LONG-RANGE ORDER AND DIFFRACTION

DEDICATED TO TAKEO YOKONUMA ON THE OCCASION OF HIS RETIREMENT FROM SOPHIA UNIVERSITY.

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ABSTRACT. The paper is intended to introduce the reader to the mathematics of long-range (aperiodic) order and to some of the recent work on diffraction, especially pure point diffraction.

To carry the self forward
and realize the ten thousand dharmas is delusion.
That the ten thousand dharmas advance
and realize the self is enlightenment. [1]

1. INTRODUCTION

For a conference which revolves around group theory and its representations, this paper seems a little out of place. Nonetheless, much of group theory is about symmetry, and symmetry is about pattern and order. And in fact we shall see that the mathematics that we are going to discuss is entirely based on group theory. More than that, it points to a whole realm of new mathematics that may be explored, of which we are only seriously looking at the Abelian part so far.

The prototype of a structure with long-range order in ordinary 3-space is a simple motif or pattern that is repeated indefinitely in three independent directions. This is periodic order and it is an extreme situation. If you look at mountainous terrain or at prairie landscape from an airplane you see in each case a scene of long-range order – any part of the scene looks much like any other. However this is far from periodic. So the notion of rigid symmetry in describing order, the precise and perfect alignment of parts under some transformation is not an appropriate tool for understanding order in the larger sense.

This is a rather philosophical discussion, but the discovery of quasi-crystalline materials, as they came to be known, in the early 1980's showed that there is unknown territory with great internal order that we know little about. D. Shechtman [38], discovered, quite unexpectedly, a metallic phase of Al-Mn that produces a crystal-like diffraction pattern, that is to say, a pattern of sharp bright spots, which has icosahedral symmetry. The sharp bright spots, **Bragg peaks**, signal long-range order, but the icosahedral symmetry violates the crystallographic restriction in 3-space. This was not a crystal, but its long-range structure was so coherent that it was sufficient to scatter an incoming beam of X-rays so as to create an interference pattern just like that of a crystal (see Figure 1).

Since that time a great deal of work has been done by mathematicians, physicists, and material scientists in trying to understand this type of order. This has heightened our awareness of just how great and wonderful world of symmetry there is between crystal-like order and randomness. As Robert Burton likes to put it, there is the perfect garden of heavenly delights on the one hand, and Bernoulli City, the more disordered place we most often live in, on the other!

The work reported in this paper is about structures and mathematics that might best be described as **almost periodic**. It has been pointed out that any society that based its calendar on the moon has

[1] EIHEI DOGEN, from *Genjokoan*, 1233 CE, translation Hakuyu Taizan Maezumi.

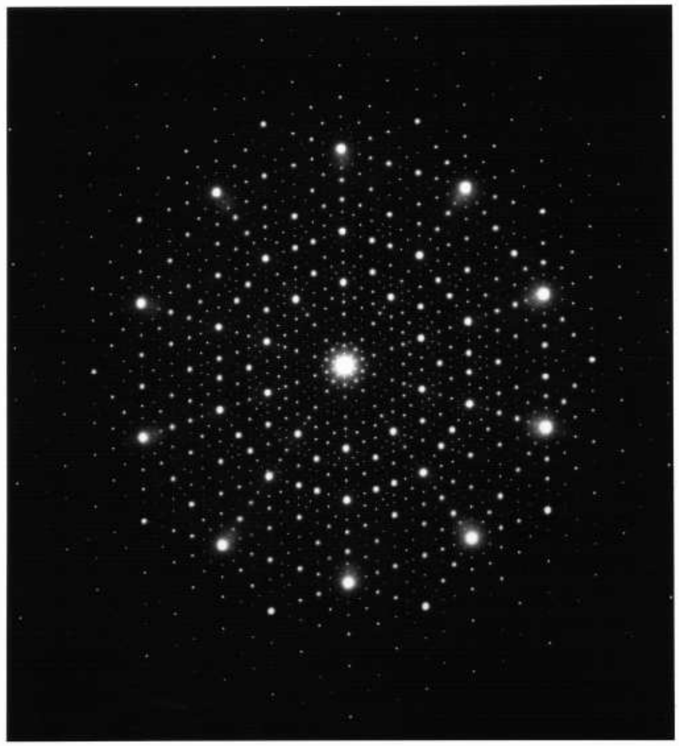

FIGURE 1. Diffraction from decagonal $Al_{70}Co_{11}Ni_{19}$ from an image by C. Beeli.

already invested a lot of time into the area of almost periodic order. The subject of almost periodic functions and measures is also well-established and is part of what we have to say. But our aim here is to survey some of the new developments, all around diffraction, that show how we are coming to see almost periodic order today. In the bibliography we have highlighted (using a five-fold star ($\star$)) a few papers and two books of papers [32, 6] which we feel offer good places to pick up further background and more detailed references to the literature. The second of these books also has its own *Guide to the Quasicrystal Literature*.

2. Discrete point sets

The setting for the mathematics that we are going to discuss is that of compactly generated locally compact Abelian groups. However, from the point of view of exposition, as well as for application, we shall stay with the case of $\mathbb{R}^d$. Doing this does not trivialize the subject in any way; in fact, even the case $d = 1$, which has existed for years as the theory of sequences [36], provides many of the characteristics of the more general theory.

We are interested in discrete and extended objects in $\mathbb{R}^d$. A subset Λ of $\mathbb{R}^d$ is called **locally finite** (alternatively closed and discrete) if for all compact subsets K of $\mathbb{R}^d$, $\Lambda \cap K$ is finite. Stronger than this is uniform discreteness: Λ is r**-uniformly discrete** if for all $x \in \Lambda$, $(x + B_r) \cap \Lambda = \{x\}$, where B_r is the ball of radius r around 0. We say that Λ is **uniformly discrete** if $r > 0$ exists for which Λ is r-uniformly discrete. Obviously every uniformly discrete set in $\mathbb{R}^d$ is countable. The set of all uniformly discrete subsets of $\mathbb{R}^d$ is denoted by $\mathcal{D} = \mathcal{D}(\mathbb{R}^d)$ and the set of r-uniformly discrete subsets by $\mathcal{D}_r$.

Uniformly discrete sets can have various further regularity properties. A uniformly discrete subset Λ of $\mathbb{R}^d$ is called **Delone** if it is also relatively dense, i.e., if there exists a compact K in $\mathbb{R}^d$ with

$\mathbb{R}^d = \Lambda + K$. Delone sets are considered to be a natural setting for idealizing atomic solids, since the uniform discreteness can be thought of as a statement about minimal separation of atoms, and the relative denseness as a statement about the homogeneous nature of the way in which space is filled with atoms (no arbitrarily large holes).

Throughout the paper Λ will be always be uniformly discrete.

Given a finite or countably infinite point set $\Lambda \subset \mathbb{R}^d$ we shall often represent it by the **Dirac comb**

$$\delta_\Lambda := \sum_{x \in \Lambda} \delta_x \,,$$

that is, the measure satisfying $\langle \delta_\Lambda, f \rangle = \sum_{x\in\Lambda} f(x)$ for all continuous compactly supported functions f on $\mathbb{R}^d$.

More realistic assumptions would allow "different types" of points, to represent different types of atoms. We will treat this later. Also one may require the atoms to have extended scattering profiles. This can be arranged simply by convolving the comb with the required profile: $c*\delta_\Lambda(t) = \sum_{x\in\Lambda} c(t-x)$. This turns out to be easy to do after the fact, so we can keep this little complication out of the picture in developing our theory.

The measure δ_Λ is a (positive) translation bounded measure on $\mathbb{R}^d$, i.e., for all compact sets K, $|\delta_\Lambda|(t+K)$ (which in our case is $\delta_\Lambda(t+K)$) is uniformly bounded in t.

Let Λ be uniformly discrete. A considerable rôle is played by the set of translation vectors $\Lambda - \Lambda$ of our set Λ. We say that Λ is of **finite local complexity** if $\Lambda - \Lambda$ is locally finite. The name comes from the equivalent condition that for every compact $K \subset \mathbb{R}^d$

$$\{(-x+\Lambda) \cap K : x \in \Lambda\}$$

is finite. In effect it says that the set of patterns formed around a point of Λ by centering the compact set K on it, is finite. This is a strong condition on the homogeneity of the set Λ and it implies that the group $\langle \Lambda - \Lambda \rangle$ is finitely generated.

3. Meyer Sets

A set $\Lambda \subset \mathbb{R}^d$ is a **Meyer set** if it is relatively dense and $\Lambda - \Lambda$ is uniformly discrete. It is automatic that a Meyer set is a Delone set with finite local complexity.

Meyer sets were introduced (as relatively dense harmonious sets) by Y. Meyer [30]. The Meyer sets are quite robust − adding or removing a finite number of points from a Meyer set does not destroy the Meyer property. They also have a remarkable number of different characterizations of which the one we have used as a definition (due to J. Lagarias [23]) is the simplest looking. Although Meyer established many of these, the most accessible account of the entire set of characterizations is [33]. To give some indication of the strong implications of the Meyer condition on the Fourier side, we give a short version of the main theorem which is to be found there.

Definition: For $\Lambda \subset \mathbb{R}^d$ and every $\epsilon \geq 0$ define the **ϵ-dual** of Λ by

$$\Lambda^\epsilon = \{\lambda \in \mathbb{R}^d : |e^{2\pi i \lambda . x} - 1| \leq \epsilon \text{ for all } x \in \Lambda\} \,.$$

This looks like a rather imprecise type of condition, but in fact it is not. For example, if Λ is relatively dense, then for all $\epsilon < 1$, Λ^ϵ is uniformly discrete. If Λ is actually a lattice and $\epsilon < \sqrt{3}$ then $\Lambda^\epsilon = \Lambda^0$ (i.e., it is the same as if ϵ were 0), which is none other than the dual lattice of Λ: $\{\lambda \in \mathbb{R}^d : \lambda . x \in \mathbb{Z} \text{ for all } x \in \Lambda\}$. This is the essence of the famous Bragg condition for diffraction in crystals.

So, the condition $|e^{2\pi\lambda . x} - 1| \leq \epsilon$ for all $x \in \Lambda$ is a statement that λ is almost in the "dual" of Λ. It is rather an amazing coherence condition. In general one cannot expect a relatively dense set Λ to have any of these almost periods. Yet we have:

Theorem 1. *Let $\Lambda \subset \mathbb{R}^d$ be relatively dense. The following are equivalent (to Λ being a Meyer set):*

(1) $\Lambda - \Lambda$ *is uniformly discrete;*

(2) *there is a finite set F so that $\Lambda - \Lambda \subset \Lambda + F$;*
(3) *for every $\epsilon > 0$, Λ^ϵ is relatively dense;*
(4) *for some $0 < \epsilon < 1/2$, Λ^ϵ is relatively dense.*

Thus the Meyer property is a strong coherence conditon which obviously relates deeply to the Fourier side of Λ. The following unexpected result reveals this more clearly:

Theorem 2 (Strungaru)**.** *If Λ is a Meyer set then the set of Bragg peaks in its diffraction pattern is relatively dense in $\mathbb{R}^d$.*

This result brings us to the subject of diffraction. It says that a diffraction images of a Meyer set (taken in appropriate directions) will show a relatively dense set of bright spots.

4. Diffraction

The diffraction of a distribution of density in space is usually described as the square absolute value of some suitably normalized Fourier transform of this density[2]. Alternatively it is the Fourier transform of the volume averaged autocorrelation. For finite sets of scatterers or for cyrstals, both lead to the same thing. With quasicrystals one has to be careful - because of issues of convergence, only the second one makes mathematical sense. Formally the definitions are as follows:

Let $\Lambda \in \mathcal{D}_r$ be locally finite and ω the corresponding Dirac comb. Define $\omega_R = \omega|_{B_R}$ and $\tilde{\omega}_R = (\omega_R)\tilde{}$. Then, the measure

$$\gamma_\omega^{(R)} \;:=\; \frac{\omega_R * \tilde{\omega}_R}{\mathrm{vol}(B_R)} \;=\; \frac{1}{\mathrm{vol}(B_R)} \sum_{x,y \in \Lambda \cap B_R} \delta_{x-y}$$

is well defined, as it is the (volume averaged) convolution of two **finite** measures[3]. The **autocorrelation** measure γ_ω of ω is the limit of $\big(\gamma_\omega^{(R)}\big)_R$ in the vague topology as $R \to \infty$, *if this limit exists*[4].

We will assume that the autocorrelation measure γ_ω exists. It is a positive definite, translation bounded measure, and as such has a well-defined Fourier transform (also defined on $\mathbb{R}^d$), which is also a positive translation bounded measure. This measure, $\widehat{\gamma}_\omega$, is the **diffraction** or **diffraction measure** of ω. The pure point part of this measure is called the **Bragg spectrum**. The set Λ is called **pure point diffractive** if $\widehat{\gamma}_\omega$ is a pure point (also called discrete or atomic) measure on $\mathbb{R}^d$.

The theory of diffraction in this form was laid out carefully in the papers of A. Hof, and his papers [19, 20] are the natural place to get into this subject. For more on the basic theory of translation bounded measures the first chapter of [9] is a good place to look.

So the essence of quasicrystals is that the Fourier transform of the autocorrelation is a pure point measure or has a significant pure point part in addition to some continuous part which may be singular continuous, absolutely continuous, or a mixture of both. There is a deliberate lack of precision in this definition. The definition is that given by the International Union of Crystallographers, and reflects the reality that experimentalists have to deal with – and increasingly so. In fact this is good for the mathematics too, because it clearly points out the need for us to understand more than just pure point diffractive sets.

Going back to the autocorrelation, it is rather easy to see why the set of translation vectors $\Lambda - \Lambda$ is so important. If Λ has finite local complexity then $\Lambda - \Lambda$ is locally finite and $\gamma_\omega = \sum_{t \in \Lambda - \Lambda} \eta(t)\delta_t$

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[2] For a physical approach to diffraction, one may consult [11]

[3] If f is a function on $\mathbb{R}^d$ then $\tilde{f}$ is the function $\tilde{f}(x) = \overline{f(-x)}$; and for a measure μ, the measure $\tilde{\mu}$ is defined by $\tilde{\mu}(f) = \overline{\mu(\tilde{f})}$ for all f.

[4] A sequence of translation bounded measures $\{\nu_i\}$ converges to the measure ν in the vague topology if for all continuous functions f of compact support the sequence $\{\nu_i(f)\}$ converges to $\nu(f)$.

where the coefficients are given by

$$\eta(t) \;=\; \lim_{R\to\infty} \frac{1}{\mathrm{vol}(B_R)} \sum_{\substack{x,y\in\Lambda\cap B_R \\ x-y=t}} 1 = \lim_{R\to\infty} \frac{1}{\mathrm{vol}(B_R)} \mathrm{card}(\Lambda\cap(t+\Lambda)\cap B_R). \tag{1}$$

The second equality uses the fact that as R becomes large the error caused by the mismatching of B_R and $t+B_R$ becomes negligible with respect to the volume of B_R. The function η can be extended from $\Lambda-\Lambda$ to all of $\mathbb{R}^d$ by setting $\eta(t)=0$ for all other t. It is a positive definite function.

What is particularly relevant here is the fact that there is a pseudo-metric defined on the space $\mathbb{X}_0$ of all $\mathbb{R}^d$- translates of Λ defined for all t,

$$\begin{aligned} d(s+\Lambda, t+\Lambda) : &= \lim_{R\to\infty} \frac{\mathrm{card}\left(((s+\Lambda)\ \triangle\ (t+\Lambda))\cap B_R\right)}{\mathrm{vol}(B_R)} \\ &= \lim_{R\to\infty} \frac{\mathrm{card}\left((\Lambda\ \triangle\ (t-s+\Lambda))\cap B_R\right)}{\mathrm{vol}(B_R)} = 2(\eta(0)-\eta(t-s))\,, \end{aligned} \tag{2}$$

as can be seen from the definition of the symmetric difference operator $\triangle : \Lambda \triangle (t+\Lambda) = (\Lambda\cup(t+\Lambda))\backslash(\Lambda\cap(t+\Lambda))$.

Thus the pseudo-metric d, which we call the **autocorrelation pseudo-metric**, and the autocorrelation coefficients $\eta(t)$ are directly related. We will say more about this later, but to end this section we offer two criteria for pure point diffraction that are relevant. The first is a very general result of J. Gil de Madrid and L. N. Argabright:

Theorem 3. [16] *The measure ω is pure point diffractive if and only if the autocorrelation measure γ_ω is strongly almost periodic.*

This key result of the theory introduces a new concept, **strong almost periodicity**, which by virtue of its appearance here is crucial for the fundamental understanding of pure point diffraction. However it is not particularly intuitive. Fortunately, under the assumption that $\Lambda-\Lambda$ is uniformly discrete (the **Meyer** condition), we have something more readily appreciated.

Define, for all $\epsilon>0$,

$$P_\epsilon := \{t\in\mathbb{R}^r \,:\, d(t+\Lambda,\Lambda)<\epsilon\} = \{t\in\mathbb{R}^d \,:\, \eta(0)-\eta(t)<\epsilon/2\}\,. \tag{3}$$

We call these the sets of **statistical ϵ- almost periods**.

Theorem 4. [7] *Suppose that Λ is a Meyer set with a well-defined autocorrelation. The autocorrelation measure γ_ω of ω is strongly almost periodic if and only if, for all $\epsilon>0$, P_ϵ is relatively dense.*

Thus, for a Meyer set Λ, pure pointedness of the diffraction hinges around a property of almost periodicity. See Theorem 13 for a generalization of this.

5. Topologies on Point Sets

We now come to the two notions of closeness of point sets. We will define two topologies, each defined by means of a uniformity.

For each pair (R,ϵ), positive real numbers define

$$U(R,\epsilon) := \{(\Lambda,\Lambda')\in\mathcal{D}_r\times\mathcal{D}_r : \Lambda\cap B_R\subset\Lambda'+B_\epsilon \quad \text{and} \quad \Lambda'\cap B_R\subset\Lambda+B_\epsilon\} \tag{4}$$

These sets form a fundamental system for a uniform structure on $\mathcal{D}_r$ whose topology has the sets

$$U_{LT}(R,\epsilon)[\Lambda] := \{\Lambda'\in\mathcal{D}_r : (\Lambda',\Lambda)\in U(R,\epsilon)\} \tag{5}$$

as a neighbourhood basis of Λ. We call it the **local topology** on $\mathcal{D}_r$.

This uniformity can also be described by a metric, though it is not particularly natural. The intuition is that two sets are close if inside some large ball around 0 each set is within ϵ of the other.

One should note that the uniformity is certainly invariant under translations, but the individual entourages $U_{LT}(R, \epsilon)$ are not. The natural translation action of $\mathbb{R}^d$ on $\mathcal{D}_r$ is continuous.

The second notion of closeness is based on average matching of the two sets. Let $\varLambda, \varLambda' \in \mathcal{D}_r$.

$$d(\varLambda, \varLambda') := \limsup_{r\to\infty} \frac{\text{card}((\varLambda \triangle \varLambda') \cap B_r)}{\text{vol}(B_r)} . \tag{6}$$

It is rather easy to see that d is a pseudo-metric on $\mathcal{D}_r$ and it is invariant under $\mathbb{R}^d$-translation.

We obtain a metric by defining the equivalence relation

$$\varLambda \equiv \varLambda' \Leftrightarrow d(\varLambda, \varLambda') = 0$$

and factoring d through it:

$$\mathcal{D}_r^{\equiv} := \mathcal{D}_r/\equiv \quad \text{and} \quad d : \mathcal{D}_r^{\equiv} \times \mathcal{D}_r^{\equiv} \longrightarrow \mathbb{R}_{\geq 0} . \tag{7}$$

Note that the translation action of $\mathbb{R}^d$ is retained on $\mathcal{D}_r^{\equiv}$.

We call the resulting topology on $\mathcal{D}_r$ the **autocorrelation topology**. As we will note below, $\mathcal{D}_r$ under the local topology and $\mathcal{D}_r^{\equiv}$ under the autocorrelation topology are both complete spaces - that is they are already their Hausdorff completions.

The action of $\mathbb{R}^d$ on $\mathcal{D}_r$ in the autocorrelation topology is not continuous. This is rectified by introducing a new uniformity defined by the basic fundamental entourages:

$$U_{mACT}(\epsilon_1, \epsilon_2) := \{(\varLambda, \varLambda') \in \mathcal{D}_r \times \mathcal{D}_r : d(v + \varLambda, \varLambda') < \epsilon_1 \text{ for some } v \in B_{\epsilon_2} .\} \tag{8}$$

The resulting topology is the **mixed autocorrelation topology**.

It is worth noting that in each of the local topology and the mixed autocorrlation topology there are two ways in which point sets can be close: by small translations by elements of $\mathbb{R}^d$ and by some overall similarity of structure. It is the latter that relates to almost periodicity.

Theorem 5. i) *$\mathcal{D}_r$ is a compact metric space in the local topology* [37].
ii) *$\mathcal{D}_r^{\equiv}$ is a complete space and is the Hausdorff completion of $\mathcal{D}_r$ in the autocorrelation topology* [35].
iii) *$\mathcal{D}_r^{\equiv}$ is a complete space in the mixed autocorrelation topology* [4].

Some idea of the local topology can be gleaned from the following observation. If one takes a large square S around the origin in $\mathbb{R}^d$ and divides it, chessboard fashion, into a grid of small squares, then for each finite selection F of some of these smaller squares one may consider the collection of all point sets in $\mathcal{D}_r$ whose intersection with S contains points of exactly those small squares of F and no others. The subsets of $\mathcal{D}_r$ so formed as S and F vary are a neighbourhood basis for the topology of $\mathcal{D}_r$. From this it is easy to see that $\mathcal{D}_r$ is totally bounded, hence, being closed, also compact.

The natural action of $\mathbb{R}^d$ on $\mathcal{D}_r$ is uniformly continuous. Typically some $\mathbb{R}^d$ probability measure μ on $\mathcal{D}_r$ is also attached to the system so $(\mathcal{D}_r, \mathbb{R}^d, \mu)$ is a dynamical system. Most commonly μ is supported on some closed $\mathbb{R}^d$-invariant subspace $\mathbb{X}$ of $\mathcal{D}_r$ and μ is at least ergodic and often uniquely ergodic. Thus more generally we shall be interested in some dynamical system of the form $(\mathbb{X}, \mathbb{R}^d, \mu)$ where $\mathbb{X} \subset \mathcal{D}_r$. This is explained in more detail below where we look at hulls of locally finite point-sets $\varLambda$.

The autocorrelation topology is natural, but we do want to point out that it actually takes some work to prove Theorem 5 (ii) and (iii). The problem is that it is not at all obvious that a Cauchy sequence of point sets in the autocorrelation topology (or its mixed version) will converge to some point set. As we have pointed out, it is only in the mixed autocorrelation topology that we obtain a continuous action of $\mathbb{R}^d$. We will also see dynamical systems in this topology.

We denote by β the natural mapping (which is an $\mathbb{R}^d$-mapping):

$$\beta : \mathcal{D}_r \longrightarrow \mathcal{D}_r^{\equiv} . \tag{9}$$

This mapping is an $\mathbb{R}^d$- mapping but it is **not** continuous. However, it can be on certain closed subsets of $\mathcal{D}_r$, and this will become a major theme in our discussion of model sets (see Theorem 6).

6. Dynamical hulls

In the dynamics of a physical system one considers a (compact) configuration space or phase space and the time evolution of points of this space. Of special importance is the notion of recurrence, in the sense of the time-orbit of a point returning very closely to the initial state.

In the geometry of point sets and tilings a parallel construction on points sets is possible, using the translation action of the underlying space as the group action, instead of time. This provides a powerful way of understanding the internal geometry of a given point set. We begin with $\mathcal{D}_r$ and its translation action by $\mathbb{R}^d$, take a single point set of interest, $\Lambda \in \mathcal{D}_r$, and then construct the closure of its orbit under translation: $\overline{\mathbb{R}^d + \Lambda}$.

Our two topologies provide two separate interpretations of the orbit closure of $\Lambda \in \mathcal{D}_r$:

$$\begin{aligned} \mathbb{X}(\Lambda) &= \overline{\mathbb{R}^d + \Lambda} \quad \text{in the local topology} \\ \mathbb{A}(\Lambda) &= \overline{\mathbb{R}^d + \Lambda} \quad \text{in the autocorrelation topology} \end{aligned}$$

which are the **local and autocorrelation hulls** respectively[5].

First of all, let us look at the local hull. Since $\mathbb{X}(\Lambda)$ is a closed subset of $\mathcal{D}_r$ it is compact. Recall that a dynamical system which is the closure of an orbit is minimal if and only if it is uniformly recurrent (in our notation this means that for each point $\Lambda' \in \mathbb{X}(\Lambda)$ and for each open neighbourhood V of Λ' the set of t in $\mathbb{R}^d$ for which $t + \Lambda'$ is in V is relatively dense in $\mathbb{R}^d$,[15]). In the case of $\mathbb{X}(\Lambda)$ this condition on Λ is called **repetitivity** and has a simple geometrical meaning: Λ is **repetitive** if and only if for each $r > 0$ there is an $R > 0$ so that for each $x \in \Lambda$ and for each $y \in \mathbb{R}^d$ there is a copy, under translation, of the cluster of points $(x + B_r) \cap \Lambda$ in $(y + B_R) \cap \Lambda$. Everything repeats, and it does so with some degree of regularity. This is a type of almost periodicity and it means that the information that one can derive by looking locally at a cluster gives no information about the global position of that cluster in the entire point-set.

Proposition 1. [40] *Let $\Lambda \in \mathcal{D}_r$ and let $\mathbb{X}(\Lambda)$ be its local hull.*

i) *$\mathbb{X}(\Lambda)$ is minimal if and only if Λ is repetitive.*
ii) *$\mathbb{X}(\Lambda)$ is uniquely ergodic if and only if it has uniform cluster frequencies.*

A **cluster** of Λ is a finite subset of its points. Let F be such a cluster. The frequency of F relative to the point $u \in \mathbb{R}^d$ is

$$\lim_{R \to \infty} \frac{\operatorname{card}\{t \in u + B_R \,:\, (t + F) \subset \Lambda\}}{\operatorname{vol} B_R}\,.$$

Uniform cluster frequency means that this limit converges uniformly in R independently of the reference point u.

Suppose that $(\mathbb{X}, \mathbb{R}^d, \mu)$ is ergodic for some invariant probability measure μ. Since $\mathbb{R}^d$ acts on $\mathbb{X}(\Lambda)$ it acts also on $L^2(\mathbb{X}(\Lambda), \mu)$ and the action is unitary. It was Koopman who in the 1930s suggested that the study of the spectrum of this unitary action should provide insight into the nature of $\mathbb{X}$. Its connection with diffraction was first pointed out by S. Dworkin in [14]. Dworkin's argument is the basis of one half of the following result.

Proposition 2. [26] *Let $\Lambda \in \mathcal{D}_r$ be of finite local complexity and have uniform patch frequencies (or equivalently it is uniquely ergodic). Then Λ is pure point diffractive if and only if the spectrum of $L^2(\mathbb{X}(\Lambda), \mu)$ is pure point (i.e. has a Hilbert basis of eigenfunctions) .*

We have offered here an explicit place to look for a complete proof of this result, but in one way or another it has been around for some time. The result also applies (without change of hypotheses) for multi-sets – see below. It has also been generalized to dynamical systems of translation bounded measures [2].

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[5]For a useful introduction to topological and measure-theoretical dynamics, see [43].

It is useful to note that both $\mathbb{X}(\Lambda)$ and $\mathbb{A}(\Lambda)$ can be interpreted as completions of our starting space $\mathbb{R}^d$. In each case one simply provides $\mathbb{R}^d$ with a new topology by pulling back of the uniform topology on $\mathcal{D}_r$ to $\mathbb{R}^d$ using the mapping $x \mapsto x + \Lambda$. In both cases, points that are usually close in $\mathbb{R}^d$ remain so. But now also $x, x' \in \mathbb{R}^d$ are close if $x + \Lambda$ and $x' + \Lambda$ are close in the local (resp. autocorrelation) topology.

$\mathbb{A}(\Lambda)$ has the structure of an Abelian group, a fact that arises from the group structure of $\mathbb{R}^d$ and the translation invariance of the autocorrelation entourages. In particular it has a unique invariant probability measure $\theta_{\mathbb{A}}$ (Haar measure). In general $\mathbb{X}(\Lambda)$ does not get a group structure in this way.

We need to know what the basic open sets for this new autocorrelation topology of $\mathbb{R}^d$ look like. It suffices to consider open sets around 0, and for these a basis consists of the sets P_ϵ which we defined in (3).

Thus both $\mathbb{X}(\Lambda)$ and $\mathbb{A}(\Lambda)$ become dynamical systems under appropriate conditions. In the case of $\mathbb{A}(\Lambda)$, mimimality comes for free with the compactness. However, the real importance of compactness from our point of view is:

Proposition 3. [7, 35] *Let $\Lambda \in \mathcal{D}_r$. Then the first two statements below are equivalent. If Λ is a Meyer set, all three are equivalent.*

i) $\mathbb{A}(\Lambda)$ *is compact;*
ii) *for all $\epsilon > 0$, P_ϵ is relatively dense;*
iii) *Λ is pure point diffractive.*

7. Model Sets

Abstractly we know what pure point diffraction means, but how do we construct interesting examples of it? One way, whose origins date back to the earliest days of quasi-cyrstallography, is to create suitable sets $\Lambda \subset \mathbb{R}^d$ by projection of a lattice in some higher dimensional space. The idea seems to have originated from the realization that to index the diffraction patterns of experimentally created quasicrystals – that is, assign systems of integer co-ordinates to the Bragg peaks – it is necessary to use 6 rather than the usual 3 co-ordinates. The Bragg peaks were lying on a $\mathbb{Z}$-module of rank 6 even though the material itself is a 3-dimensional solid. This is in striking contrast to crystals which are always indexed by the same number of co-ordinates as the dimension [6]. So the thought arose to view the atomic sites of the quasicrystal as points projected from a lattice in a higher dimensional space (6 in this case). However, this has to be mitigated in some way, for the projected lattice has either accumulation points or just reduces to a 3D lattice again. The idea is to cut the higher dimensional lattice by a cylinder in the direction of the given space of the crystal so that the cross-section is a compact set with non-empty interior in the orthogonal direction, and project only the lattice points falling in this cylinder.

Interestingly enough, Meyer [30] had also created such sets, though in more generality and for entirely different reasons. His method, turned around a bit, has become the basic formalism for the cut and project formalism, and the resulting sets are called model sets, as he had named them.

With these preliminaries we go directly to the general definitions. One feature of this is that the "higher dimensional space" is best taken to be of the form $\mathbb{R}^d \times H$ where H is some locally compact Abelian group. Doing this allows the theory to cover many more interesting examples – the chair tiling, for instance, which is shown in Figure 2 – and, as we shall see, is actually necessary for some parts of the theory.

A **cut and project scheme** is a triple $(\mathbb{R}^d, H, \mathcal{L})$ of locally compact Abelian groups in which $\mathcal{L}$ is a lattice in $\mathbb{R}^d \times H$ and for which the natural projections π_1, π_2 satisfy the conditions that $\pi_1|_{\mathcal{L}}$ is injective and $\pi_2(\mathcal{L})$ is dense in H:

[6]The phenomenon higher rank indexing had also appeared, earlier, in the context of modulated structures [11].

$$\begin{array}{ccccc} \mathbb{R}^d & \xleftarrow{\pi_1} & \mathbb{R}^d \times H & \xrightarrow{\pi_2} & H \\ & & \bigcup & & \\ & & \mathcal{L} & & \end{array} \quad . \tag{10}$$

We let $L := \pi_1(\mathcal{L})$ and $^\star : L \longrightarrow H$ be the mapping $\pi_2 \circ (\pi_1|_{\mathcal{L}})^{-1}$. So $\mathcal{L} = \{(t, t^\star)|t \in L\}$, and that it is a lattice means that it is a discrete group and the group $\mathbb{T} := (\mathbb{R}^d \times H)/\mathcal{L}$ is compact. It is worth noting for the next section that the obvious $\mathbb{R}^d$-action on $\mathbb{T}$, namely, $x + (t, t^\star) + \mathcal{L} \mapsto (x + t, t^\star) + \mathcal{L}$, makes it into a minimal dynamical system.

A **model set** (defined by the cut and project scheme (10)) is a non-empty set of the form

$$\varLambda = x + \curlywedge(W) := x + \{t \in L : t^\star \in W\}$$

where $W \subset H$ satisfies the condition $\overline{W} = \overline{W^\circ}$ and is compact, and $x \in \mathbb{R}^d$. If in addition $\theta_H(\partial W) = 0$, where θ_H is Haar measure on H, it is called a **regular** model set.

A recent development [28, 4] has been to introduce **inter-model sets**, which are defined as sets $\varLambda$ of the form

$$x + \curlywedge(W^\circ) \subset \varLambda \subset x + \curlywedge(\overline{W})$$

where W is above. We then have **regular** inter-model sets in the same way.

The advantage of inter-model sets is that for them it is possible to replace the cut and project scheme by one with a smaller H if necessary, so that for $u \in H$, $u + W = W$ if and only if $u = 0$ [39, 28]. We will assume that this condition - called **irredundancy** – holds in what follows.

The regular model set $\varLambda$ is **generic** if $\partial W \cap L^\star = \emptyset$. Generic model sets are repetitive. Since $L^\star$ is countable, the set of $u \in H$ for which the boundary of translated window $u + W$ meets $L^\star$ is actually a meagre set. It is in this sense that they represent the generic situation.

It is not hard to show that model sets are always Delone sets [30, 33] the uniform discreteness coming from the compactness of W and the relative denseness from its non-empty interior. In fact model sets are even Meyer sets, as can be seen by applying the previous sentence to the model set $\varLambda - \varLambda = \{t \in L : t^\star \in W - W\}$.

Regular model sets have uniquely defined autocorrelations[7], so we can consider the autocorrelation group $\mathbb{A}(\varLambda)$. A key point is that $\mathbb{A}(\varLambda)$ and $\mathbb{T}$ are isomorphic as topological groups [35], so in fact $\mathbb{T}$ for a regular model set has a very natural interpretation – namely the completion of the orbit of $\varLambda$ under the autocorrelation topology.

Theorem 6. [40, 4] *Let $\varLambda$ be a regular inter-model set. Then the mapping β of (9) provides a continuous surjective $\mathbb{R}^d$-mapping*

$$\beta : \mathbb{X}(\varLambda) \longrightarrow \mathbb{A}(\varLambda)\,. \tag{11}$$

This mapping β is $1-1$ almost everywhere, in the sense that the set of elements of $\mathbb{A}(\varLambda)$ over which there lie more than one point of $\mathbb{X}(\varLambda)$ is of Haar measure 0.

If we add into this the result of Theorem 3 we obtain the result that makes model sets so interesting:

Theorem 7. *Regular inter-model sets are pure point diffractive. The intensity of the Bragg peak at $k \in \mathbb{R}^d$ is $|\widehat{\mathbf{1}_W}(k^\star)|^2$, where $\mathbf{1}_W$ is the indicator function on W.* [8]

[7]The autocorrelation can be expressed, using a Weyl-type theorem for uniform distributiion [39, 34], as an integral over H which is dependent only on W.

[8]The statement about the intensities of the Bragg peaks in Theorem 7 requires some explanation. Along with our given cut and project scheme $(\mathbb{R}^d, H, \mathcal{L})$ there is a dual one $(\widehat{\mathbb{R}^d} = \mathbb{R}^d, \hat{H}, \mathcal{L}^\circ)$ where $\mathcal{L}^\circ = \hat{\mathbb{T}}$ and the projection into $\mathbb{R}^d$ is the dual of the mapping $x \mapsto (x, 0) + \mathcal{L}$. The Bragg peaks all occur in the projection of $\mathcal{L}^\circ$. As with the original cut and project scheme, there is a mapping of the projection of the lattice $\mathcal{L}^\circ$ over into $\hat{H}$, which we again denote by the superscript *. The indicator function on the window W has a Fourier transform defined on $\hat{H}$. This is the function that occurs in determining the intensities of the Bragg peaks.

Model sets are thus an easily defined class of sets that are in general completely without periods, yet are also in general pure point diffractive. This important result on model sets was first established by A. Hof [19] for polygonal type windows, and later generalized to the arbitrarily locally compact Abelian groups by M. Schlottmann [40]. The proof through the use of the ϵ-almost periods is from [7].

Example The most famous of all aperiodic tilings are those of R. Penrose. Here we discuss the vertex set of the rhombic Penrose tiling. It is, in fact, easy to reconstruct the tiling from its vertices, so there is no loss in information in passing to the point set. The point set is a model set, and its construction is highly algebraic.

Start with the primitive 5th root of unity $\zeta = e^{2\pi i/5}$. Then $\mathbb{Z}[\zeta]$ is the ring of integers of the cyclotomic field $\mathbb{Q}[\zeta]$. Let $\nu : \mathbb{Z}[\zeta] \longrightarrow \mathbb{Z}/5\mathbb{Z}$ be reduction modulo the prime $\sqrt{5}$ – it is given by $\sum a_j \zeta^j \mapsto \sum a_j$. Let $(\ )^\star$ denote the Galois automorphism defined by $\zeta \mapsto \zeta^3$. We obtain as our cut and project scheme:

$$\begin{array}{ccccc} \mathbb{C} & \stackrel{\pi_1}{\longleftarrow} & \mathbb{C} \times (\mathbb{C} \times \mathbb{Z}/5\mathbb{Z}) & \stackrel{\pi_2}{\longrightarrow} & (\mathbb{C} \times \mathbb{Z}/5\mathbb{Z}) \quad . \\ & & \bigcup & & \\ & & \mathbb{Z}[\zeta] & & \\ x \in \mathbb{Z}[\zeta] & \longleftrightarrow & (x, x^\star, \nu(x)) & \mapsto & (x^\star, \nu(x)) \end{array}$$

Let P denote the pentagon which is the convex hull of the fifth roots of 1 in the complex plane. Then we define the window

$$W = (P, 1) \cup (-\tau P, 2) \cup (\tau P, 3) \cup (-P, 4) \subset \mathbb{C} \times \mathbb{Z}/5\mathbb{Z}\,,$$

where τ is the Golden ratio $(1 + \sqrt{5})/2$. The generic model sets of the form $x + \curlywedge(u + W)$, $u \in \mathbb{C}$ are the Penrose sets [12].

8. Characterizing Model Sets

Model sets have all the kinds of properties that we would like to have. But how can we know if we are looking at a model set? It is hard to see how to recover the cut and project scheme and the window out of the resulting point set.

Here are two closely related solutions to this problem, both of which relate back to the dynamical system $\mathbb{X}$. In the first we see that the link between the local and autocorrelation topologies that exists for model sets (Theorem 6) essentially characterizes them:

Theorem 8. [4] *Let Λ be a Meyer subset of $\mathbb{R}^d$ such that the canonical map $\beta : \mathbb{X}(\Lambda) \longrightarrow \mathbb{A}(\Lambda)$ is continuous and $1:1$ almost everywhere, with respect to the Haar measure on $\mathbb{A}(\Lambda) = \beta(\mathbb{X}(\Lambda))$. Then, $\mathbb{X}(\Lambda)$ is uniquely ergodic and Λ agrees with a regular model up to a set of density zero. Furthermore, if Λ is repetitive then $\mathbb{X}(\Lambda)$ is actually associated to a regular model set.*

Where does the cut and project scheme for the model set come from? On the group $L := \langle \Lambda - \Lambda \rangle$ define the structure of a topological group by using the sets P_ϵ, $\epsilon > 0$, of (3) as a basis for the open sets at 0. Let $\phi : L \longrightarrow H$ be the Hausdorff completion of L. Then H is the internal group of the cut and project scheme, $\mathcal{L} := \{(x, \phi(x)) \,:\, x \in L\}$ is the lattice, and L its projection in $\mathbb{R}^d$.

We can pull Theorem 8 completely back to the dynamical system one dynamical system in the local topology:

Theorem 9. [4] *Let $(\mathbb{X}, \mathbb{R}^d)$ be a dynamical system formed out of point sets that lie in $\mathcal{D}_r$. Then, for $(\mathbb{X}, \mathbb{R}^d)$ to be the dynamical system associated to a repetitive regular model set, it is necessary and sufficient for the following four conditions to be satisfied.*

(1) *All elements of $\mathbb{X}$ are Meyer sets;*
(2) *$(\mathbb{X}, \mathbb{R}^d)$ is strictly ergodic, i.e., uniquely ergodic and minimal;*

(3) $(\mathbb{X}, \mathbb{R}^d)$ *has pure point dynamical spectrum with continuous eigenfunctions;*
(4) *The eigenfunctions of* $(\mathbb{X}, \mathbb{R}^d)$ *separate almost all points of* $\mathbb{X}$ (*i.e., the set* $\{\Gamma \in \mathbb{X} : \text{there exists } \Gamma' \neq \Gamma \text{ with } f(\Gamma) = f(\Gamma') \text{ for all eigenfunctions } f\}$ *has measure zero*).

It is interesting to note the requirement of almost 1-1-ness and almost separation that occurs in these two results. They really contain the essence of the aperiodicity that we are studying. If the 1-1-ness or separation are actually *everywhere* then the result is that the sets are crystallographic – that is, periodic with periods in d-independent directions [4].

9. Pure pointedness beyond Meyer sets

Up to now we have concentrated on Meyer sets. However, the Meyer condition is by no means necessary for pure point diffractiveness. Of course if a finite number of points of a pure point diffractive set are removed or moved elsewhere it makes no difference to the diffraction. But there are more drastic looking alterations that one can do without destroying the property.

For example, the **visible points** of the lattice $\mathbb{Z}^d$ in $\mathbb{R}^d$, that is the set of all points whose integer coordinates are relatively prime, is a not a Meyer set (it is not relatively dense, although it has a well-defined density positive density) but it is pure point diffractive [8, 7].

In another direction, we can start shifting the points of a model set around in a significant way:

Theorem 10. *Let* $(\mathbb{R}^d, H, \mathcal{L})$ *be a cut and project scheme and* $\curlywedge(W)$ *a regular model set. Let* $\theta : H \longrightarrow \mathbb{R}^d$ *be a continuous mapping. Then, providing that it is a Delone set,*

$$\curlywedge_\theta(W) := \{x + \theta(x) \; : \; x \in L, x^\star \in W\}$$

is pure point diffractive.

Such sets are called **deformed model sets**. This theorem was proved by G. Bernuau and M. Duneau in [10]. A more more general version by M. Baake and D. Lenz based on deforming dynamical systems may be found in [3]. Deformed model sets need not be Meyer sets.

Jean-Baptiste Gouéré has a more general version of Proposition 4 that requires nothing but the uniform discreteness of Λ:

Theorem 11. [17] *Let* $\Lambda \in \mathcal{D}_r$ *admit an autocorrelation measure* γ*. Then* Λ *is pure point if and only if for all* $R > 0$ *and for all* $\epsilon > 0$ *the set*

$$\{t \in \mathbb{R}^d \; : \; \gamma(t + B_R) \geq \gamma(\{0\}) - \epsilon\}$$

is relatively dense.

Another approach, which is more oriented to the study of classes of related point sets and is in some sense is more physical, is to deal again with collections of point sets that collectively form a dynamical system. We have already used the local hull $\mathbb{X}(\Lambda)$ of a point set Λ to determine information about its internal structure. However, instead of starting with a single point set, we may start with the dynamical system $(\mathcal{D}_r, \mathbb{R}^d, \mu)$ where μ is some invariant regular Borel probability measure, that we shall assume here to be ergodic. We may interpret the dynamical system $(\mathcal{D}_r, \mathbb{R}^d, \mu)$ as the possible outcomes of a random variable whose values are point sets in $\mathcal{D}_r$. Then for any Borel subset B of $\mathcal{D}_r$, $\mu(B)$ is the probability of finding the outcome in B.

In practice the support of the measure μ will be some proper closed invariant subspace of $\mathcal{D}_r$, so it is more intuitive to restrict to such a subspace in the first place. So our assumption will be that we have a dynamical system $(\mathbb{X}, \mathbb{R}^d, \mu)$ where $\mathbb{X}$ is a closed invariant subspace of $\mathcal{D}_r$ and μ is an invariant ergodic probability measure on $\mathbb{X}$. For example, given a point set $\Lambda \in \mathcal{D}_r$ we may take the set $\mathbb{X}$ of all the point sets in $\mathcal{D}_r$ that are locally indistinguishable from Λ. In other words $\Lambda' \in \mathbb{X}$ if and only if for all $r > 0$ and for all $x \in \Lambda'$, there is $y \in \Lambda$ so that $\Lambda' \cap (x + B_r) = \Lambda \cap (y + B_r)$ and vice-versa. Locally it is impossible to say which of the two sets you are in. This set $\mathbb{X}$ is called the

local indistinguishability class of $\varLambda$ and is a closed $\mathbb{R}^d$-invariant subset of $\mathcal{D}_r$. It always carries some ergodic measures. If $\varLambda$ is repetitive, $\mathbb{X}$ is the same as $\mathbb{X}(\varLambda)$. If it has finite local complexity and uniform patch frequency then it is uniquely ergodic. Generally, in a physical system whose states can be represented by uniformly discrete point sets it is not unreasonable to expect the set of all states to be representable is the form $(\mathbb{X}, \mathbb{R}^d, \mu)$ for some ergodic probability measure.

For each measurable set $A \subset \mathbb{R}^d$ we define

$$N_A : \mathcal{D}_r \longrightarrow \mathbb{R} \cup \{\infty\}, \quad N_A(\varLambda) := \mathrm{card}(\varLambda \cap A)\,.$$

These functions N_A are μ-measurable

For any bounded A, the function N_A is also bounded, say by the constant $C(A)$, on $\mathcal{D}_r$. Since the function $A \mapsto \int_{\mathcal{D}_r} N_A \mathrm{d}\mu$ is an $\mathbb{R}^d$-invariant Borel measure on $\mathbb{R}^d$, it is a multiple of Lebesgue measure, so for all measurable $A \subset \mathbb{R}^d$,

$$\int_{\mathcal{D}_r} N_A \mathrm{d}\mu = I_0 \lambda(A)\,.$$

The non-negative number $I_0 = I_0(\mu)$ is, in effect, the μ-averaged density of points in the sets $\varLambda \in \mathcal{D}_r$, [17, 31]. We will assume that $I_0 > 0$.

It will not in general happen that the autocorrelation of elements $\varLambda$ of $\mathbb{X}$ is independent of the choice of $\varLambda$. However, ergodicity allows us to show that there is a single measure that is the measure of the $\varLambda \in \mathbb{X}$, μ-almost surely. This measure can be defined explicitly in the following way:

Define a measure q' on $\mathbb{R}^d \times \mathcal{D}_r$ by

$$q'(B \times F) = \int_{\mathcal{D}_r} \sum_{x \in \varLambda \cap B} \mathbf{1}_F(-x + \varLambda) \mathrm{d}\mu(\varLambda)$$

for all $B \times F \in \mathcal{B} \times \mathcal{H}$. It is easily seen to be translation invariant in B, and hence for F fixed it is a multiple $q(F)\lambda(B)$ of Lebesgue measure. Thus $F \mapsto q(F) := q'(B \times F)/\lambda(B)$ is a measure on $\mathcal{D}_r$ that is independent of the choice of $B \in \mathcal{B}$ (B assumed to have finite positive measure) and this is the definition of the **Palm measure**.

The **intensity of the Palm measure** is the measure I_q on $\mathbb{R}^d$ defined by

$$I_q(A) := \int_{\mathcal{D}_r} N_A(\varLambda)\, \mathrm{d}q(\varLambda)\,.$$

Theorem 12. [17] *Let $(\mathbb{X}, \mathbb{R}^d, \mu)$ be a dynamical system where $\mathbb{X}$ is a closed invariant subspace of $\mathcal{D}_r$ and μ is an invariant ergodic probability measure on $\mathbb{X}$. Then the autocorrelation $\gamma_\varLambda$ of $\varLambda \in \mathbb{X}$ exists μ-a.s. This measure is μ-a.s. independent of $\varLambda$ and equal to the intensity I_q of the Palm measure.* □

It follows from this, or directly, that I_q is a positive and positive definite translation bounded measure. The same then goes for its Fourier transform $\widehat{I_q}$. Since the intensity of the Palm measure is almost surely the autocorrelation, its Fourier transform $\widehat{I_q}$ is almost surely the diffraction.

Theorem 13. [17] *Let $(\mathbb{X}, \mathbb{R}^d, \mu)$ be a dynamical system where $\mathbb{X}$ is a closed invariant subspace of $\mathcal{D}_r$ and μ is an invariant ergodic probability measure on $\mathbb{X}$. Then the following are equivalent:*

i) *The elements of $\mathbb{X}$ are pure point diffractive μ-almost surely;*
ii) *For all Borel sets B of $\mathbb{X}$ and for all $\epsilon > 0$,*

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

is relatively dense.

Using the intensity of the Palm measure we can get some insight into why there is a connection between the diffraction and dynamical spectra as we had noted in Theorem 2 above. Form the two Hilbert spaces $L^2(\mathbb{R}^d, \widehat{I_q})$ and $L^2(\mathcal{D}_r, \mu)$. Since the translation action of $\mathbb{R}^d$ on $\mathcal{D}_r$ is measure preserving, it gives rise to a unitary representation T of $\mathbb{R}^d$ on $L^2(\mathcal{D}_r, \mu)$ by the usual prescription

$$T_t f(\varLambda) = f(-t + \varLambda)\,.$$

We also have a unitary representation U of $\mathbb{R}^d$ on $L^2(\mathbb{R}^d, \widehat{I_q})$ defined by

$$U_t f(x) = \exp(-2\pi i t.x) f(x)\,.$$

Theorem 14. [13] *There is a natural injective Hilbert space mapping*

$$\theta : L^2(\mathbb{R}^d, \widehat{I_q}) \longrightarrow L^2(\mathcal{D}_r, \mu)$$

that intertwines the two representations of $\mathbb{R}^d$.

This map is actually a bijection in the case that either side is pure point diffractive, though in general it is not surjective.

10. Tilings and Multi-sets

Our discussion shows that pure pointedness goes beyond the realm of model sets, even though we do not yet understand how far. However, when it comes to point sets which arise from substitutions, the situation is much clearer: effectively the regimes of model set and pure point sets become equivalent. In this section we discuss the background for this and provide the exact statements.

A great part of the theory of aperiodic order arose through the creation of the first aperiodic tilings. Many of the famous tilings are **substitution tilings**: Penrose, chair, Fibonacci, square-triangle tilings. The basic idea is simple. One has a finite set of tile types – prototiles. These are so cleverly designed that there is an inflation factor σ so that if each of the prototiles is expanded by σ then the resulting inflated tiles can be dissected into translated copies of the original prototiles. Now, starting with one prototile one repeatedly expands and dissects it to form larger and larger sets of tiles, that in the limit, can be arranged to cover space (see Figure 2).

We have already indicated that a tiling might be reduced to a point set, say by taking its vertices, as we did with the Penrose tiling. Likewise given a point set we can obtain a tiling by taking, for instance the Voronoi regions of each of the points. These are by no means the only ways to make such transitions, but still one might hope for a theory of substitution point sets matching that of tilings, along with a way to pass between the two. In fact there is such a theory, that we shall now describe, and because of the extra information that is inherent in the substitution process and in the ability to move over to tilings, there are better results for substitution point sets than we can achieve otherwise. The results are to be found in four papers [24, 27, 29, 25], all of which are accessible.

The first thing that we do is to move from straight point-sets to point sets in which points may have different types or colours, so that we can associate different point types to different tile types. This is a good thing to do in any case since in realistic atomic models different types of atoms ought to be distinguished from one another. In addition we want to set things up so that we can pass between point-sets and tilings in a way which respects the substitution process. We now describe what happens in more detail.

10.1. **Multi-colour sets and tilings.** A **multi-colour set** or m**-multi-colour set** in $\mathbb{R}^d$ is a subset $\mathbf{\Lambda} = \mathit{\Lambda}_1 \times \cdots \times \mathit{\Lambda}_m \subset \mathbb{R}^d \times \cdots \times \mathbb{R}^d$ (m copies) where $\mathit{\Lambda}_i \subset \mathbb{R}^d$. We also write $\mathbf{\Lambda} = (\mathit{\Lambda}_1, \ldots, \mathit{\Lambda}_m) = (\mathit{\Lambda}_i)_{i\le m}$. Although $\mathbf{\Lambda}$ is a product of sets, we like to think of it as a set whose points come in various colours, i being the colour of the points in Λ_i. We call multi-colour sets **multi-sets** for brevity.[9]

A **cluster** of $\mathbf{\Lambda}$ is, by definition, a family $\mathbf{P} = (P_i)_{i\le m}$ where $P_i \subset \Lambda_i$ is finite for all $i \le m$. Define $A \cap \mathbf{\Lambda} := (A \cap \Lambda_i)_{i\le m}$, for a compact set $A \subset G$. There is a natural translation $\mathbb{R}^d$-action on the set of multi-sets and their clusters in $\mathbf{\Lambda}$. The translate of a cluster $\mathbf{P}$ by $x \in G$ is $x + \mathbf{P} = (x + P_i)_{i\le m}$.

All usual concepts move over to multi-sets, so we will mostly let the reader make the extensions as needed. For example, we say that $\mathbf{\Lambda}$ is **locally finite** if for any compact set K in $\mathbb{R}^d$, $K \cap \mathbf{\Lambda}$ is finite (equivalently each $\mathit{\Lambda}_i$ is discrete and closed). We say that $\mathbf{\Lambda}$ is **Delone** if each component $\mathit{\Lambda}_i$ is Delone and if $\cup_{i=1}^m \mathit{\Lambda}_i$ is Delone.

[9] Our use of the word multi-set is not standard in the mathematical literature. Often the term refers to point sets with multiplicities.

Analogously to the multi-sets we have tilings. Begin with a set of types (or colours) $\{1, \ldots, m\}$. A **tile** in $\mathbb{R}^d$ is defined as a pair $T = (A, i)$ where $A = \text{supp}(T)$ (the support of T) is a compact set in $\mathbb{R}^d$ which is the closure of its interior, and $i = l(T) \in \{1, \ldots, m\}$ is the type of T. The analogous concept to clusters is patches: a set P of tiles is a **patch** if the number of tiles in P is finite and the tiles of P have mutually disjoint interiors. The **support of a patch** is the union of the supports of the tiles that are in it. Translation is defined in the obvious way: $g + T = (g + A, i)$ for $g \in \mathbb{R}^d$ and similarly for patches. We say that two patches P_1 and P_2 are **translationally equivalent** if $P_2 = g + P_1$ for some $g \in \mathbb{R}^d$. A tiling of $\mathbb{R}^d$ is a set $\mathcal{T}$ of tiles such that $\mathbb{R}^d = \cup\{\text{supp}(T) : T \in \mathcal{T}\}$ and distinct tiles have disjoint interiors. Given a tiling $\mathcal{T}$, finite sets of tiles of $\mathcal{T}$ are called $\mathcal{T}$-patches.

We assume that

a) any two $\mathcal{T}$-tiles with the same colour are translationally equivalent.
(Hence there are finitely many $\mathcal{T}$-tiles up to translation.)

b) the tiling $\mathcal{T}$ has **finite local complexity**, that is, for any $R > 0$ there are finitely many $\mathcal{T}$-patches of diameter less than R up to translation equivalence.

Let $\mathbb{X}_{\mathcal{T}} = \overline{\{-g + \mathcal{T} : g \in \mathbb{R}^d\}}$, where $\mathbb{X}_{\mathcal{T}}$ carries the topology, analogous to the local topology (5) for $\mathbb{X}_{\Lambda}$, relative to which it is compact (equivalent to finite local complexity). We have a natural action of $\mathbb{R}^d$ on $\mathbb{X}_{\mathcal{T}}$ which makes it a topological dynamical system. The set $\{-g + \mathcal{T} : g \in \mathbb{R}^d\}$ is the orbit of $\mathcal{T}$. As before, the minimality of dynamical system $(\mathbb{X}_{\mathcal{T}}, \mathbb{R}^d)$ is equivalent to the repetitivity of $\mathcal{T}$. .

10.2. **Tile-substitutions.** Let $Q : \mathbb{R}^d \to \mathbb{R}^d$ be a linear map that is **expansive** – i.e., all the eigenvalues of Q lie outside the closed unit disk in $\mathbb{C}$. Let $\mathcal{A} = \{T_1, \ldots, T_m\}$ be a finite set of tiles in $\mathbb{R}^d$ such that $T_i = (A_i, i)$; we will call them **prototiles**. Denote by $\mathcal{P}_{\mathcal{A}}$ the set of patches made of tiles each of which is a translate of one of T_i's. A **tile-substitution** (with expansive map Q) is a mapping $\omega : \mathcal{A} \to \mathcal{P}_{\mathcal{A}}$ for which there exist finite sets $D_{ij} \subset \mathbb{R}^d$ (some of which may be empty) for $i, j \le m$, such that

$$\omega(T_j) = \{u + T_i : \ u \in D_{ij}, \ i = 1, \ldots, m\} \quad \text{for } j \le m, \tag{12}$$

with

$$Q(A_j) = \bigcup_{i=1}^{m} (D_{ij} + A_i).$$

All sets in the right-hand side are assumed to have disjoint interiors.

The substitution (12) is extended to all translates of prototiles by $\omega(x + T_j) = Qx + \omega(T_j)$, and to patches and tilings by $\omega(P) = \cup\{\omega(T) : \ T \in P\}$. The substitution ω can be iterated, producing larger and larger patches $\omega^k(T_j)$. To the substitution ω we associate its $m \times m$ substitution matrix S, with $S_{ij} := \text{card}(D_{ij})$. The substitution ω is called **primitive** if the substitution matrix S is primitive, i.e., if there is an $l > 0$ for which S^l has no zero entries.

A patch will be called **legal** if it is a translate of a **subpatch** of $\omega^k(T_i)$ for some $i \le m$ and $k \ge 1$. A tiling $\mathcal{T}$ with finite local complexity is said to be **self-affine** with the prototile set $\mathcal{A}$, expansive map Q, and primitive substitution ω, if every $\mathcal{T}$-patch is legal.

The set of self-affine tilings associated with $(\mathcal{A}, \omega)$ is a dynamical system $\mathbb{X}_{\mathcal{A},\omega}$ under the translation action of $\mathbb{R}^d$. The topology is defined in the same way as we defined the local topology above: closeness means agreement to within ϵ-sized errors on large balls around the origin. In the case of finite local complexity (which is mostly assumed here), the agreement is exact on large balls around the origin after a very small shift. A tiling $\mathcal{T}$ is called a **fixed point** of the substitution ω if $\omega(\mathcal{T}) = \mathcal{T}$. One can always find a **periodic point** for ω in the space $\mathbb{X}_{\mathcal{A},\omega}$ i.e. there is $\mathcal{T} \in \mathbb{X}_{\mathcal{A},\omega}$ such that $\omega^N(\mathcal{T}) = \mathcal{T}$ for some $N \ge 1$. In this case we can always use ω^N in place of ω to obtain a tiling which is a fixed point of ω.

Theorem 15. [27] *Let $\mathcal{T}$ be a fixed point of a primitive substitution ω with expansive map Q and prototiles $\mathcal{A}$. Then $\mathcal{T}$ is repetitive if and only if every $\mathcal{T}$-patch is legal, i.e. $\mathcal{T} \in \mathbb{X}_{\mathcal{A},\omega}$.*

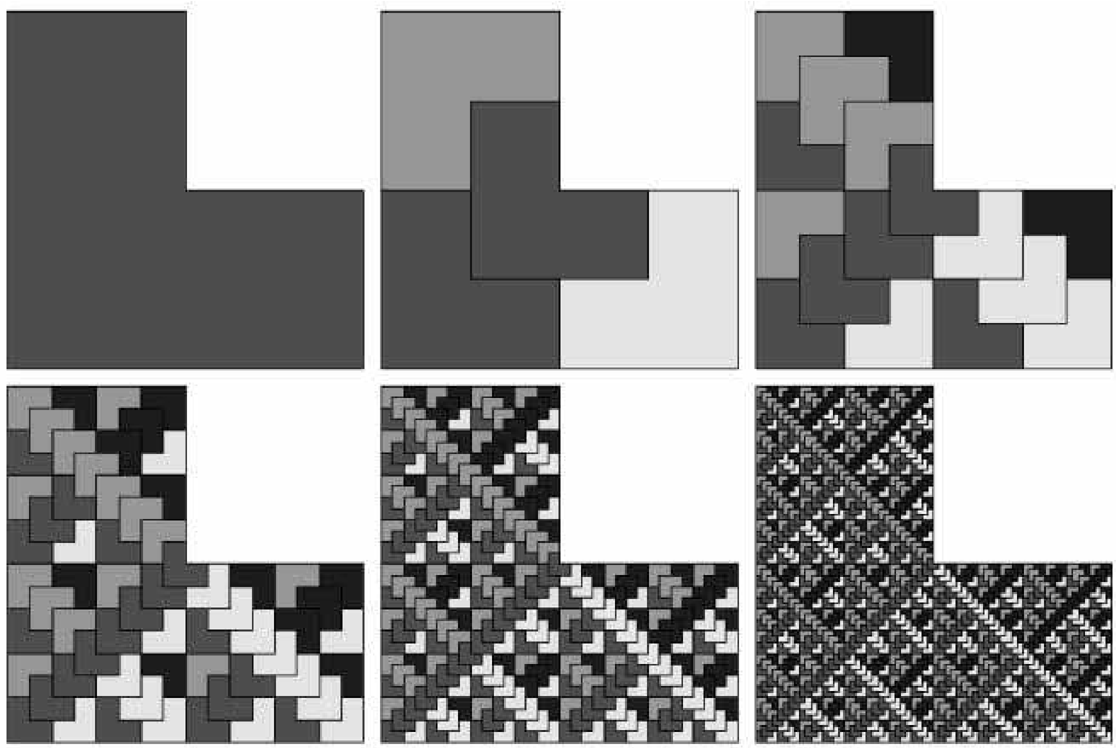

FIGURE 2. Several iterations of the chair tiling. The chairs occur in 4 orientations and appear in different shades of grey here.

10.3. **From substitution Delone multi-sets to tilings.** We now link the theory of multi-sets and tilings through the notion of representable Delone multi-sets. The concept was introduced by Lagarias and Wang [24], under the name of self-replicating Delone set families.

$\mathbf{\Lambda} = (\Lambda_i)_{i\le m}$ is called a **substitution Delone multi-set** if $\mathbf{\Lambda}$ is a Delone multi-set and there exist an expansive map $Q:\mathbb{R}^d \to \mathbb{R}^d$ and finite sets D_{ij} for $i,j\le m$ such that

$$\Lambda_i = \bigcup_{j=1}^{m} (Q\Lambda_j + D_{ij}), \quad i\le m,$$

where the unions on the right-hand side are disjoint.

For each primitive substitution Delone multi-set there is an **adjoint system** of equations

$$QA_j = \bigcup_{i=1}^{m} (D_{ij} + A_i), \quad j\le m \tag{13}$$

which looks, of course, exactly like the formula for substitution tilings. From Hutchinson's Theory, it follows that (13) always has a unique solution for which $(A_i)_{i\le m}$ is a family of non-empty compact sets of $\mathbb{R}^d$ (see for example [5], Thm. 1.1). It is proved in [24, Thm. 2.4 and Thm. 5.5] that if $\mathbf{\Lambda}$ is a primitive substitution Delone multi-set, then all the sets A_i from (13) have non-empty interior and, moreover, each A_i is the closure of its interior.

We say that our substitution Delone multi-set $\mathbf{\Lambda} = (\Lambda_i)_{i\le m}$ is **representable** (by tiles) if the tiles $T_i = (A_i, i), i\le m$, arising from this solution to the adjoint system satisfy

$$\{x + T_i:\ x\in\Lambda_i,\ i\le m\} \quad \text{is a tiling of } \mathbb{R}^d, \tag{14}$$

that is, $\mathbb{R}^d = \bigcup_{i\le m}\bigcup_{x\in\Lambda_i}(x+A_i)$, and the sets in this union have disjoint interiors.

A cluster will be called **legal** if it is a translate of a subcluster of $\Phi^k(x_j)$ for some $x_j \in \Lambda_j$, $j \le m$ and some $k \in \mathbb{Z}_+$.

Lagarias and Wang have a condition, namely existence of a fundamental cycle of period 1, which ensures representability [24, Th.7.1]. The next theorem is based on this, though it uses the more general concept of legality.

Theorem 16. [27] *Let $\mathbf{\Lambda}$ be a repetitive primitive substitution Delone multi-set. Then every $\mathbf{\Lambda}$-cluster is legal if and only if $\mathbf{\Lambda}$ is representable.*

How hard is legality to check? If $\mathbf{\Lambda}$ is a substitution Delone multi-set, then there is a finite multi-set (cluster) $\mathbf{P} \subset \mathbf{\Lambda}$ for which $\Phi^{n-1}(\mathbf{P}) \subset \Phi^n(\mathbf{P})$ for $n \ge 1$ and $\mathbf{\Lambda} = \lim_{n\to\infty}\Phi^n(\mathbf{P})$ [24, Lemma 3.2]. We call such a multi-set $\mathbf{P}$ a **generating multi-set**. In order to check that every $\mathbf{\Lambda}$-cluster is legal, we only need to see if some cluster that contains a finite generating multi-set for $\mathbf{\Lambda}$ is legal.

Any tiling $\mathcal{T}$ can be converted into a Delone multi-set by simply choosing a point $x_{(A,i)}$ for each tile (A,i) so that the chosen points for tiles of the same type are in the same relative position in the tile: $x_{(g+A,i)} = g + x_{(A,i)}$. We define $\Lambda_i := \{x_{(A,i)} : (A,i) \in \mathcal{T}\}$ and $\mathbf{\Lambda} := (\Lambda_i)_{i\le m}$[10]. Clearly $\mathcal{T}$ can be reconstructed from $\mathbf{\Lambda}$ given the information about how the points lie in their respective tiles. This bijection establishes a topological conjugacy of $(\mathbb{X}_\Lambda, \mathbb{R}^d)$ and $(\mathbb{X}_\mathcal{T}, \mathbb{R}^d)$. Concepts and theorems can clearly be interpreted in either language (finite local complexity, uniform cluster frequency, unique ergodicity, pure point dynamical spectrum, etc.).

On the other hand, suppose that $\mathbf{\Lambda}$ is a representable primitive substitution Delone multi-set. Consider $T_i = (A_i, i)$, $i \le m$, as prototiles, where A_i's are defined by (13). Let $\mathcal{T} = \mathcal{T}(\mathbf{\Lambda})$ be the tiling in (14), with the colours added, that is, $\mathcal{T} = \{x_i + T_i :\ x_i \in \Lambda_i,\ i \le m\}$, and let $\mathcal{A} = \{T_1, \ldots, T_m\}$. By (13) and the definition of representable primitive substitution Delone multi-set, we have a tile-substitution $\omega :\ \mathcal{A} \to \mathcal{P}_\mathcal{A}$.

Lemma 1. [27] *The dynamical systems $(\mathbb{X}_\Lambda, \mathbb{R}^d)$ and $(\mathbb{X}_\mathcal{T}, \mathbb{R}^d)$ are topologically conjugate.*

We had intimated above that by passing through tilings one could glean information that might otherwise be hard to obtain. One such example is this:

Theorem 17. [27] *If $\mathbf{\Lambda}$ is a primitive substitution Delone multi-set with finite local complexity such that every $\mathbf{\Lambda}$-cluster is legal, then the dynamical system $(\mathbb{X}_\mathbf{\Lambda}, \mathbb{R}^d)$ is uniquely ergodic.*

We have already seen that the Meyer hypothesis is an important ingredient in results about model sets and pure point diffraction. But there is a general feeling that the Meyer condition might follow from other conditions that seem physically or mathematically more natural. One such example is the open question of J. Lagarias: is a Delone set with finite local complexity and repetitivity which is pure point diffractive necessarily a Meyer set? Here is a version of this (for multi-sets even!) in the context of substitution Delone multi-sets:

Theorem 18. [29] *Let $\mathbf{\Lambda}$ be a primitive substitution Delone multi-set with expansion Q for which every $\mathbf{\Lambda}$-cluster is legal and $\mathbf{\Lambda}$ has finite local complexity. Suppose that $(X_\mathbf{\Lambda}, \mathbb{R}^d, \mu)$ has pure point dynamical spectrum. Then $\Lambda := \cup_{i=1}^m \Lambda_i$ is a Meyer set.*

Theorem 18 has been effectively used in the recent result of J.-Y. Lee:

Theorem 19. [25] *Let $\mathbf{\Lambda}$ be a non-periodic primitive substitution Delone multi-set such that every $\mathbf{\Lambda}$-cluster is legal. Then the following are equivalent;*

(i) $\mathbf{\Lambda}$ *has pure point dynamical spectrum.*

[10] A more subtle way to do this is to choose for each tile $T \in \mathcal{A}$ a tile $\gamma(T)$ in $\omega(T)$ and extend γ to all tiles of $\mathcal{T}$ by translation. Then one may define the control points $c(T) = \cap_{n=0}^\infty Q^{-n}\gamma^n(T)$, $T \in \mathcal{T}$. The idea goes back to Kenyon and Thurston [22]. Also see [29] for an example of this.

(ii) $\mathbf{\Lambda}$ *is a model multi-set.*

This result is an abbreviated version of the theorem that also involves several notions of coincidence.

11. Concluding Remarks

This little paper has been directed to the question of diffraction, and mostly towards questions around pure point diffraction. There are two directions which seem ripe for investigation. First, it seems like the right time to move towards systems with mixed spectra – a pure point part of Bragg peaks plus a background part that is continuous. There are some well-known substitution systems that have mixed spectra, the most famous being the Thue-Morse (pure point + singular continuous) and the Rudin-Shapiro (pure point + absolutely continuous) substitutions that serve as starting points for this investigation [36]. Then there are purely random sequences. Interesting examples are the Bernoulli sequences which are constructed by choosing for each $n \in \mathbb{Z}$ either to take it or throw it away with probabilities $\{p, 1-p\}$. The remaining integers, seen on the real line, form a point set. The diffraction from these is almost surely pure point + absolutely continuous. A. Hof [21] has looked at diffraction from model sets disturbed by random (high temperature) fluctuations in position.

This is difficult ground. There are few theorems that allow any simple insight into the nature of the continuous part of a measure (see [1]). Nor does the geometrical structure of a point set give as much information about the diffraction as one might imagine. It is a remarkable fact that the diffraction from a Bernoulli sequence with $p = 1/2$ is almost surely identical with the diffraction from the Rudin-Shapiro sequence even though the first is random and the second deterministic [18].

Another direction is to move away from the dominance of translations in the theory. Up to now the theory has been based primarily on translational almost periodicity. Our dynamical systems have been based on the translation group $\mathbb{R}^d$ of Euclidean space. But what would happen if one allowed the full Euclidean group to be involved? A fundamental example is the pinwheel tiling of John Conway and Charles Radin in which the tiles occur in a countable infinity of directions. Translational symmetry is no longer appropriate, but under the full Euclidean group, there is still finite local complexity. Interestingly the diffraction of the pinwheel tiling is circularly symmetric. The radial profile of the diffraction is, however, unknown at this point. Recent work of T. Yokonuma [44] has looked into some foundational questions of this non-Abelian theory.

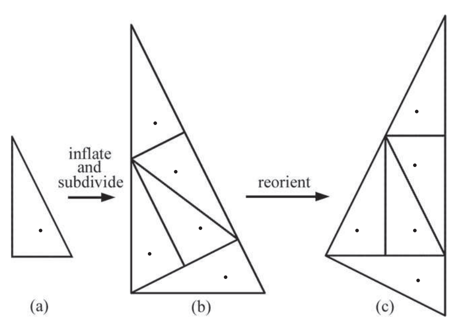

Figure 3. The pinwheel substitution. The figure also indicates the positions of the corresponding control points by which it may be turned into a point-set.

Symmetry is a term whose meaning in mathematics has continued to evolve over time. Long-range aperiodic order requires a theory where symmetry does not mean the exact perfect matching that we are used to, but rather a theory of "almost" matching. This almost matching manifests itself in interesting mathematical structures like the dynamical hulls that we have seen in this paper. One might even consider the dynamical system as the true object encoding the symmetry of an almost periodic system. In any case we seem to be entering a rich world with unexpected turns and new insights. We may have taken only a few steps towards Bernoulli City but we can see already that the views from the path offer a beauty and fascination of their own.

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