

## Pure point diffraction

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Dedicated to Peter Kramer on the occasion of his 70th birthday

### Abstract

Many important mathematical models of distributions of matter with pure point diffraction arise out of the cut and project formalism. As we show here, under some basic assumptions, the latter emerges very naturally from inherent data of pure point diffractive structures. Moreover, the internal space, whose physical meaning is often questioned, is the expression of a naturally occurring topology (the autocorrelation topology) that is part of the physical picture, though very different from the usual topology of space. We also indicate some of the recent progress in the geometrical properties that can be inferred from knowing that a uniformly discrete structure is pure point diffractive.

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### 1. Introduction

Diffraction experiments are the key tool of structure determination in crystallography and materials science. In its simplest form, known as kinematic diffraction [12], one is confronted with the Fourier transform of the autocorrelation (or Patterson) function of the underlying atomic structure, and tries to infer as much as possible about the latter. Even though kinematic diffraction is only an approximation to the full quantum mechanical scattering process involved, many important phenomena already show up and can be explained in this setting.

One is therefore justified in studying the central questions of kinematic diffraction in a more abstract mathematical language, with focus on the conceptual issues, while completely abstracting from the potential practical problems. This is very much our point of view here. In particular, we address the old and important question of which distributions of atoms diffract, in the sense that their diffraction images consist of Bragg peaks

only and show no diffuse scattering. This allows a relatively complete answer, compare also [8] and references given there. Furthermore, we start to address the inverse problem: What conclusions may be drawn from a pure Bragg diffraction image?

This is a very difficult question, and no complete answer is known at present, or even in sight. However, if one knows a bit more about the underlying structure on top of the pure point diffractivity, such as some essential uniform discreteness, significant conclusions are possible, some of which we are going to describe here.

A very natural setting for all this is the theory of translation bounded measures and their Fourier theory [1,10]. To simplify the presentation, we will restrict our discussion to Dirac combs, i.e., to measures that consist of (possibly weighted) point measures ( $\delta$ -functions) only. This way, an atom is modelled by its position and weight (scattering strength). Convolutions with more realistic profiles are not considered here, but can easily be treated by the convolution theorem of Fourier analysis, compare [10].

The primary conclusion to be drawn from this work is that Kramer's cut and project formalism [18,20], which has always been a primary modelling device for quasicrystals (see [21] and references given there for recent applications) is, under certain circumstances,

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already inherent in the pure point diffraction, and that internal spaces and projection lattices have straight forward interpretations from the physical side. Under additional conditions, which we will mention towards the end of this article, one can even decide whether a given point set is a (regular) model set.

## 2. Dirac combs and their autocorrelations

The basic object of interest is a countable set  $S$  of scatterers in  $\mathbb{R}^d$  with (bounded) scattering strengths  $w(x)$ ,  $x \in S$ , where we assume that the set  $S$  is locally finite.<sup>1</sup> This can be represented as a non-zero regular complex Borel measure in the form of a *weighted Dirac comb*

$$\omega = \sum_{x \in S} w(x) \delta_x, \quad (1)$$

where  $\delta_x$  is the unit point (or Dirac) measure located at  $x$ , and  $w : S \rightarrow \mathbb{C}$  is a function with the restriction that, for each compact set  $K \subset \mathbb{R}^d$ ,  $\sum_{x \in S \cap (y+K)} |w(x)|$  is uniformly bounded as  $y$  runs over  $\mathbb{R}^d$ . The most obvious example is the simple comb  $\omega = \delta_S := \sum_{x \in S} \delta_x$  that represents a uniformly discrete<sup>2</sup> point set  $S \subset \mathbb{R}^d$ .

In the sequel, the set

$$\Delta = \Delta(S) := S - S := \{x - y | x, y \in S\} \quad (2)$$

of ‘inter-atomic distances’ and the subgroup  $L'$  of  $\mathbb{R}^d$  generated by  $\Delta$  play important roles. For  $S$  a lattice,  $S = \Delta = L'$ . However, in quasicrystal theory,  $L'$  is generally not discrete. We assume that  $\Delta$  is locally finite. If the set  $S$  is constructed or obtainable through any cut and project method (with flat atomic surfaces) then  $\Delta$  is not only discrete, but even *uniformly* discrete. In this paper, we will make this stronger assumption for a closely related set which we will now construct.

Let us first introduce the autocorrelation measure of  $\omega$  and, from there, the diffraction pattern. Let us define  $\tilde{\omega} := \sum_{x \in S} \overline{w(x)} \delta_{-x}$ , where the bar denotes complex conjugation, and let  $B_n$  be the (open) ball of radius  $n$  around 0, with volume  $v_n$ , where  $n \in \mathbb{N} = \{1, 2, \dots\}$ . Set  $\omega_n = \omega|_{B_n}$  and  $\tilde{\omega}_n = (\tilde{\omega})|_{B_n}$ . Then, the measure

$$\gamma_\omega^{(n)} := \frac{\omega_n * \tilde{\omega}_n}{v_n} = \frac{1}{v_n} \sum_{x, y \in S \cap B_n} w(x) \overline{w(y)} \delta_{x-y} \quad (3)$$

is well defined, since it is the (volume averaged) convolution of two *finite* measures. The *autocorrelation* of  $\omega$  exists (then denoted by  $\gamma_\omega$ ) if  $(\gamma_\omega^{(n)})_{n \in \mathbb{N}}$  converges in the vague topology [16]. It is then a positive definite measure

with  $\gamma_\omega = \sum_{z \in \Delta} \eta(z) \delta_z$  where, in view of our assumption on  $\Delta$ , the coefficients are given by

$$\eta(z) = \lim_{n \rightarrow \infty} \frac{1}{v_n} \sum_{\substack{x, y \in S \cap B_n \\ x-y=z}} w(x) \overline{w(y)}. \quad (4)$$

The function  $\eta$  can be extended from  $\Delta$  to all of  $\mathbb{R}^d$  by setting  $\eta(z) = 0$  for all  $z \notin \Delta$ . It is a positive definite function, so in particular  $|\eta(z)| \leq \eta(0)$  and

$$|\eta(z) - \eta(z+t)|^2 \leq 2\eta(0)(\eta(0) - \operatorname{Re}(\eta(t))) \quad (5)$$

for all  $z, t \in \mathbb{R}^d$  (see [10, p. 12, Eq. (4)]). The set of  $t$  for which  $\eta(t) = \eta(0)$  thus forms a subgroup of  $L'$ , called the group of *statistical periods* of  $\omega$ . Extending this to ‘almost equality’ gives a fundamental tool to understand pure point diffraction; for all  $0 < \varepsilon < 1$ , we define the set of  $\varepsilon$ -almost periods (see also [29]) of  $\omega$ :

$$P_\varepsilon := \left\{ t \in \mathbb{R}^d : \left| 1 - \frac{\eta(t)}{\eta(0)} \right| < \varepsilon \right\}. \quad (6)$$

We clearly have<sup>3</sup>  $P_\varepsilon \subset L'$  and  $P_\varepsilon \subset P_{\varepsilon'}$  for  $\varepsilon \leq \varepsilon'$ . At this point, we make a slight refinement to  $\Delta$  and  $L'$  introducing  $\Delta^{\text{ess}} := \bigcup_{0 < \varepsilon < 1} P_\varepsilon \subset \Delta$  and  $L := \langle \Delta^{\text{ess}} \rangle_{\mathbb{Z}} \subset L'$ . Thus, we are only interested in the interatomic differences with non-zero autocorrelation coefficient and in the group that they generate. From now on, we make the **basic assumption**:

$$\Delta^{\text{ess}} \text{ is uniformly discrete.} \quad (7)$$

If the original (weighted) set  $S$  is repetitive,<sup>4</sup> nothing happens in this refinement.

## 3. Fourier transform and diffraction

The autocorrelation measure  $\gamma_\omega$  is a positive definite, translation bounded measure and, as such, has a well-defined Fourier transform  $\hat{\gamma}_\omega$  (also defined on  $\mathbb{R}^d$ ), which is a positive and also translation bounded measure [10,16]. This is, by definition, the *diffraction* of  $\omega$ . The measure  $\omega$  is *pure point diffractive* if  $\hat{\gamma}_\omega$  is a pure point (also called discrete or atomic) measure on  $\mathbb{R}^d$ . Let us consider a measure  $\omega$  whose autocorrelation  $\gamma_\omega$  exists.

**Theorem 1** [15]. *The measure  $\omega$  is pure point diffractive if and only if the autocorrelation measure  $\gamma_\omega$  is strongly almost periodic.*

This key result of the theory introduces a new concept – strong almost periodicity. There are many forms

<sup>1</sup>  $S$  is called *locally finite*, if its intersection with any compact subset of  $\mathbb{R}^d$  is a finite set.

<sup>2</sup>  $S$  is *uniformly discrete* if there is an  $r > 0$  so that the balls of radius  $r$  centered on the points of  $S$  are mutually disjoint.

<sup>3</sup> In [6], the set  $P_\varepsilon$  as defined in (6) is denoted by  $P_\varepsilon$ . Making this replacement makes the presentation here easier and makes no difference to the statements of the results.

<sup>4</sup> A point set  $S \subset \mathbb{R}^d$  is called *repetitive* if each cluster, i.e.,  $S \cap K$  for  $K$  compact, reappears in  $S$  with bounded gaps (resp. holes) under translation.

of almost periodicity [31], but most of them can be summarized as follows:  $\lambda$  is  $\Omega$ -almost periodic if the  $\Omega$ -closure of the translation orbit of  $\lambda$  under the action of  $\mathbb{R}^d$  is compact. Here,  $\lambda$  may be a function or a measure and  $\Omega$  is some topology on the corresponding space of functions or measures. In our case, it is a topology called the strong topology on the space of translation bounded measures of  $\mathbb{R}^d$ . Fortunately, under the assumption that our autocorrelation is supported on  $\Delta^{\text{ess}}$ , which is uniformly discrete, there is a far simpler way of understanding this.

**Theorem 2** [6]. *The autocorrelation measure  $\gamma_\omega$  of  $\omega$  is strongly almost periodic if and only if, for all  $0 < \varepsilon < 1$ ,  $P_\varepsilon$  is relatively dense.*<sup>5</sup>

Thus, for our  $\omega$ , pure pointedness of the diffraction hinges around the relative denseness of the sets  $P_\varepsilon$ .

#### 4. Application: Cut and project sets

The well-known cut and project mechanism provides examples of weighted point sets which satisfy the conditions above, and for which we can quite easily see how the relative denseness of the  $P_\varepsilon$  appears. Most often, in examples from the physics literature, cut and project comes by cutting a lattice in a higher dimensional space  $\mathbb{R}^{d+m}$  by a cylinder of the form  $\mathbb{R}^d \times W$  (where  $W$  is some set with non-empty interior and compact closure in the internal space  $\mathbb{R}^m$ ) and projecting the resulting point set into  $\mathbb{R}^d$ . In fact, the internal space can be replaced by any locally compact Abelian (LCA) group (of which real spaces are only one special type) without changing the basic geometrical consequences much at all. In view of our goal of characterizing pure point diffractivity, it is absolutely essential for us to make this generalization (see also [9]).

A *cut and project scheme* is a triplet  $(\mathbb{R}^d, H, \tilde{L})$  consisting of a pair of LCA groups  $\mathbb{R}^d, H$  and a lattice<sup>6</sup>  $\tilde{L} \subset \mathbb{R}^d \times H$  for which the canonical projections  $\pi : \mathbb{R}^d \times H \rightarrow \mathbb{R}^d$  and  $\pi_H : \mathbb{R}^d \times H \rightarrow H$  satisfy the conditions that  $\pi|_{\tilde{L}}$  is one-to-one and that  $\pi_H(\tilde{L})$  is dense in  $H$ .

We write  $L := \pi(\tilde{L})$ , so  $L$  is a subgroup of  $\mathbb{R}^d$  and note that the mapping  $(\cdot)^{\star} := \pi_H \circ (\pi|_{\tilde{L}})^{-1} : L \rightarrow H$  has dense image in  $H$ . To determine volumes, we will use Lebesgue measure on  $\mathbb{R}^d$  and a fixed Haar measure  $\theta_H$  on  $H$ .

A set  $A \subset \mathbb{R}^d$  is a *model set* [24] for the cut and project scheme  $(\mathbb{R}^d, H, \tilde{L})$  if there is a non-empty compact set

$W \subset H$  which is the closure of its interior and an  $x \in \mathbb{R}^d$  such that

$$A = x + \Lambda(W) = x + \{t \in L : t^{\star} \in W\}. \tag{8}$$

Such sets are always *Delone sets*.<sup>7</sup> There are variations on the definition of model set which arise by assuming more about  $W$  and its relation to its closure. For example, the model set is *regular* if the boundary  $\partial W$  of  $W$  has Haar measure 0 and *generic* if  $L^{\star} \cap \partial W = \emptyset$ .

**Theorem 3.** *Let  $\Lambda$  be a regular model set and  $w$  a weighting function on  $\Lambda$  defined by  $w(x) := f(x^{\star})$  for some complex-valued function  $f$  on  $H$  which is supported and continuous on the compact set  $W$ . Then, the Dirac comb  $\omega_f = \sum_{x \in \Lambda} w(x)\delta_x = \sum_{x \in \Lambda} f(x^{\star})\delta_x$  has a well-defined autocorrelation, satisfies the basic assumption (7), and is pure point diffractive.*

This result is constructive in the sense that the diffraction measure can be calculated explicitly [14,16,19,28].

This theorem, in various degrees of generality, has been proved by Hof [16], Solomyak [29], and Schlottmann [28].<sup>8</sup> The hard part is the pure point diffractivity, and all these proofs are based upon the pointwise ergodic theorem for uniformly ergodic dynamical systems, following or extending Dworkin’s argument [13]. However, according to Theorems 1 and 2, the pure point diffractivity of our weighted model set is equivalent to the relative denseness of the corresponding sets of  $\varepsilon$ -almost periods. In fact, this is fairly easy to see from the uniform distribution property of the cut and project formalism [25,27] that for any complex-valued function  $g$ , continuous and supported on  $W$ ,

$$\lim_{n \rightarrow \infty} \frac{1}{v_n} \sum_{x \in \Lambda(W) \cap B_n} g(x^{\star}) = C \int_W g d\theta_H, \tag{9}$$

where  $C$  is a positive constant that depends only on the choice of the Haar measure  $\theta_H$  on  $H$  and on the lattice  $\tilde{L}$ . Using the function  $fT_{z^{\star}}(f)$  in (9) (where  $T_a$  denotes the shift by  $a$ ) we obtain

$$\begin{aligned} \eta(z) &= \lim_{n \rightarrow \infty} \frac{(\omega_n * \tilde{\omega}_n)(\{z\})}{v_n} \\ &= C \int_W f(u) \overline{f(u - z^{\star})} d\theta_H(u). \end{aligned} \tag{10}$$

In particular, the autocorrelation exists and  $|\eta(0) - \eta(z)|$  is bounded by

<sup>7</sup> A set  $A \subset \mathbb{R}^d$  is *Delone* iff it is relatively dense and uniformly discrete.

<sup>8</sup> There are two notions of pure pointedness that appear in these works: pure point dynamical spectrum and pure point diffraction spectrum. It is the latter that we are dealing with here. For uniquely ergodic systems, these two notions are the same [4,23].

<sup>5</sup>  $P \subset \mathbb{R}^d$  is *relatively dense* if a radius  $R > 0$  exists so that every ball of radius  $R$  in  $\mathbb{R}^d$  contains a least one point of  $P$ .

<sup>6</sup> A *lattice* in  $\mathbb{R}^d \times H$  is a closed subgroup  $\tilde{L}$  such that the factor group  $(\mathbb{R}^d \times H)/\tilde{L}$  is compact.

$$C \int_W |f(u)| |f(u) - f(u - z^\star)| d\theta_H(u).$$

Let  $\varepsilon > 0$  and write  $W = (W \cap (z^\star + W)) \cup (W \setminus (z^\star + W))$ , splitting the integral accordingly. Using the uniform continuity of  $f$  on  $W \cap (z^\star + W)$  and the uniform continuity of  $\int_{W \setminus (u+W)} 1 d\theta_H = \theta_H(W) - (\mathbf{1}_W * \mathbf{1}_W)(u)$  as a function of  $u$ , we can find a neighbourhood  $V$  of 0 so that  $|\eta(0) - \eta(z)| < \eta(0)\varepsilon$  for all  $z \in A(V)$ . Since this set is relatively dense ( $V$  is open) and a subset of  $P_\varepsilon$ , the latter is also relatively dense.

One advantage of our new approach, without reference to unique ergodicity, is that it establishes pure point diffraction also for a wider class of systems, including examples such as the visible points of a lattice or the square-free integers (see [6,7]).

### 5. Construction of a cut and project scheme

We now turn to the inverse problem where we start with a countable weighted set  $S$  of scatterers in  $\mathbb{R}^d$  for which the corresponding weighted Dirac comb is pure point diffractive. Our assumptions are as before:  $\Delta^{\text{ess}}$  is uniformly discrete and (necessarily, since we are talking about the diffraction) the autocorrelation exists. Note that uniform discreteness of  $\Delta^{\text{ess}}$  is a crucial ingredient – it does not follow from the pure point diffractivity of  $S$ . According to Theorem 2, the pure point diffractivity is now equivalent to the relative denseness of the sets of  $\varepsilon$ -almost periods,  $0 < \varepsilon < 1$ , which we can thus assume. This leads us to a suitable cut and project scheme with an internal space  $H$  and a lattice  $\tilde{L}$ .

The key point is to start with our group  $L = \langle \Delta^{\text{ess}} \rangle_{\mathbb{Z}}$ . Inside this are the sets  $P_\varepsilon$  which we now treat as open neighbourhoods of 0 for a new group topology (the *autocorrelation topology*) on  $L$ . Thus we take the topology on  $L$  generated by the sets  $x + P_\varepsilon$  where  $x$  ranges over  $L$  and  $\varepsilon$  over  $(0,1)$ . This topology can also be defined via the pseudo-metric

$$\varrho(s, t) = \left| 1 - \frac{\eta(s - t)}{\eta(0)} \right|^{1/2},$$

(which is indeed non-negative, symmetric, and satisfies the triangle inequality). Also, it is immediate that one has  $\varrho(s + r, t + r) = \varrho(s, t)$  for all  $r \in G$  which shows that  $\varrho$  is translation invariant. It is not a metric in general – the almost-periods  $t$  all satisfy  $\varrho(t, 0) = 0$ . In terms of this pseudo-metric,  $P_\varepsilon$  is just the open ball of radius  $\varepsilon^2$ .

The group  $L$ , equipped with this topology, admits a Hausdorff completion  $H$  (essentially made in the same way as  $\mathbb{R}$  is made from  $\mathbb{Q}$ , by providing limits for every Cauchy sequence) which is a locally compact Abelian group. This means that there is a continuous group homomorphism  $\varphi : L \rightarrow H$ ,  $\varphi(L)$  is dense in  $H$ , and for every set  $P_\varepsilon$  in  $L$  there is an open set  $B(\varepsilon)$  of  $H$  so that

$\varphi(P_\varepsilon) = \varphi(L) \cap B(\varepsilon)$ . The relative denseness of the  $P_\varepsilon$  is crucial here, giving the compactness of  $\overline{B(\varepsilon)}$  and hence the local compactness of  $H$ .

We now also have a mapping from  $L$  to  $\mathbb{R}^d \times H$ , sending  $t \in L$  to the point  $(t, \varphi(t))$ . Let  $\tilde{L} \subset \mathbb{R}^d \times H$  be the image of  $L$  under this mapping.

**Theorem 4** [6].  $\tilde{L}$  is a lattice in  $\mathbb{R}^d \times H$ , and  $(\mathbb{R}^d, H, \tilde{L})$  is a cut and project scheme, with the homomorphism  $\varphi$  as its  $\star$ -map.

The internal space and the lattice both arise from the group  $L$  via the new topology in which closeness is given by  $\varepsilon$ -almost periodicity (i.e., by the  $\varepsilon$ -almost-periods). In spite of its apparent abstraction, the procedure gives back the familiar real internal spaces of the well-known examples such as the Fibonacci chain in one dimension, the octagonal Ammann–Beenker tiling of the Euclidean plane or the icosahedrally symmetric Ammann–Kramer and Danzer tilings of 3-space.

In the case of the rhombic Penrose tilings (resp. its vertex set), the method gives  $H = \mathbb{R}^2 \times (\mathbb{Z}/5\mathbb{Z})$ , which has been known for some time to be the minimal internal space possible for representing them in the cut and project formalism. For other tilings, such as the chair or the sphinx tilings, the internal spaces may be  $p$ -adic spaces, or other more exotic locally compact Abelian groups [7,9]. It is useful to note that the completion map  $\varphi$  is not one-to-one in general; in fact, its kernel is  $\bigcap_{0 < \varepsilon < 1} P_\varepsilon$ . For example, suppose that our original weighted set is a lattice with all weights equal. Then,  $S = L$  and  $\varphi$  is the 0-map,  $H = 0$ , and  $\tilde{L} = L$ , so the cut and project formalism collapses into a triviality. This is of course exactly what is needed! In general, the internal space  $H$  ignores the periodic part of  $\omega$ , for which no additional structure is required, and reflects only the aperiodic, but ‘nearly periodic’, parts.

It is natural to consider the meaning of the quotient group  $\mathbb{T} := (\mathbb{R}^d \times H) / \tilde{L}$  which has arisen in this discussion. Since  $\tilde{L}$  is a lattice,  $\mathbb{T}$  is a compact Abelian group. The importance of  $\mathbb{T}$  (for ‘torus’) was first noted in [2,28], in terms of the so-called torus parametrization of model sets. Below, we provide a natural interpretation of it in terms of dynamical systems and, in doing so, establish a closer connection between pure pointedness and model sets.

### 6. Dynamical systems

In this section, we restrict ourselves to the case of unweighted scatterers – or, in terms of Dirac combs, those for which the weighting function  $w \equiv 1$ .

Let  $\mathcal{D}$  be the set of locally finite subsets of  $\mathbb{R}^d$  and put on it the topology for which two discrete sets are close if and only if, after a small shift, their symmetric difference

has small density. This is a uniform topology, very closely connected to the autocorrelation, and  $\mathcal{D}$  is complete with respect to it (though the process identifies sets which differ in density 0). Clearly,  $\mathcal{D}$  admits the action of  $\mathbb{R}^d$  by translation. For any locally finite set  $S$  in  $\mathbb{R}^d$ , we can define the orbit closure  $\mathbb{T}(S)$  of  $S$  in  $\mathcal{D}$ .

**Theorem 5** [26]. *Let  $S \subset \mathbb{R}^d$  be a locally finite set for which  $\Delta(S)$  is uniformly discrete. Then,  $\mathbb{T}(S)$  is compact if and only if  $S$  is pure point diffractive. If  $S$  is a regular model set,  $\mathbb{T}(S)$  is precisely the group  $\mathbb{T}$  of the cut and project formalism that defines  $S$ .*

In the case that  $\mathbb{T}(S)$  is compact,  $(\mathbb{T}(S), \mathbb{R}^d)$  is a (minimal) dynamical system. There is another more common dynamical system associated with  $S$ . We declare two locally finite subsets  $S', S''$  to be close iff, for some large  $n$  and some small shift  $u \in \mathbb{R}^d$ ,  $(u + S') \cap B_n = S'' \cap B_n$ . The closure  $\mathbb{X}(S)$  of the  $\mathbb{R}^d$ -orbit of a locally finite set  $S$  in the resulting topology is called the *dynamical hull* of  $S$ . Provided that  $\Delta(S)$  is locally finite,  $\mathbb{X}(S)$  is compact and  $(\mathbb{X}(S), \mathbb{R}^d)$  is a dynamical system (see [4] for a more general approach in terms of measures).

These two dynamical systems arise from  $S$  in two very different ways, one using average coincidence over all of space, the other based on exact coincidence on large patches. In general, there is no reason to expect them to be related. However, one has

**Theorem 6** [5,26,28]. *Let  $S$  be a repetitive Meyer set. Then,  $S$  is a regular model set if and only if there exists a continuous surjective and almost everywhere 1–1  $\mathbb{R}^d$ -mapping  $\mathbb{X}(S) \rightarrow \mathbb{T}(S)$ .*

In general, although this map is almost everywhere one-to-one, its structure is very complicated and depends intimately on the boundary of the window defining  $S$ .

The connections between  $\mathbb{X}(S)$  as a dynamical system and the geometry of  $S$  as a point set are profound. Of particular relevance here is the following result (which has been recently improved and generalized to translation bounded measures [4]):

**Proposition 1** [23]. *Let  $S \subset \mathbb{R}^d$  be locally finite and let  $\mathbb{X}(S)$  be its dynamical hull, with  $U$  the associated unitary representation of  $\mathbb{R}^d$  on  $L^2(\mathbb{X}(S))$ . Then,  $S$  has uniform cluster frequencies if and only if  $(\mathbb{X}(S), \mathbb{R}^d)$  is uniquely ergodic. If so, then  $S$  is pure point diffractive if and only if the spectrum of  $U$  is pure point (pure point dynamical spectrum).*

Regular model sets are prime examples of pure point diffractive sets, and indeed most of the famous examples of pure point diffractive sets are model sets or multi-

coloured model sets. Is it possible to characterize regular model sets through pure point diffractivity? Here we offer an example of the type of result that seems like a highly plausible conjecture:

**Conjecture 1** [5]. *Let  $S$  be a repetitive and locally finite subset of  $\mathbb{R}^d$  for which  $\Delta(S)$  is uniformly discrete. Then,  $S$  is a regular model set if and only if the following three conditions are satisfied.*

- *The dynamical hull,  $\mathbb{X}(S)$ , is strictly ergodic, as a dynamical system over  $\mathbb{R}^d$ ;*
- *The eigenfunctions of the associated unitary representation  $U$  of  $(\mathbb{X}(S), \mathbb{R}^d)$  are continuous;*
- *$S$  is pure point diffractive.*

## 7. Final comments

The sine qua non of our whole investigation is the uniform discreteness of  $\Delta^{\text{ess}}$ . As an indication of just how powerful this type of condition is, even on its own, we mention a recent result of Strungaru:

**Theorem 7** [30]. *Let  $S \subset \mathbb{R}^d$  be relatively dense and suppose that  $\Delta(S)$  is uniformly discrete (in other words,  $S$  is a Meyer set). Then, assuming the autocorrelation of  $S$  exists, the diffraction of  $S$  contains a relatively dense (in particular infinite) set of Bragg peaks.*

Can we relax our strong basic assumption? The evidence points to some sort of fundamental barrier here beyond which things may be considerably different. The class of deformed model sets [11,16] requires a more advanced repertoire of dynamical systems theory, but seems tractable with the theory of factors in full generality. Examples such as the visible lattice points [7] demonstrate that pure point diffractivity is, in a way, also quite robust towards significant deviations from uniquely ergodic systems. A better understanding of these connections will also require a detailed analysis of the homometry problem, which is concerned with the characterization of all measures that share the same autocorrelation. This is also at the heart of the full inverse problem of crystallographic structure determination.

Finally, in view of the rapidly improving experimental tools and methods in crystallography, deviations from pure point diffraction gain importance. Stepping into the territory of mixed spectra, where there is still strong internal order manifested by a well-defined Bragg spectrum but also absolutely continuous and singular continuous parts, seems particularly timely (see [3,17,22] and references given there).

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