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Recent developments in the mathematics of diffraction

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Abstract

This is a survey of some recent results in the mathematics of diffraction, concentrating on the use of dynamical systems and stochastic point processes.

1 Introduction

The characterizing feature of physical cyrstals and quasicrystals is often taken as the prominent appearance of Bragg peaks in their diffraction diagrams. Thus arises the fascinating question of what this suggestive, but rather vague, characterization really implies, both in physical and mathematical terms. In this short paper we outline some recent mathematical advances in the study of diffraction.

Our approach here is to use a setting familiar from statistical mechanics and from the theory of tilings and long-range aperiodic order, augmented with ideas from the theory of point processes. A good deal of the paper is involved in setting this up. Rather than deal with a single quasicrystal Λ, we work instead with translation invariant families of them. The intuition is that such a family X will consist of all those quasicrystals which are in some sense locally indistinguishable from one another, or which cannot be isolated from one another by the physical considerations at hand. As for the individual quasicrystals, initially we model these simply as point sets in space, representing the positions of the atoms, and assume them to satisfy a minimal separation requirement (uniform discreteness). Later on the situation naturally generalizes to more general distributions of density in space.

The main points that we wish to discuss can be summed up as:

1. X may be construed in the context of dynamical systems and spatial point processes.
2. All relevant information about a system like X is contained in its collection of n-point correlations, the diffraction being the Fourier transform of the 2-point correlation.
3. Extinctions play an important role in the complexity of the diffraction.
4. Pure pointed-ness is directly and precisely related to almost periodicity.
5. Model sets (cut and project sets) are completely determined by their 2- and 3-point correlations.

2 Point sets and local hulls

We work in general d-dimensional space $\mathbb{R}^d$, since the dimension does not play any special role here[1]. Throughout the paper C_R, $R > 0$, denotes the open cube $(-R/2, R/2)^d \subset \mathbb{R}^d$. The translates of C_R shall be called R-cubes. A subset Λ of d-dimensional space $\mathbb{R}^d$ is *uniformly discrete* (or more specifically r-uniformly discrete) if there is an $r > 0$ so that no r-cube can contain more than one point of Λ. This is often called a *hard core* condition. The collection of all such r-uniformly discrete subsets is denoted by $\mathcal{D}_r = \mathcal{D}_r(\mathbb{R}^d)$.

Given two elements Λ and Λ' in $\mathcal{D}_r$ we decree that Λ and Λ' are 'close' if on some 'large' region K around the origin in $\mathbb{R}^d$ and for some 'small' $\epsilon > 0$, the points of Λ that are within K also lie in the ϵ-cubical neighbourhoods of points of Λ', and vice-versa. This is a very natural physical definition and provides a topology on $\mathcal{D}_r$, which we call the *local topology.* The easiest way to think of this is that Λ and Λ' are close if and only if they make essentially the same pattern Π on large grids G with fine mesh, around the origin, see Fig. 1. The set of all Λ with pattern Π form a *cylinder set* $B(\Pi)$ of X. From an experimenter's point of view, a finite sample of a material, supposedly representative of some class X, and a level of positional tolerance $\epsilon > 0$, specify a cylinder set of possible infinite structures in X from which it could have come.

Translating points sets around in $\mathbb{R}^d$, $T_x(\Lambda) := x + \Lambda \in \mathcal{D}_r$, for $x \in \mathbb{R}^d$, is continuous in the local topology.

An important property of $\mathcal{D}_r$ is that it is compact, a consequence of the finiteness of the number of patterns that can occur in a grid of fixed size and mesh.

The basic objects of interest in this paper are pairs (X, μ) with the properties that X is a closed translation invariant subset of $\mathcal{D}_r(\mathbb{R}^d)$ and μ is a translation invariant ergodic probability Borel measure (TIEPM) on X.

[1] Virtually everything we say can be transported to the setting of arbitrary locally compact Abelian groups, but this extra generality adds nothing essentially new to the understanding and is of lesser physical value.

[2] Dynamical systems usually refer to systems with an action of $\mathbb{R}$, acting as time. In this paper the action is translation. Nothing other than what is stated here is implied by the term. The pictorial representation of X as a torus in Fig. 2 is more measure theoretic than topological. The torus mapping, of § 5 shows that there is a significant singular topological structure that the measure does not "see".

Since $\mathcal{D}_r$ is compact, so is X. Thus already we have a topological dynamical system[2] $(X, \mathbb{R}^d)$. Fig. 2 gives a schematic idea of the appearance of X and an orbit on it for the case $d = 1$. The existence of TIEPMs is guaranteed by general theory. We think of such a measure μ as the giving pattern frequencies for the elements of X; for any pattern Π of cells from any grid $\mu(B(\Pi))$ is the frequency of this pattern in the sense that it measures the relative proportion of $\Lambda \in X$ which have points around 0 in precisely the pattern Π. Thus (X, μ) is both a probability space and an ergodic dynamical system. The importance of creating dynamical systems in this kind of way derives from [22, 5].

Examples:

1. The set X of all Penrose tilings with the same basic tiles and the same underlying orientations are locally indistinguishable from one another and form what is called an LI (local indistinguishability) class of point sets. Penrose tilings have natural pattern frequencies which determine the measure. In this case it is the only TIEPM that X has (the system is *uniquely ergodic*).

2. Begin with a particular point set $\Lambda \in \mathcal{D}_r$ of interest. Along with Λ consider all its translates $t + \Lambda$, $t \in \mathbb{R}^d$. The closure $X(\Lambda)$ of the entire set of translates in $\mathcal{D}_r$ is called the *local hull* of Λ. As long as Λ is regular enough to have well-defined pattern frequencies, we will obtain an invariant measure μ which gives the pattern frequences, and $(X(\Lambda), \mu)$ will satisfy the two axioms above. For instance, if Λ were a Penrose tiling $(X(\Lambda), \mu)$ would be its LI class. Other well-known examples come from regular model sets, see §5.

3. The bi-infinite Bernoulli system. Fix a number $0 < p < 1$ and then start at an arbitrary point on the real line and move in unit steps along the line, in both directions, at each step laying down (resp. not laying down) a point with probability p (resp. $1 - p$). The set of all bi-infinite point sets arising this way constitutes X. The probability of any finite pattern of points appearing is the obvious one and this determines a TIEPM μ_p on X. Notice that X is the same, no matter what p is! It is the choice of the p which determines the measure μ_p and assigns the pattern frequencies.

4. Randomize any of the above, subject only to the hard core condition. See [16, 1] for more on this type of process.

The measure μ gives the information about what patterns are possible and what their probabilities of occurrence are. The assumption of ergodicity coincides with the original concept of ergodicity in statistical mechanics: the set of all translates of a 'typical'[3]element $\mathit{\Lambda}$ of X seen from a fixed point in space, say the origin, faithfully reproduces the statistics of local patterns of the entire ensemble X.

Along with (X, μ) we associate the space $L^2(X, \mu)$ of all square integrable $\mathbb{C}$-valued functions F on X. The translation action of $\mathbb{R}^d$ on X produces a corresponding action on functions: $T_t F$ is the function $(T_t F)(\Lambda) := F(T_{-t}\Lambda) = F(-t + \Lambda)$. Since μ is shift invariant, this action is unitary: the translation action on functions preserves the inner product $\langle F|G \rangle := \int_X F\overline{G}\, \mathrm{d}\mu$ on $L^2(X, \mu)$. The importance of this sort of idea, dating back to Koopmann in the 1930s, is that it relates the spectral analysis of this action to the properties of μ and ultimately to the typical members of X, see §4.

Although the connection between the ambient space $\mathbb{R}^d$ and (X, μ) is apparent from our discussion, there is a formal and crucial way of expressing this: for $f : \mathbb{R}^d \longrightarrow \mathbb{C}$ define

$$N_f : X \longrightarrow \mathbb{C} \quad \text{by} \quad N_f(\Lambda) := \sum_{x \in \Lambda} f(x)\,. \tag{1}$$

This produces a function N_f on X (sometimes called a *counting function*) for each function f on $\mathbb{R}^d$, as long as the sum involved in N_f makes sense. This happens, for instance, for all continuous and compactly supported functions on $\mathbb{R}^d$, since then only finitely many points of Λ can contribute to the sum. As long as the function is reasonable the resulting function on X is square integrable with respect to μ. Furthermore, the mapping $f \mapsto N_f$ intertwines the $\mathbb{R}^d$-actions on functions on $\mathbb{R}^d$ and on functions on X.

[3]'Typical' means that this is true except possibly on some subset of X of μ-measure 0: synonyms are 'almost surely true', or that it happens 'almost everywhere'.

Let us summarize what we have achieved: we have a probability space (X,μ), consisting of discrete point sets of $\mathbb{R}^d$ and a measure indicating pattern frequencies. $\mathbb{R}^d$ acts on X in a measure preserving way and there is a continuous $\mathbb{R}^d$-invariant mapping

$$N : C_c(\mathbb{R}^d) \longrightarrow L^2(X,\mu)\,. \qquad (2)$$

This is what is called a *stationary ergodic spatial point process* (SEPP). As such it fits into the well-developed theory of point processes [8], albeit the situation is atypical since we have the hard core assumption and are interested in highly ordered situations, even ones that are deterministic. The interpretation of randomness in something like the LI class of a Penrose tiling is that $\mu(\Pi)$ is the probability that a randomly chosen Penrose tiling has the pattern Π around the origin.

We take the attitude that the knowledge of μ and N are all that we can hope to know about our physical system. The function N describes the outcomes of observations of X. Our objective is to determine μ from other, physically observable, data gleaned from N.

In our case this other data will be the various correlations of the system (X,μ).

If $A \subset \mathbb{R}^d$ is a bounded region then we have the corresponding function $N_A := N_{1_A}$, and it is simply a counting function; $N_A(\Lambda)$ is the number of points of Λ in A, whence the name.

If A is small enough that it is covered by a a single r-cube (A is *r-small*), then N_A is nothing but an indicator function that indicates whether or not a point set $\Lambda \in X$ does or does not have a point in A, giving the values 1 or 0 accordingly.

3 Correlations and diffraction

Let (X,μ,N) be a SEPP. The $(n+1)$-moment of the measure μ is the measure $\mu^{(n+1)}$ on $\mathbb{R}^d \times \cdots \times \mathbb{R}^d$ ($n+1$ factors) defined (on functions) by

$$\mu^{(n+1)}(f_0,\ldots,f_n) = \int_X N_{f_0}(\Lambda)\ldots N_{f_n}(\Lambda)\,\mathrm{d}\mu(\Lambda)\,,$$

[8]. The intuitive meaning of these moments becomes clear if the functions f_j are taken to be of the form 1_{A_j} where the A_j are r-small measurable subsets of $\mathbb{R}^d$. Then for a fixed Λ in X we have from the assumption of ergodicity that, almost surely,

$$\begin{aligned}&\mu^{(n+1)}(A_0,\ldots,A_n) := \mu^{(n+1)}(1_{A_0},\ldots,1_{A_n})\\ =\;& \int N_{A_0}\ldots N_{A_n}\,\mathrm{d}\mu\\ =\;& \lim_{R\to\infty}\frac{1}{\operatorname{vol}C_R}\int_{C_R} N_{A_0}(-t+\Lambda)\ldots N_{A_n}(-t+\Lambda)\,\mathrm{d}t\,,\end{aligned}$$

which gives the average frequency in which elements of X have points simultaneously in each of the sets $A_0,\ldots,A_n$. In other words, it is picking up pattern frequencies. Notice that the moment measure belongs to the pair (X,μ), but it is also expressible on the individual elements of X, at least almost surely.

The first moment, $\mu^{(1)}(A) = \int N_A(\Lambda)\,\mathrm{d}\mu(\Lambda)$ is the average number of points in $\Lambda \cap A$ as Λ runs over X. Since this average is independent of the position of A, $\mu^{(1)}$ is an invariant measure on $\mathbb{R}^d$ and so is just a multiple I_0 of ordinary Lebesgue measure: $\mu^{(1)}(A) = I_0\operatorname{vol}(A)$ for all measurable A. This number I_0 is called the *intensity of the process* and represents the average number of points per unit volume of the point sets making up X and also, almost surely, the average number of points per unit volume of any Λ in X.

The way in which translation is factored out of the first moment is also applicable to all the higher moments, and leads to the correlation measures $\gamma^{(n)}$ for which $\gamma^{(n)}(A_1,\ldots,A_n)$ is the frequency of the sets of points of the form $t + \{0,x_1,\ldots,x_n\}$ with $x_j \in A_j$, $j = 1,\ldots,n$ in a typical element Λ of X. This measure looks more familiar when acting on functions (of n variables):

$$\gamma^{(n)}(f) = \lim_{R\to\infty}\frac{1}{\operatorname{vol}C_R}\sum_{t,x_1,\ldots x_n} f(-t+x_1,\ldots,-t+x_n)\,,$$

where the sum runs over all $t,x_1,\ldots,x_n \in \Lambda\cap C_R$. This ostensibly belongs to Λ, but the theory shows that this limit exists and is the same for almost all Λ in X, so we can ignore its apparent dependence on a particular element of X, see [5, 13] for $n=2$, [9] in general.

The 2-point correlation, which we write simply as γ, is called the *autocorrelation*. The *diffraction* is **by definition** the Fourier transform $\widehat{\gamma}$ of the autocorrelation[4].

[4]For a *finite* sample or set of points Λ the diffraction can be defined as $|\rho|^2$ (suitably normalized), where $\rho(k) := \sum_{x\in\Lambda} e^{-2\pi i k.x}$.

The diffraction is a measure and may have a point-like part and a continuous part. The diffraction is *pure point* (and X is *pure point diffractive*) if this measure is entirely a point measure. In this case the point-sets comprising X are almost surely pure point diffractive.

Theorem 3.1 *[9] Given a SEPP* (2)*, the n-point correlations $\gamma^{(n)}$, $n = 1, 2, \ldots$, exist and collectively they determine the measure μ.*

The proof of this depends on proving that μ is determined by its moments. This is not necessarily the case for arbitrary point processes, but the uniform discreteness makes our point processes special. Of course knowing the diffraction is equivalent to knowing the 2-point correlation (they are Fourier transforms of one another). The fundamental question is how much does the 2-point correlation tell us about (X, μ).

4 Dynamics and diffraction

The unitary action of $\mathbb{R}^d$ on $L^2(X, \mu)$ leads one to look at spectral features. For instance, $f_k \in L^2(X, \mu)$ is an *eigenfunction* for the frequency vector $k \in \mathbb{R}^d$ if $T_t f_k = \exp(2\pi i k.t) f_k$ for all $t \in \mathbb{R}^d$. These k lie in the Fourier dual of $\mathbb{R}^d$, which is another copy of $\mathbb{R}^d$, and form a subgroup E of it. Ergodicity guarantees the non-degeneracy of the corresponding eigenspaces. We say that $L^2(X, \mu)$ has *pure point dynamical spectrum* if it has a Hilbert basis of eigenfunctions. Surprisingly, there is a direct connection between the notions of pure pointedness in dynamics and diffraction:

Theorem 4.1 *[18, 13, 3] X is pure point diffractive if and only if (X, μ) has pure point dynamical spectrum.*

In order to understand this result we need a way to relate the diffraction to the dynamics. This comes via (2). We consider the diffraction measure $\widehat{\gamma}$ on $\mathbb{R}^d$ and the corresponding space $L^2(\mathbb{R}^d, \widehat{\gamma})$ of functions f on $\mathbb{R}^d$ that are $\widehat{\gamma}$-square integrable, that is, $\int |f|^2 \, \mathrm{d}\widehat{\gamma} < \infty$. Define an action U of $\mathbb{R}^d$ on $L^2(\mathbb{R}^d, \widehat{\gamma})$ by

$$(U_t f)(x) = e^{-2\pi i t.x} f(x)$$

for all $t, x \in \mathbb{R}^d$, $f \in L^2(\mathbb{R}^d, \widehat{\gamma})$. This effects only phase factors in the values of f.

Theorem 4.2 *Let (X, μ, N) be a SEPP. Then:*

(i) There is a unique isometric embedding

$$N^\vee : L^2(\mathbb{R}^d, \widehat{\gamma}) \longrightarrow L^2(X, \mu)$$

with $N^\vee(\widehat{f}) = N_f$ for all rapidly decreasing functions[5] f on $\mathbb{R}^d$. It intertwines U and T.

(ii) The algebra of functions generated by $N^\vee(L^2(\mathbb{R}^d, \widehat{\gamma}))$ is dense in $L^2(X, \mu)$.

(iii) $k \in \mathbb{R}^d$ is an eigenvalue for U if and only if $\widehat{\gamma}(\{k\}) > 0$, i.e. there is a Bragg peak at k. The corresponding eigenfunction in $L^2(\mathbb{R}^d, \widehat{\gamma})$ is the function $\mathbf{1}_k$, and $N^\vee(\mathbf{1}_k)$ is a k-eigenfunction for $L^2(X, \mu)$. The equation

$$N^\vee(\mathbf{1}_k)(\Lambda) = \lim_{R\to\infty} \frac{1}{\operatorname{vol} C_R} \sum_{x \in \Lambda \cap C_R} e^{2\pi i k.x}$$

holds, where the limit is taken in the L^2 sense [6].

The $N^\vee$ is not in general surjective. If it is then the theorem says that the diffraction really determines μ. But this does not usually happen, even in the case that both sides are pure point. However, the eigenfunctions for U are exactly the strange looking functions $\mathbf{1}_k$, $\widehat{\gamma}(\{k\}) > 0$, which take the value 1 at k and zero everywhere else.

Unfortunately, outside the context of point sets supported on a lattice, sums like this cannot be construed as measures once Λ becomes infinite, and it is the infinite case that we are primarily interested in. One option would be to try and average out these sums as one goes along: $\rho(k) := \lim_{R\to\infty} \frac{1}{\operatorname{vol} C_R} \sum_{x\in\Lambda\cap C_R} e^{2\pi i k.x}$. These are the sums that show up in a series of results known as the Bombieri-Taylor conjecture [7, 14], §4, but they are not the correct objects for the diffraction. The mathematical way out, formulated by A. Hof, is to define the autocorrelation (i.e. the two point correlation) first and then Fourier transform this measure, and this results in $\lim_{R\to\infty} \frac{1}{\operatorname{vol} C_R} \sum_{t,x\in\Lambda\cap C_R} e^{2\pi i k.(-t+x)}$, which is just the Fourier transform of the 2-point correlation above. The individual summands are just normalized versions of the usual diffraction for finite sets. However, the limit has to be taken with care. The diffraction is not usually a function, but only a measure. The summands here are taken as (continuous) measures and the limit is taken in the vague topology.

[5] Infinitely differentiable functions which, along with their derivatives, decay rapidly at infinity.

[6] For a point-wise version of this see [17].

The direct definition of $N^\vee$ given by the formula (1) is not applicable for $\mathbf{1}_k$. Part (iii) comes through the process of the L^2-completion. This is a form of the Bombieri-Taylor conjecture [7, 14], and is derived by a limit process using rapidly decreasing functions. The content of (i) is an elaboration of an idea that was first formulated in this context by S. Dworkin [11]. Thms. 4.1 and 3.1 are consequences of Thm. 4.2. Thm. 4.2 as stated here appears in [9].

Theorem 4.3 *[13] With (X, μ) as above, μ is a pure point measure (and hence $\Lambda \in X$ is almost surely pure point diffractive) if and only if every measurable subset B of X satisfies the condition that for all $\epsilon > 0$ the set*

$$\{t \in \mathbb{R}^d \,:\, \mu(B \triangle (-t + B)) < \epsilon\}$$

is relatively dense[7].

Here $\triangle$ is the symmetric difference. What does this actually say? If we think of B as designating all the Λ of X which have a certain pattern, then $B \triangle (-t + B)$ denotes those Λ for which exactly one of Λ and $-t + \Lambda$ has the pattern. With ϵ small it means that with high probability either both or neither has the pattern. So, in this sense, t is an ϵ-*almost period* of X. Pure pointedness is always related to relative denseness of ϵ-almost periods, see also [4].

Suppose that (X, μ, N) is a pure point SEPP. The diffraction consists of Bragg peaks in Fourier space, which is $\mathbb{R}^d$. Let S denote the set of positions of the Bragg peaks. Via the mapping $N^\vee$ the eigenfunctions of U, namely the functions 1_k, $k \in S$, are mapped to eigenfunctions of T in $L^2(X, \mu)$. The eigenvalue group E introduced in §4 is generated by S, but in general $S \neq E$. The points of $E \backslash S$ are often called *extinctions*, places where potentially there could be a Bragg peak but where, in fact, there are none. We know that $S = -S$ and S generates E. Thus $E = \cup_{n=1}^{\infty} n\, S$, where $nS := S + \cdots + S$ (n summands). The complexity of the diffraction seems to be related deeply to the nature of the extinctions. One indication of this is:

Proposition 4.4 *[19] Let (X, μ, N) be a pure point stationary ergodic point process. If $nS = E$ then μ is entirely determined by the $2, 3, \ldots, 2n+1$-correlations. In particular, if $S = E$ then the process is determined by the 2 and 3-point correlations*[8].

5 Model sets

Model sets, or cut and project sets, are very familiar to the quasicrystal community and afford natural examples of SEPPs. One extends physical space $\mathbb{R}^d$ by an internal space H for which there is a lattice $\mathcal{L} \subset \mathbb{R}^d \times H$ with the properties that the projection mappings of the *cut and project scheme* (cps)

$$\begin{array}{ccccc} \mathbb{R}^d & \xleftarrow{\pi_1} & \mathbb{R}^d \times H & \xrightarrow{\pi_2} & H \\ & & \cup & & \\ L & \xleftrightarrow{\simeq} & \mathcal{L} & & \end{array} \qquad (3)$$

satisfy $\pi_1|_{\mathcal{L}}$ of π_1 is injective and $\pi_2(\mathcal{L})$ is dense in H.

Let $L := \pi_1(\mathcal{L})$ and $(\cdot)^\star\colon\, L \longrightarrow H$ be the mapping $\pi_2 \circ (\pi_1|_{\mathcal{L}})^{-1}$. A *regular model set* is a set of the form $\mathit{\Lambda}(W) := \{x \in L : x^\star \in W\}$, or some translate of this, where W is a compact subset of H which is the closure of its interior and the boundary of W has measure 0. Model sets are uniformly discrete.

Often people use a Euclidean space as internal space H, but mathematically H needs only to be a locally compact Abelian group. As $\mathcal{L}$ is a discrete and co-compact subgroup of $\mathbb{R}^d \times H$, the quotient $\mathbb{T} := (\mathbb{R}^d \times H)/\mathcal{L}$ is a compact Abelian group[9]. In the standard cut and project setting with Euclidean spaces only, this group is a torus. There is an obvious action of $\mathbb{R}^d$ on $\mathbb{T}$ given by $x + \big((t,h) + \mathcal{L}\big) := (x+t, h) + \mathcal{L}\,, \quad x \in \mathbb{R}^d$, through which $(\mathbb{T}, \mathbb{R}^d)$ is a minimal and uniquely ergodic dynamical system with respect to the Haar measure $\theta_{\mathbb{T}}$ of $\mathbb{T}$. The hull $X(\Lambda)$ of Λ is the closure in $\mathcal{D}_r$ of the set of

[7] A subset P of $\mathbb{R}^d$ is relatively dense if there is an R so that every R-cube contains at least one point of P.

[8] The importance of moments in the study of crystallography (and quasicrystallography) was emphasized in a paper of N. D. Mermin [21]. Although the formalism there cannot be applied to infinite discrete point sets, nonetheless forerunners of Prop. 4.4 and Prop. 5.1 are stated there.

[9] Although H is not uniquely determined by Λ, it is possible to arrange things so that W generates H as a group and there are no non-zero $t \in H$ with $t + W = W$. With these conditions H is unique up to isomorphism (e.g. for the Penrose tilings it is $\mathbb{R}^2 \times \mathbb{Z}/5\mathbb{Z}$). In this form H has a description which shows that it has a direct physical meaning which relates to the way L looks from the point of view of almost periodicity, see [4].

translations of Λ. It is uniquely ergodic and, using the counting function N of (1), we obtain a SEPP (X, μ, N). We shall assume that X is mininal[10]. It reasonable to think of $X(\Lambda)$ as looking like $\mathbb{T}$: there is a continuous $\mathbb{R}^d$-invariant surjective mapping $\beta : X(\Lambda) \longrightarrow \mathbb{T}$ which is $1-1$ almost everywhere [23]. However, the points at which $1-1$-ness fails are dense in $\mathbb{T}$, so this is a primarily a measure theoretical similarity. It is, however, enough to obtain $L^2(X, \mu) \simeq L^2(\mathbb{T}, \theta_{\mathbb{T}})$, from which the pure pointedness of model sets follows pretty much immediately.

The correlations for model sets look particularly nice in internal space: they are of the form $\theta_H(W \cap \bigcap_{j=1}^n (x_j^\star + W))$, where θ_H is a Haar measure on H. This leads to a strengthening of Prop. 4.4:

Proposition 5.1 *[10] Let (X, μ, N) be determined by the local hull of a model set with internal space of the form $\mathbb{R}^m \times$ (Finite Group). Then (X, μ, N) is completely determined within the class of all model sets on $\mathbb{R}^d$ by the second and third correlations.*

6 The limits of diffraction?

There is an extensive literature on the famous inverse problem of diffraction: given the diffraction of something, what distribution of matter produced it? In effect one is asking for a convolution 'square root' of the autocorrelation. The trouble is that with this bare information the solution need not be unique. This is known as the *homometry problem*. The article by Baake and Grimm [2] in this issue gives some explicit examples of how counter-intuitive this problem can be, even when restricted to point sets.

The diffraction of a point set, or more generally any distribution of matter in $\mathbb{R}^d$, is a measure ω on $\mathbb{R}^d$ with the following properties: it is positive, centrally symmetric, and translation bounded (i.e. for each compact set $K \subset \mathbb{R}^d$ the set $\omega(t + K)$ as t runs over all of $\mathbb{R}^d$ is bounded). Here we pose the general problem of whether an arbitrary *pure point* measure with just these three properties is necessarily the diffraction of something. What makes the problem particularly difficult is that one is not sure at the outset what kinds of 'distributions of matter' one is supposed to be looking for: point sets, continuous functions, measures, something more general?[11]

Remarkably there is an affirmative answer to the question, [20]. Given such a measure there is a way to construct a compact probability space (X, μ) with a pure point ergodic $\mathbb{R}^d$-action, and a continuous mapping $N : C_c(\mathbb{R}^d) \longrightarrow L^2(X, \mu)$ which is $\mathbb{R}^d$-equivariant, so that for all $f \in C_c(\mathbb{R}^d)$,

$$\int_{\mathbb{R}^d} f * \tilde{f} d\gamma = \int_X N_f \overline{N_f} d\mu = \langle f | f \rangle .$$

The elements of X may be interpreted as 'distributions of density' on $\mathbb{R}^d$ and have, almost surely, a naturally defined autocorrelation whose Fourier transform is ω. The construction is not unique but depends on the choice of phase factors, whose freedom can be classified. In this way one achieves what one may call an overview of all solutions to the homometry problem.

There is a penalty for such generality. The stochastic process (X, μ, N) is no longer necessarily a point process. Measure theoretical dynamical systems and measure theoretic point processes have been studied [3, 15], but the situation here seems to be more general still: the elements of X here may not be interpretable as measures on $\mathbb{R}^d$. Rather their structure is to be inferred by testing them with functions $f \in C_c(\mathbb{R}^d)$. The functions N_f, their sums, products, etc. then test the elements of X. From this such properties as uniform discreteness, pattern frequencies, etc. may be inferred. This seems to have a rather physical feel to it. Being a characterization of pure pointedness, it seems to point directly at what really underlies pure point diffraction. There remain, of course, the much deeper problems of classifying those choices of phase factors that lead to point sets, continuous distributions of matter, measures, etc.

Acknowledgements The brief bibliography below is a small indication of the work that has gone into the

[10] There are numerous variations on the definition of models sets, none of which make much difference to what we are saying here. Minimality is equivalent to repetitivity. This is easy to arrange: $\mathit{\Lambda}(W)$ is repetitive if there are no points of $L^\star$ on the boundary of W.

[11] There is an explicit class of solutions to the convolution root problem under the name of Boas-Kac theorems, see [6, 12] which hold under conditions in which, among other things, all the objects in question have to be functions and to have compact support. In their presently available forms it seems difficult to apply them to the problem that we are addressing.

mathematics of diffraction and relates only to the material discussed here. Thanks to my colleagues and coauthors who have done so much to make the time that I have spent on this subject so congenial. Thanks also to Michael Baake and Uwe Grimm for their valuable comments. The author acknowledges the on-going support of the Natural Sciences and Engineering Research Council of Canada.

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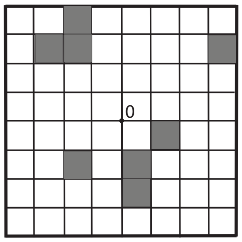

Figure 1: A grid pattern Π: point-sets $\Lambda, \Lambda' \in X$ are close if they make the same grid pattern for some large fine-meshed grid around 0. The proportion of X taken up by the set $B(\Pi)$ of elements $\Lambda \in X$ sharing the same pattern Π is given by $\mu(B(\Pi))$.

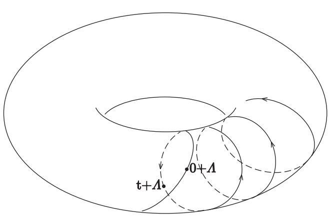

Figure 2: A schematic view of a point-set dynamical system X over $\mathbb{R}$. Each point of X represents an entire discrete point set in $\mathbb{R}$. Part of the orbit of a single point-set Λ is shown. Orbits close only if there is periodicity. Close returns of the orbit to Λ indicate point sets $t + \Lambda$ that match Λ closely on a region around the origin. This type of picture is accurate from the measure theoretical point of view, but omits much of the fine topological detail. It is the former that is most important for the theory of diffraction.