffraction of lattice gases (without interaction) and its connection to entropy density. This gives us the opportunity to review some well known results in a different setting that matches the generalizations derived later. We hope that the reader can adjust to our approach that way without too much pain. This is followed by our general set-up, where we introduce a rather general type of point sets which are accessible with our methods. Common examples such as model sets (or cut-and-project sets) are contained as special cases.

The remainder of the article is then devoted to the diffraction of point sets with independent stochastic occupation of sites. First, the focus is on the situation of independent, but identically distributed (i.i.d.) random variables, the case most frequently studied. Theorem 1 gives the result for this case. This is illustrated by some examples, and model sets in particular.

More general, and less obvious, is the treatment of independent, but not necessarily identically distributed, random variables, which leads to theorem 2. Among the applications are weighted model sets and their stochastic counterpart, and, more specifically, weighted model sets where the weights are determined by a so-called invariant density [2, 3]. This way, we are able to keep certain aspects of point and inflation symmetries. We believe that this application is of particular value in the discussion of perfect versus random tiling order, as it really is a first step of an intermediate picture.

Our concluding remarks try to relate the results to other investigations and to point towards the next steps that should be taken.

2. Diffraction from a lattice gas

In order to keep things simple, and to familiarize the reader with our approach, we start with the description of the lattice situation and give proper definitions for the general set-up later. Let Γ be a lattice in \mathbb{R}^n , i.e. a discrete Abelian subgroup of \mathbb{R}^n such that \mathbb{R}^n/Γ is compact [35]. Equivalently, there are n linearly independent vectors $\mathbf{b}_1, \dots, \mathbf{b}_n$, called the basis vectors of Γ , so that $\Gamma = \mathbb{Z}\mathbf{b}_1 \oplus \dots \oplus \mathbb{Z}\mathbf{b}_n$. Since we will be talking about Fourier transforms, we will also need the dual (or reciprocal) lattice of Γ , defined by

$$\Gamma^\circ := \{x \in \mathbb{R}^n \mid x \cdot y \in \mathbb{Z} \text{ for all } y \in \Gamma\} \tag{1}$$

where $x \cdot y$ denotes the Euclidean scalar product.

Next, define *Dirac's comb* as the characteristic distribution

$$\omega = \omega_\Gamma := \sum_{x \in \Gamma} \delta_x \tag{2}$$

on Γ , where δ_x is Dirac's distribution at point x , i.e.

$$(\delta_x, \phi) := \phi(x) \tag{3}$$

for all test functions ϕ . In particular, one gets

$$(\omega, \phi) = \sum_{x \in \Gamma} \phi(x) \tag{4}$$

which is well defined for all rapidly decreasing functions (Schwartz functions), hence ω_Γ is a tempered distribution [28].

To deal with diffraction, we need the corresponding autocorrelation distribution, γ_ω , of Γ , also called its Patterson function (although it is a distribution[†]). With the abbreviation

$$\Gamma_r := \Gamma \cap B_r(0) = \{x \in \Gamma \mid |x| \leq r\} \tag{5}$$

γ_ω can be defined and calculated as follows

$$\gamma_\omega := \lim_{r \rightarrow \infty} \frac{1}{\text{vol}(B_r(0))} \sum_{x, y \in \Gamma_r} \delta_{x-y} = d \cdot \omega \tag{6}$$

where d is the density of Γ , i.e. the number of lattice points per unit volume.

By the Fourier transform of a Schwartz function ϕ we mean

$$\hat{\phi}(k) := \int_{\mathbb{R}^n} e^{-2\pi i k \cdot x} \phi(x) \, dx \tag{7}$$

which is again a Schwartz function [28]. The inverse operation is given by

$$\check{\psi}(x) = \int_{\mathbb{R}^n} e^{2\pi i x \cdot k} \psi(k) \, dk. \tag{8}$$

This definition results in the usual properties, such as $\check{\check{\phi}} = \phi$ and $\hat{\hat{\psi}} = \psi$. The convolution theorem takes the form $\widehat{\phi_1 * \phi_2} = \hat{\phi}_1 \cdot \hat{\phi}_2$ where convolution is defined by

$$\phi_1 * \phi_2(x) = \int_{\mathbb{R}^n} \phi_1(x - y) \phi_2(y) \, dy. \tag{9}$$

Finally, the matching definition of the Fourier transform of a distribution T is

$$(\hat{T}, \phi) := (T, \hat{\phi}) \tag{10}$$

for all Schwartz functions ϕ , as usual.

Now, the diffraction by the lattice Γ is described by the Fourier transform of its autocorrelation [9], and in this case we have $\hat{\gamma}_\Gamma = d \cdot \hat{\omega}_\Gamma$. To calculate the latter, we employ Poisson's summation formula for tempered distributions, cf p 254 of [30], which reads

$$\sum_{x \in \Gamma} \delta_x = d \cdot \sum_{k \in \Gamma^\circ} \delta_k \tag{11}$$

[†] It would actually be slightly more appropriate to adopt the set-up of measure theory, where γ_ω would represent a tempered measure, see [12] for this complementary approach.

and can easily be proved from the corresponding Poisson summation formula for Schwartz functions. So we get

$$\hat{\gamma}_\omega = d^2 \cdot \sum_{k \in \Gamma^\circ} \delta_k \tag{12}$$

which is the well known result that the diffraction from point scatterers of equal strength on the points of a lattice is a pure point measure, consisting of periodically placed point measures on the dual lattice. Note that the strength of the peak at $k = 0$ is d^2 , the square of the density of Γ , as it must be.

Let us now move on to the corresponding lattice gas, i.e. to the point set obtained from Γ by removing points from it stochastically. To describe this, we define a new measure ω_s (with suffix s for *stochastic*) by

$$\omega_s = \sum_{x \in \Gamma} \eta(x) \delta_x \tag{13}$$

where $\eta(x)$ is a random variable at site x which takes only the values 0 and 1, meaning empty or occupied. We assume that these random variables are independent of one another and identically distributed, i.e. they constitute a (countable) family of i.i.d. random variables [8, 36]. In fact, we parametrize the probability P that $\eta(x)$ takes the value 1 by a number $0 \leq p \leq 1$, i.e.

$$P(\{\eta(x) = 1\}) = p \quad P(\{\eta(x) = 0\}) = 1 - p. \tag{14}$$

With this definition, ω_s of (13) describes scatterers on the sites of a lattice, each single site being occupied with the same independent probability p . Clearly, the mean value of each random variable is $m_1 = p$, the second moment is $m_2 = p$ and the variance is thus $v = m_2 - (m_1)^2 = p(1 - p)$.

Referring now to the strong law of large numbers [8, 36], we can deduce (details will be given below in a more general context) that, almost surely,

$$\lim_{r \rightarrow \infty} \frac{1}{\text{vol}(B_r(0))} \sum_{x \in \Gamma_r} \eta(x) \eta(x - y) = d \cdot p(p + (1 - p)\delta_{y,0}) \tag{15}$$

i.e. the limit exists and equals the right-hand side with probability one. Here, $\delta_{a,b}$ denotes Kronecker's delta. With this expression, one can calculate the new autocorrelation to be, with probability one,

$$\gamma_{\omega_s} = p^2 \cdot \gamma_\omega + d \cdot p(1 - p) \cdot \delta_0. \tag{16}$$

Fourier's transformation then gives

$$\hat{\gamma}_{\omega_s} = p^2 \cdot \hat{\gamma}_\omega + d \cdot p(1 - p) \tag{17}$$

i.e. we retrieve the point part of the full lattice case, reduced by a factor of p^2 as it should according to the reduced density of points, plus a constant diffuse background which is the absolutely continuous part of the diffraction. This term is related to the entropy density $s = s(p)$,

$$s(p) = -p \log(p) - (1 - p) \log(1 - p) \tag{18}$$

which is a measure of the complexity of the ensemble of point sets we are actually dealing with in this example. The presence of entropy is usually connected to continuous components in the diffraction spectrum, and one can clearly see that $s(p)$ vanishes if, and only if, $p = 0$ or $p = 1$, i.e. iff the random variables are sharp. Also, $s(p)$ is maximal at $p = \frac{1}{2}$, which corresponds to the value of p where the diffraction (17) shows the largest

amount of white noise. Finally, in this case, we have an essentially unique relationship between the entropy and the background intensity, up to the symmetry $p \leftrightarrow (1 - p)$.

Note that the continuous part vanishes if and only if the variance of our random variable vanishes, i.e. if and only if $p = 0$ or $p = 1$. Also, the pure point part vanishes if and only if the mean of the random variable vanishes, i.e. if and only if $p = 0$. We shall meet this situation again later in a much more general context.

3. General set-up

The previous section should have served to get a feeling of what we are after, and to introduce the type of notation we wish to apply. Let us now develop the theory with more precision and in more generality. In what follows, we will only consider uniformly discrete point sets $\Lambda \subset \mathbb{R}^n$, i.e. point sets with the property that there is a positive radius ε such that each point $x \in \Lambda$ can be surrounded by an open ball of radius ε that does not contain any point from Λ other than x . With this assumption, the corresponding Dirac comb ω_Λ defines a translationally bounded distribution (i.e. for each compact set K , there is a constant c_K so that for all $x \in \mathbb{R}^n$, $(\omega_\Lambda, \chi_{K+x}) \leq c_K$, where χ_S denotes the characteristic function of a set S). This is sufficient, though certainly not necessary, to make ω_Λ a tempered distribution. As before, we write Λ_r for the intersection $\Lambda \cap B_r(0)$. Now, we have to tie this together with Fourier analysis.

Definition 1. Let Λ be a uniformly discrete point set of (existing) natural density $d > 0$, and let $\omega = \omega_\Lambda = \sum_{x \in \Lambda} \delta_x$ be its Dirac comb. We say that Λ has a natural *autocorrelation* if

$$\gamma_\omega := \lim_{r \rightarrow \infty} \frac{1}{\text{vol}(B_r(0))} \sum_{x, y \in \Lambda_r} \delta_{x-y} \quad (19)$$

exists as a limit in the weak topology (i.e. as a limit of tempered distributions), and thus is a tempered distribution. Then, γ_ω is called an *autocorrelation distribution* or simply an *autocorrelation* of Λ .

Note that, if this situation applies, then γ_ω is translation bounded (γ_ω inherits this property from ω) and is a distribution of positive type, compare [12]. Let us briefly comment on the more general set-up in terms of measures. If we only had existence of an autocorrelation as a measure in the vague topology, translation boundedness would guarantee that it is actually tempered—so, in our context of uniformly discrete sets, the restriction to tempered distributions is reasonable.

Note that existence of an autocorrelation, as we have defined it here, is specific to the type of region (in this case balls, as implied above by the attribute ‘natural’) over which we compute our averages. Replacing balls by other (convex) objects, centred at 0, the limit $r \rightarrow \infty$ (with r the radius of inscribed balls, say) might give a different answer or might not even exist. For the purposes of this article we do not need to deal with limiting processes over more than one type of shape at the same time, so we will phrase the arguments in terms of convergence based on sequences of balls. The arguments for sequences based on other shapes work in the same way. However, for other purposes it is important to specify *uniqueness* of the autocorrelation. For example, this can be done as follows:

Let $(C_n)_{n \in \mathbb{N}}$ be a family of convex bodies, centered at 0, with the properties that, as $n \rightarrow \infty$, the radius of the maximal inscribed balls tends to ∞ and the quotient of the radii

of circum- and inscribed balls is bounded. If

$$\gamma_\omega := \lim_{n \rightarrow \infty} \frac{1}{\text{vol}(C_n)} \sum_{x,y \in \Lambda \cap C_n} \delta_{x-y} \tag{20}$$

exists for each such sequence as a tempered distribution and is unique, we say that Λ has a *unique autocorrelation*, γ_ω .

In any case, a point set with a natural autocorrelation has a positive measure $\hat{\gamma}_\omega$ as its Fourier transform (due to the Bochner–Schwartz theorem [28]). It is this measure that describes the diffraction [9, 12], and it is very natural that a positive measure shows up here: after all, diffraction is all about the amount of intensity scattered into a certain (measurable) region of space. Also, this positive measure can now, according to Lebesgue’s decomposition theorem, uniquely be decomposed into an absolutely continuous part, a singular continuous part, and a pure point part. The pure point part (usually called ‘Bragg part’ in physics) will always contain a trivial term of the form $d^2 \cdot \delta_0$ where d is the (by assumption existing) density of Λ per unit volume. This motivates the following.

Definition 2. A point set Λ with autocorrelation γ_ω is called *diffractive* (with respect to the convergence process adopted) if $(\hat{\gamma}_\omega)_{pp}$ is non-trivial, i.e. contains Dirac distributions different from $d^2 \cdot \delta_0$. Λ is called *perfectly diffractive* or *pure point* if $\hat{\gamma}_\omega$ has no continuous part at all.

The simplest example of a perfectly diffractive point set is a lattice, where the statement follows from Poisson’s summation formula. Another class of examples is given by regular model sets with sufficiently nice windows (see the last section for more on this) or by extensions of them to certain limit-periodic or limit-quasiperiodic point sets usually described by means of inflation [37, 6]. All these examples are not only uniformly discrete, but also relatively dense, so they are Delone sets. What is more, they are actually Meyer sets, i.e. not only are they Delone but they have the additional property that their difference set, $\Lambda - \Lambda$, is also Delone. Note, however, that the Delone property is not necessary for perfectly diffractive sets, as can be seen from the example of the set of visible points of a lattice [5] which has holes of arbitrary size (and this even with positive density) and is thus neither Delone nor a density 0 deviation of one. Note that removing or adding points of density zero from a perfectly diffractive set does not change its autocorrelation, and the set thus stays perfectly diffractive.

On the other hand, Meyer sets need not be perfectly diffractive, as can be seen from the union of $2\mathbb{Z}$ with various subsets of $2\mathbb{Z} + 1$. This is always a Meyer set, but one can easily construct cases with continuous components (and positive entropy density). This indicates that the class of Meyer sets, or even Delone sets, and the class of perfectly diffractive sets are rather different, though they have some sets in common. In general, perfectly diffractive sets will not be Delone, and hence not Meyer. One interesting class of point sets in this context is that of uniformly discrete sets S with the extra property that $S - S$ is Delone, or at least that $S - S$ is closed and discrete. They are the ones we shall consider here.

4. Point sets with independent stochastic occupation of sites

In this section, we will develop an appropriate generalization of the lattice gas (with i.i.d. random variables) to much more general point sets. From now on, let Λ be a uniformly discrete point set which has a *natural autocorrelation*. Let us also assume that Λ is of *finite local complexity*, i.e. that $\Delta := \Lambda - \Lambda$ is discrete and closed, compare [21] for a detailed discussion in the context of Delone sets. Finite local complexity of a set Λ implies that, for

every radius $r > 0$, there are, up to translations, only finitely many different configurations of points in a ball of radius r . In particular, Λ is uniformly discrete. This is so because Δ discrete forces $0 \in \Delta$ to be isolated, so different points in Λ must have a uniform minimal distance from one another.

If $\omega = \sum_{x \in \Lambda} \delta_x$ is the Dirac comb of Λ , as usual, it is now certainly translation bounded, and the autocorrelation is given by equation (19). We then have

$$\gamma_\omega = \sum_{z \in \Delta} v(z) \delta_z \quad (21)$$

where $v(z)$ is the *autocorrelation coefficient* at z , defined by

$$v(z) = \lim_{r \rightarrow \infty} \frac{1}{V_r} \sum_{\substack{x, y \in \Lambda_r \\ x-y=z}} 1. \quad (22)$$

Here, $\Lambda_r := \Lambda \cap B_r(0)$ as before, and $V_r := \text{vol}(B_r(0))$. Note that, in order to establish the existence of an autocorrelation, it is sufficient to show the existence of the limits in (22), i.e. the existence of the coefficients, because Δ discrete then implies existence of the autocorrelation as a measure in the vague topology, and translation boundedness ensures temperedness, see [12] for further details.

Let us now turn to a stochastic ‘lattice gas’ version of Λ . It is defined by the characteristic distribution

$$\omega_s = \sum_{x \in \Lambda} \eta(x) \delta_x \quad (23)$$

where $\eta(x)$ is a family of i.i.d. random variables taking the values 0 and 1, parameterized as in equation (14), each with mean p and variance $v = p(1-p)$.

We first address the question of the existence of the corresponding stochastic autocorrelation. In analogy to equation (22), we now have the coefficients

$$v_s(z) := \lim_{r \rightarrow \infty} \frac{1}{V_r} \sum_{\substack{x, y \in \Lambda_r \\ x-y=z}} \eta(x) \eta(y) = \lim_{r \rightarrow \infty} \frac{1}{V_r} \sum_{x, x-z \in \Lambda_r} \eta(x) \eta(x-z). \quad (24)$$

We will show that under mild assumptions these coefficients exist, at least in a probabilistic sense. In order to do this, we need to be able to decompose the sum involved in $v_s(z)$ into two parts, because the various terms in the sum of (24) are still random variables, but not necessarily independent ones any more. Fix $z \in \mathbb{R}^n$. Define

$$S(z) := \{x \mid x, x-z \in \Lambda\} \quad (25)$$

and its restricted version $S(z, r)$, where the $x, x-z$ appearing in the definition are required to lie in Λ_r . We distribute the points of $S(z)$ (and, by proper restriction, also those of $S(z, r)$) into *two* sets $S(z)^{(0)}$ and $S(z)^{(1)}$. This may be done in an arbitrary fashion, subject only to the two conditions that:

- (1) if $x, x-z$ both lie in $S(z)$, then they are *not* in the same $S(z)^{(i)}$, and
- (2) the two sets $S(z)^{(i)}$ have well-defined densities:

$$v^{(i)}(z) := \lim_{r \rightarrow \infty} \frac{1}{V_r} \sum_{x \in S(z, r)^{(i)}} 1. \quad (26)$$

Evidently, (26) implies $v(z) = v^{(0)}(z) + v^{(1)}(z)$. Let us say that the set Λ can be *decoupled* if, for every $z \in \Delta$, we can find such a partition.

We note that there may be many ways of decoupling a set Λ . For lattices, for example, we can take each line of points $x + \mathbb{Z}z$ and distribute it into the two subsets according to

whether the coefficient of z is even or odd. For aperiodic model sets (see definitions below), each of the sets $\{x|x+z, x-kz \notin \Lambda; x, x-z, \dots, x-(k-1)z \in \Lambda\}$ is finite, of bounded length k and, for each k , the set of such strings has a definite density. We can place the points $x, x-z, x-2z, \dots$ alternately into $S(z)^{(0)}$ and $S(z)^{(1)}$ and again obtain sets with well-defined density this way; see [13] for a very similar approach to thermal fluctuations which establishes the usual form of the Debye–Waller factor for essentially the same kind of structures that we are dealing with here.

The decoupling property is some kind of ergodicity assumption. It is certainly fulfilled for point sets with uniform frequencies of all finite patches (as is the case for usual model sets), but it is more general than this. In particular, it is still valid for objects such as the pinwheel tiling, compare the brief discussion in [13]. At present, we do not know any equivalent characterization simpler than that given above, which is very much designed for its (technical) purpose.

Proposition 1. Let Λ be a point set of finite local complexity which has a natural autocorrelation. Assume further that the set Λ can be decoupled. Then each coefficient of the stochastic autocorrelation (i.e. the corresponding limit) exists with probability 1, and is given by

$$v_s(z) = v(z) \cdot ((m_1)^2 + (m_2 - (m_1)^2)\delta_{z,0}) \tag{27}$$

where $m_1(= p)$ is the common mean of the i.i.d. random variables $\eta(x)$ and m_2 is their common second moment.

Proof. This is an application of the strong law of large numbers. Forming a sequence of random variables out of a family $(\eta(x))_{x \in \Lambda}$ etc is rather canonical. Since Λ is uniformly discrete, we number the $\eta(x)$ with x in finite sets Λ_r for increasing r . Each such sequence, by the general assumptions made, is a sequence that conforms to the strong law of large numbers.

Let us consider $z = 0$ first. Here, the relevant random variable is actually $\eta(x)^2$, with mean m_2 , the second moment of $\eta(x)$. These variables are independent and, almost surely,

$$\lim_{r \rightarrow \infty} \frac{1}{V_r} \sum_{\substack{x \in \Lambda_r \\ x-z \in \Lambda}} \eta(x)^2 = d \cdot m_2$$

where $d = v(0)$ is the (existing) natural density of Λ .

Next, let $z \neq 0, z \in \Delta$, be arbitrary, but fixed. If $v(z) = 0$, also $v_s(z) = 0$, and our assertion is trivial. So, assume $v(z) > 0$, which means that the density of points $x \in \Lambda$, such that also $x - z \in \Lambda$, exists and is positive. For each such $x, \eta(x)\eta(x - z)$ is a random variable with mean $(m_1)^2$, where $m_1 = p$ is the (identical) mean of all random variables $\eta(y)$ involved. We now have to consider

$$\lim_{r \rightarrow \infty} \frac{1}{V_r} \sum_{\substack{x \in \Lambda_r \\ x-z \in \Lambda_r}} \eta(x)\eta(x - z).$$

This sum has only non-negative terms and decomposes as two sums:

$$v_s(z) = \lim_{r \rightarrow \infty} \frac{1}{V_r} \sum_{x \in S(z,r)^{(0)}} \eta(x)\eta(x - z) + \lim_{r \rightarrow \infty} \frac{1}{V_r} \sum_{x \in S(z,r)^{(1)}} \eta(x)\eta(x - z).$$

Now each of the two sums is an averaged sum over a set of *independent* random variables. Hence, by the strong law, we get almost sure convergence to

$$v_s(z) = v^{(0)}(z)m_1^2 + v^{(1)}(z)m_1^2 = v(z)m_1^2 \tag{28}$$

because the mean of each random variable $\eta(x)\eta(x-z)$ is m_1^2 . Together with the first step, this establishes our claim. \square

The autocorrelation γ_{ω_s} of ω_s is defined as the distribution whose value on any test function ϕ is

$$(\gamma_{\omega_s}, \phi) = \lim_{r \rightarrow \infty} \frac{1}{V_r} \sum_{x,y \in \Lambda_r} \eta(x)\eta(y)\phi(x-y). \quad (29)$$

Although we know this already from the above abstract arguments, it might be instructive to check explicitly that γ_{ω_s} is indeed a tempered distribution, at least in the sense of almost sure convergence. First, let ϕ be a C^∞ function of compact support, lying in the ball $B_s(0)$ of radius s . Then

$$(\gamma_{\omega_s}, \phi) = \lim_{r \rightarrow \infty} \sum_{z \in \Delta} \frac{1}{V_r} \left(\sum_{\substack{x,y \in \Lambda_r \\ x-y=z}} \eta(x)\eta(y) \right) \phi(z). \quad (30)$$

This limit exists because in reality the outer sum is over the finite set Δ_s and for $r \gg s$ we have $\Delta_s \subset \Lambda_r - \Lambda_r$. Thus, as $r \rightarrow \infty$, the sum converges, almost surely, to

$$\sum_{z \in \Delta} v_s(z)\phi(z). \quad (31)$$

Now if $\phi \in \mathcal{S}$, the space of Schwartz functions, and $\{\phi_i\}$ is a sequence of C^∞ -functions of compact support that converge to ϕ in the standard topology of \mathcal{S} , then

$$\sum_{z \in \Delta} v_s(z)\phi_i(z) = (m_1)^2 \sum_{z \in \Delta} v(z)\phi_i(z) + (m_2 - (m_1)^2)v(0)\phi_i(0) \quad (32)$$

and the latter converges in i to

$$(m_1)^2 \sum_{z \in \Delta} v(z)\phi(z) + (m_2 - (m_1)^2)v(0)\phi(0) \quad (33)$$

by our assumptions on the existence of the autocorrelation density of Λ .

Let us summarize these findings as follows.

Theorem 1. Let Λ be a point set of finite local complexity which has a natural autocorrelation and density d . Suppose that Λ can be decoupled. Then, the autocorrelation of Λ and that of its stochastic version are, with probability one, related by

$$\gamma_{\omega_s} = (m_1)^2 \gamma_\omega + d(m_2 - (m_1)^2)\delta_0. \quad (34)$$

As a consequence, their Fourier transforms fulfil

$$\hat{\gamma}_{\omega_s} = (m_1)^2 \hat{\gamma}_\omega + d(m_2 - (m_1)^2). \quad (35)$$

So, the stochastic version has the same ‘main’ part of the diffraction, multiplied by a factor of $(m_1)^2$ (hence vanishing if and only if the mean of the joint probability distribution is 0) plus an extra absolutely continuous part that is constant and represents the ‘white noise’ of the uncorrelated random processes. The constant is essentially given by the variance of the joint distribution, and thus this part vanishes if and only if the i.i.d. random variables are all sharp. The interpretation, and also the connection with the entropy density, is thus the same as in the lattice case, as expected.

At this point, generalizations are rather obvious, and we just want to mention a few. First of all, it is by no means essential to restrict to the particular types of random variables that we have just discussed. Here we were motivated by the idea of a lattice gas and its

generalization to uniformly discrete point sets, but we can also think of any other (non-negative) i.i.d. random variable with (existing) mean m_1 and second moment m_2 (so, the variance would be $v = m_2 - (m_1)^2$). This does not change the result, and would correspond to a situation where we place, at each point x of the set Λ , a scatterer of random strength $\eta(x)$. Again, we get the result of theorem 1.

Note also that at no point did we need to assume that $\hat{\gamma}_\omega$ was pure point. This is not necessary, and indeed, the result of theorem 1 also applies to situations where $\hat{\gamma}_\omega$ is singular continuous, absolutely continuous, or of mixed type. This same situation is met in Hof's treatment of thermal fluctuations [13].

5. Applications to lattices and model sets

The obvious first application is to *lattices*. This results in a rigorous derivation of what we described in section 2. The diffraction from a lattice gas, with i.i.d. random variables for the strength of the Dirac distributions at the lattice points, shows a point part that is the one from the lattice itself, reduced in intensity, plus a homogeneous diffuse background.

Another application is to characteristic decorations on tilings[†] that are obtained by a primitive substitution rule. Here, it was shown [22] that the autocorrelation is unique, and convergence of its coefficients is even uniform. In general, the Fourier transform will not be pure point, see [37] for a more detailed discussion. We also refer to [13] for a brief discussion of the decoupling property in situations without finite local complexity such as the pinwheel tilings of the plane.

Lattice gas versions of *model sets* provide another class of examples, of rather recent interest. Recall that a model set [25, 33] is defined via projection onto \mathbb{R}^n of a lattice in some higher-dimensional space, or, more generally, in some locally compact Abelian group. More precisely, it is assumed that $G = \mathbb{R}^n \times H$ is a locally compact Abelian group and that D is a lattice in G . Thus D is a discrete subgroup of G for which the quotient space G/D is compact. Further, we assume that the projection $\pi_1(D)$ of D into \mathbb{R}^n is *injective* and its projection $\pi_2(D)$ into H is *dense*, where π_1 and π_2 denote the canonical projections. The resulting set is aperiodic, i.e. has no translational symmetries, if and only if π_2 is injective on D . The most common examples take $H = \mathbb{R}^m$ for some m . In any case, define the composite map $*$:= $\pi_2 \circ \pi_1|_D^{-1} : \pi_1(D) \rightarrow H$. Then for any set $\Omega \subset H$ with non-empty interior and compact closure, we have the *model set*

$$\Lambda = \{x \in \pi_1(D) \mid x^* \in \Omega\}. \tag{36}$$

Provided that the boundary of Ω has measure 0 (with respect to the Haar measure μ of H), the density of such a set exists uniformly and is given by $\mu(\Omega)/\text{vol}(D)$. Here, $\text{vol}(D)$ is the volume of any fundamental domain for D in G , the volume taken relative to the product measure on G derived from the Lebesgue measure on \mathbb{R}^n and the Haar measure μ on H [32, 33]. Such a model set is a Meyer set, i.e. both Λ and $\Delta = \Lambda - \Lambda$ are Delone. Also, Λ is perfectly diffractive [34], and the obvious lattice gas version of it, with i.i.d. random variables attached to each position, falls under our theorem 1.

A large number of well known point sets can be interpreted in this setting, including the Fibonacci and many other chains, the vertex sets of various planar tilings (such as the Ammann–Beenker, the Penrose, the Tübingen triangle tiling etc) or of tilings in higher dimensions (such as the various icosahedral examples in 3D or the Elser–Sloane quasicrystal in 4D). But even decorations of the chair tiling and other limit-periodic and

[†] We call a point set of finite local complexity a characteristic decoration of a locally finite tiling if they are locally equivalent, i.e. if both objects represent the same MLD-class, see [7] for details.

limit-quasiperiodic structures fall under this class, see [6] for details. So, for all these cases, we have the following.

Corollary 1. If Λ is a model set as described above, it fulfils the conditions of theorem 1, and the diffraction of the stochastic versus the deterministic Dirac comb is, almost surely, given by equation (35).

6. Beyond identical distribution

So far, we have restricted our attention to the case of i.i.d. variables. We will now broaden our point of view to the situation where the random variables are still independent, but not necessarily identically distributed any more. Before we give proper definitions, let us have another look at the lattice gas. Above, we compared the deterministic Dirac comb $\omega = \sum_{x \in \Gamma} \delta_x$ with the stochastic one, $\omega_s = \sum_{x \in \Gamma} \eta(x) \delta_x$, where $\eta(x)$ were i.i.d. random variables of common mean m_1 . This led to theorem 1.

Alternatively, consider now the deterministic, but weighted distribution

$$\omega_a := \sum_{x \in \Gamma} m_1 \delta_x. \quad (37)$$

Clearly, ω_a has an autocorrelation if ω itself does, and we get

$$\gamma_{\omega_a} = (m_1)^2 \cdot \gamma_{\omega} \quad (38)$$

and the result of theorem 1 may be restated as

$$\hat{\gamma}_{\omega_s} = \hat{\gamma}_{\omega_a} + d(m_2 - (m_1)^2) \quad (39)$$

which holds almost surely.

This indicates how we have to generalize our previous findings properly. Let Λ again be a uniformly discrete set of finite local complexity (i.e. $\Delta = \Lambda - \Lambda$ discrete and closed), and suppose that Λ can be decoupled in the sense described above. Furthermore, let $(\eta(x))_{x \in \Lambda}$ be a family of independent random variables with non-negative means $m_1(x)$ which are bounded from above and with bounded variances $v(x)$, $v(x) \leq c$, say. Under these assumptions, this family conforms to the strong law of large numbers. This can be seen as follows. Let $(\eta_m)_{m \in \mathbb{N}}$ be any sequence made from the random variables $\eta(x)$, e.g. by numbering the points of Λ in balls of growing radius. We then obtain

$$\sum_{m=1}^{\infty} \frac{v(\eta_m)}{m^2} \leq c \sum_{m=1}^{\infty} \frac{1}{m^2} = c \cdot \zeta(2) = \frac{c\pi^2}{6} < \infty. \quad (40)$$

The assertion now follows from Kolmogorov's criterion, see [8] or [36, theorem 12.3], and we can continue to develop the appropriate analogue of theorem 1.

To this end, let us now compare the two distributions

$$\omega_a = \sum_{x \in \Lambda} m_1(x) \delta_x \quad (41)$$

which may be thought of as a toy model for an arrangement of different atoms (hence the suffix a), and

$$\omega_s = \sum_{x \in \Lambda} \eta(x) \delta_x \quad (42)$$

the former being deterministic and the latter probabilistic. We can now formulate the appropriate theorem for this situation.

Theorem 2. Let Λ be a set of finite local complexity that can be decoupled, and let $(\eta(x))_{x \in \Lambda}$ be a family of independent random variables with non-negative means $m_1(x)$ (bounded from above) and bounded variances $v(x)$ whose average is assumed to exist,

$$\bar{v} = \lim_{r \rightarrow \infty} \frac{1}{|\Lambda_r|} \sum_{x \in \Lambda_r} v(x). \tag{43}$$

If ω_a has a natural autocorrelation, in the sense we used this term above, then ω_s also possesses, almost surely, a natural autocorrelation, namely, with $d = \text{dens}(\Lambda)$

$$\gamma_{\omega_s} = \gamma_{\omega_a} + d\bar{v}\delta_0 \tag{44}$$

and its Fourier transform reads

$$\hat{\gamma}_{\omega_s} = \hat{\gamma}_{\omega_a} + d\bar{v}. \tag{45}$$

The proof is very similar to the one given above and need not be repeated.

This theorem is a little less explicit than the previous one, and one can see the potential extra complication from the following simple example. Consider $\Lambda = \mathbb{Z}$ and independent random variables $\eta(m)$ with values in $\{0, 1\}$ and parametrization

$$P(\{\eta(m) = 1\}) = \begin{cases} p & m \text{ even} \\ q & m \text{ odd} \end{cases} \tag{46}$$

where $0 \leq p, q \leq 1$. Here, $\omega_a = q \sum_{x \in \mathbb{Z}} \delta_x + (p - q) \sum_{x \in 2\mathbb{Z}} \delta_x$ which clearly has a unique autocorrelation γ_{ω_a} , with Fourier transform

$$\hat{\gamma}_{\omega_a} = \frac{(p + q)^2}{4} \sum_{y \in \mathbb{Z}} \delta_y + \frac{(p - q)^2}{4} \sum_{y \in \mathbb{Z} + \frac{1}{2}} \delta_y. \tag{47}$$

So, the diffraction spectrum depends on the values of p and q , and the second term on the right-hand side vanishes for $p = q$.

The corresponding stochastic version, ω_s , reflects this and produces the same point diffraction, plus a constant diffuse background ('white noise'), i.e. by application of theorem 2 we have, almost surely,

$$\hat{\gamma}_{\omega_s} = \hat{\gamma}_{\omega_a} + \frac{1}{2}[p(1 - p) + q(1 - q)]. \tag{48}$$

The entropy density of this little example is immediate:

$$s = -\frac{1}{2}[p \log(p) + (1 - p) \log(1 - p) + q \log(q) + (1 - q) \log(1 - q)]. \tag{49}$$

Note that, in general, a perfectly diffractive point set Λ together with a family of independent random variables $\eta(x)$ is not enough to apply theorem 2; we really have to know that not only γ_ω but also γ_{ω_a} exists. This is a rather subtle (and non-constructive) set of conditions upon the means of the random variables. There is one situation where we can escape this extra complication: if the random variables are distributed statistically, i.e. in such a way that their means $m_1(x)$ are themselves the result of a stationary Bernoulli process, we are back to the situation of theorem 1, which may then be applied with

$$m_1 = \lim_{r \rightarrow \infty} \frac{1}{|\Lambda_r|} \sum_{x \in \Lambda_r} m_1(x) \tag{50}$$

provided this limit exists.

7. Further examples: weighted model sets

Let us now return to the situation of a model set $\Lambda = \Lambda(\Omega)$, as described above. Assume that we have a family of independent random variables parametrized by the points x^* of the window Ω . Suppose that $p(x^*)$ is a continuous function on Ω , with values in $[0, 1]$. Then, $\omega_a = \sum_{x \in \Lambda} p(x^*)\delta_x$ is perfectly diffractive (this follows from a slight modification of the arguments given in [12] by means of an application of Weierstrass' approximation theorem). Explicitly, one has

$$\hat{\gamma}_{\omega_a} = \sum_{k \in \pi_1(D^\circ)} |a(k)|^2 \delta_k \quad (51)$$

where D° is the dual lattice of D and the amplitudes are given by [12]

$$a(k) = \frac{d}{\text{vol}(\Omega)} \int_{\Omega} e^{2\pi i k^* \cdot x^*} p(x^*) d\mu(x^*) = \frac{d \cdot \hat{p}(-k^*)}{\text{vol}(\Omega)} \quad (52)$$

where d denotes, as before, the density of the model set Λ .

Let us turn to the stochastic counterpart

$$\omega_s = \sum_{x \in \Lambda} \eta(x) \delta_x \quad (53)$$

where $\eta(x)$ is the random variable that decides whether x is occupied or not. Let us define it as follows

$$P\{\eta(x) = 1\} = p(x^*) \quad P\{\eta(x) = 0\} = 1 - p(x^*). \quad (54)$$

Observe that $\eta(x)$ has mean $p(x^*)$ and variance $p(x^*)(1 - p(x^*))$, the latter being bounded by $\frac{1}{4}$. So, by Kolmogorov's criterion, this family of random variables conforms to the strong law of large numbers.

Let us see whether the mean of the variances exists. We note first that we have the mean occupancy per point of Λ as

$$\bar{p} = \lim_{r \rightarrow \infty} \frac{1}{|\Lambda_r|} \sum_{x \in \Lambda_r} p(x^*). \quad (55)$$

Due to the fact that the projection into internal space H is uniform and the fact that p is continuous, it is possible to use Weyl's theory of uniformly distributed sets [20] to show that this limit indeed exists and is given by

$$\bar{p} = \frac{1}{\text{vol}(\Omega)} \int_{\Omega} p(y) d\mu(y). \quad (56)$$

In the same way, we can also calculate the averaged variance as

$$\bar{v} = \frac{1}{\text{vol}(\Omega)} \int_{\Omega} p(y)^2 d\mu(y) - \bar{p}^2. \quad (57)$$

So, we can apply theorem 2 and obtain, with probability one,

$$\hat{\gamma}_{\omega_s} = \hat{\gamma}_{\omega_a} + d\bar{v}. \quad (58)$$

The resulting set also has a positive entropy density. Clearly, for a single point, this is

$$s(x) = -p(x^*) \log(p(x^*)) - (1 - p(x^*)) \log(1 - p(x^*)) \quad (59)$$

and we would be interested in the quantity

$$\bar{s} := \lim_{r \rightarrow \infty} \frac{1}{|\Lambda_r|} \sum_{x \in \Lambda_r} s(x) \quad (60)$$

provided this limit exists. Again, this follows from the uniform distribution of the points of a model set and, using Weyl's lemma, we obtain

$$\bar{s} = -\frac{1}{\text{vol}(\Omega)} \int_{\Omega} [p(y) \log(p(y)) + (1 - p(y)) \log(1 - p(y))] d\mu(y). \quad (61)$$

As a relevant example, let us consider a special function $p(x^*)$, namely one that reflects the inflation structure of a given model set and is related to the recently investigated invariant densities on them [2, 3]. Assume that $G = \mathbb{R}^n \times \mathbb{R}^m$ and suppose that $\Lambda = \{x \in \pi_1(D) | x^* \in \Omega\}$. We are interested here in the situation in which Λ admits self-similarities of the form

$$t_{Q,v} : x \mapsto Qx + v \quad (62)$$

where Q is an inflational linear map, i.e. a rotation followed by a scalar inflation. We call such self-similarities *Q-inflations*. Remarkably, for fixed Q , the set

$$T := \{v \in \mathbb{R}^n | t_{Q,v}\Lambda \subset \Lambda\}$$

is itself a model set. In this situation, there is a unique absolutely continuous probability measure $p = p_Q$ supported on Ω which is invariant under the set of Q -inflations in the sense that

$$p = \lim_{s \rightarrow \infty} \frac{1}{|T_s|} \sum_{v \in T_s} t_v^* \cdot p \quad (63)$$

where t_v^* is the induced mapping in internal space and $(t_v^* \cdot p)(y) := p((t_v^*)^{-1}y)$.

The corresponding stochastic model set with site occupancy probability $P(\{\eta(x) = 1\})$, is likewise invariant in the sense that

$$P(\{\eta(x) = 1\}) = \lim_{s \rightarrow \infty} \frac{|\det(Q)|}{V_s} \sum_{v \in T_s} \sum_{y \in t_{Q,v}^{-1}x \cap \Lambda} P(\{\eta(y) = 1\}). \quad (64)$$

Such invariant densities in internal space are supported on the window and typically display bell-shaped form. We refer the reader to [2–4] for more details on this and for various examples.

Since this is a special case of the general situation met above, the measure

$$\omega_s := \sum_{x \in \Lambda} \eta(x) \delta_x \quad (65)$$

is (almost surely) diffractive with the *same* pure point part ω_a , since

$$\lim_{r \rightarrow \infty} \frac{1}{V_r} \sum_{x, x-z \in \Lambda_r} \eta(x) \eta(x-z) = \lim_{r \rightarrow \infty} \frac{1}{V_r} \sum_{x, x-z \in \Lambda_r} p(x^*) p(x^* - z^*). \quad (66)$$

It is an interesting feature of this situation that the probability distributions p_{Q^k} , as $k \rightarrow \infty$, tend towards the constant distribution on Ω .

8. Concluding remarks

The analysis of diffraction from point sets with stochastic occupation of sites, or with random scattering strength on the sites, can be developed in a rather general setting which goes considerably beyond the lattice situation. It was the aim of this contribution to outline some of the methods needed. For related aspects, we also recommend Hof's treatment of thermal fluctuations [13].

One concrete reason to look into this type of problem stems from the discussion of quasicrystalline order and the evidence of stochastic elements in it [15, 16]. Based upon the random tiling scenario, one would expect the $*$ -image (lift) of a ‘real world’ point set (e.g. one obtained from a tiling overlay of a high resolution electron micrograph) to show a Gaussian shaped distribution or at least a bell-shaped curve with maybe a somewhat flatter centre—in contrast to the uniform distribution obtained from a perfect model set.

Since such bell-shaped distributions have been observed and appear to be rather typical [16], it is an important question as to what extent they really support the random tiling picture. In other words: are there alternatives to explain such profiles? One is provided by the stochastic occupation of a model set, if we start from an invariant density on the window that resembles such a bell curve, see [2, 4] for the specific example of the Penrose tiling and invariant densities attached to it. With a $*$ -image of a finite patch its stochastic point set realization would reproduce the bell-shaped invariant density profiles.

We do not claim that this is enough to establish this simple stochastic approach as a real alternative—there are various other objectives to be met, such as width of the profile as a function of the patch size, structured diffuse scattering background (other than white noise), or maximization of entropy as a function of suitable parameters for the non-crystallographic phase. We believe, nevertheless, that there are interesting possibilities along the lines presented here, and it would be nice to find (solvable) examples with extra correlations that appear more realistic in the sense mentioned.

One first step in this direction is the calculation of the diffraction of a stochastic version of \mathbb{Z} with random variables that stem from a stationary ergodic Markov system, as is well known in the literature [39]. This results in a pure point part which is that of \mathbb{Z} , reduced in intensity, plus an absolutely continuous background that now shows a structure, i.e. that is no longer white noise. We hope to report on proper generalizations of this scenario soon, and also on an extension to the diffraction theory of random tilings.

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