SPECTRAL NOTIONS OF APERIODIC ORDER

MICHAEL BAAKE
Fakultät für Mathematik, Universität Bielefeld
Postfach 100131, 33501 Bielefeld, Germany

DANIEL LENZ
Mathematisches Institut, Friedrich-Schiller-Universität
Jena, 07743 Jena, Germany

Abstract. Various spectral notions have been employed to grasp the structure and the long-range order of point sets, in particular non-periodic ones. In this article, we present them in a unified setting and explain the relations between them. For the sake of readability, we use Delone sets in Euclidean space as our main object class, and present generalisations in the form of further examples and remarks.

1. Introduction. After the discovery of quasicrystals by Shechtman in 1982, which was only published two years later [64], many people realised that our common understanding of what 'long-range order' might mean is incomplete (to put it mildly). In particular, little is known in the direction of a classification, which — despite the effort of many — still is the situation to date. One powerful tool for the analysis of order phenomena is provided by Fourier analysis, as is clear from the pioneering work of Meyer [52]. Moreover, it is not surprising that methods from physical diffraction theory, most notably the diffraction spectrum and diffraction measure of a spatial structure, have been adopted and developed.

From another mathematical perspective, taking into account proper notions of equivalence (which are needed for any meaningful classification attempt), a similar situation is well-known from dynamical systems theory. Here, the spectrum defined by Koopman [41] and later developed by von Neumann [72] and Halmos–von Neumann [34], led to a complete classification of ergodic dynamical systems with pure point spectrum up to (metric) isomorphism; see [22, 27, 59] for general background on spectral theory of dynamical systems, and [62] for some results in our context.

It is an obvious question how these spectral notions are related, and part of this article aims at a systematic comparison, building on the progress of the last 15 years or so. Since this means that large parts of the paper will have review character, our exposition will be informal in style. In particular, there will be no formal theorems. Instead, we discursively present relevant statements, concepts and underlying ideas, and refer to the original literature for more details and formal proofs as well as for generalisations. We hope that the general ideas and results, supported by several examples, transpire more naturally this way, and that the general flavour of the development is transmitted, too.

2010 Mathematics Subject Classification. 37B10, 52C23, 43A25.
Key words and phrases. Symbolic and Delone dynamical systems, diffraction versus dynamical spectrum, distributions and measures, aperiodic order and quasicrystals.
The paper is organised as follows. After recalling some notions from point sets and spectral theory in Section 2, we begin with the diffraction spectrum of an individual Delone set in Section 3. This part is motivated by the description of the physical process of (kinematic) diffraction, where one considers a single solid in a particle beam (photons or neutrons, say) in order to gain insight into its internal structure, and by the general mathematical aspects of Delone sets highlighted in [42]. Next, in Section 4, we extend the view by forming a dynamical system out of a given Delone set and by extending the notion of the individual diffraction to that of a diffraction measure of an (ergodic) dynamical system. The two pictures (diffraction of individual sets and diffraction of dynamical systems) are equivalent when the dynamical system is uniquely ergodic, but we will not only look at this case.

Then, in a third step, we look at the dynamical spectrum of a Delone dynamical system in Section 5 and how it is related to its diffraction spectrum in Section 6. Beyond the equivalence in the pure point case, which has been known for a while and is discussed in Section 7, we also look into the more general case of mixed spectra, at least for systems of finite local complexity (Section 8). In this case, the entire dynamical spectrum can still be described by diffraction. However, one might have to consider the diffraction of a whole family of systems that are constructed from factors.

We then turn to the maximal equicontinuous factor in Section 9. This factor stores information on continuous eigenfunctions and can be used to understand a hierarchy of Meyer sets via dynamical systems. Continuous eigenfunctions also play a role in diffraction theory via the so-called Bombieri–Taylor approach. Finally, in Section 10, we have a look at our theory if the Delone set is replaced by suitable quasiperiodic functions. We compute autocorrelation and diffraction in this case and discuss how the arising dynamical hull can be seen as the maximal equicontinuous factor of the hull of a Delone set. Moreover, we discuss an important difference between the diffraction of quasiperiodic functions and that of Delone sets.

Our article gives an introduction to a field which has seen tremendous developments over the last two decades, with steadily increasing activity. In our presentation of the underlying concepts and ideas of proofs, we do not strive for maximal generality but rather concentrate (most of) the discussion to Delone sets and present examples in various places. We have also included some pointers to work in progress, as well as to some open questions. Part of the material, such as the ideas concerning an expansion of sets into eigenfunctions in Sections 7 and the discussion of (diffraction of) quasiperiodic functions in Section 10 do not seem to have appeared in print before (even though they are certainly known in the community).

2. Preliminaries. Let us begin by recalling some basic notions tailored to our later needs. We do not aim at maximal generality here but will rather mainly be working in Euclidean space \( \mathbb{R}^d \). Some extensions will be mentioned in the form of remarks.

We start with discussing point sets, see [6, Sec. 2.1] and references therein for further details. A set consisting of one point is called a singleton set, while countable unions of singleton sets are referred to as point sets. A point set \( A \subset \mathbb{R}^d \) is called locally finite if \( K \cap A \) is a finite set (or empty), for any compact \( K \subset \mathbb{R}^d \). Next, \( A \) is discrete if, for any \( x \in A \), there is a radius \( r > 0 \) such that \( A \cap B_r(x) = \{ x \} \), where \( B_r(x) \) denotes the open ball of radius \( r \) around \( x \). If one radius \( r > 0 \) works for all
$x \in \Lambda$, our point set is called \textit{uniformly discrete}. Next, $\Lambda$ is called \textit{relatively dense} if a compact $K \subset \mathbb{R}^d$ exists such that $K + \Lambda = \mathbb{R}^d$, where $A + B := \{a + b \mid a \in A, b \in B\}$ denotes the Minkowski sum of two sets. Clearly, if $\Lambda$ is relatively dense, there is a radius $R > 0$ such that we see the condition satisfied with $K = B_R(0)$.

A \textit{Delone set} in $\mathbb{R}^d$ is a point set that is both uniformly discrete and relatively dense, so it can be characterised by two radii $r$ and $R$ in the above sense. They are therefore also called $(r,R)$-sets in the literature. Delone sets are mathematical models or idealisations of atomic positions in solids, which motivates their detailed study in our context.

A locally finite point set $\Lambda \subset \mathbb{R}^d$ is said to have \textit{finite local complexity} (FLC) with respect to translations if, for any compact neighbourhood $K$ of 0, the collection of $K$-clusters of $\Lambda$,

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

is a finite set. Again, it suffices to consider closed $R$-balls around 0 for all $R > 0$, and $\Lambda$ is an FLC set if and only if $\Lambda - \Lambda$ is locally finite; compare \cite[Prop. 2.1]{6}. Note that clusters (or $R$-patches in the case that we use a ball) are always defined around a point of $\Lambda$, so that the empty set is not a cluster in our sense.

A considerably stronger notion than that of a Delone set with finite local complexity is that of a \textit{Meyer set}, where one demands that $\Lambda$ is relatively dense while $\Lambda - \Lambda$ is uniformly discrete; see \cite[Lemma 2.1 and Rem. 2.1]{6} for details and \cite{55,56} for a thorough review. Clearly, every lattice in Euclidean space (by which we mean a co-compact discrete subgroup of $\mathbb{R}^d$) is a Meyer set. Thus, Meyer sets can be thought of as natural generalisations of lattices and this has been a very fruitful point of view for the theory of Meyer sets.

Meyer sets are always subsets of so-called \textit{model sets} \cite{52,55,6}, and they are important idealisations of the atomic positions of quasicrystals. Here, we do not go further into the theory of model sets and their cut-and-project schemes. Instead, we refer to \cite{52,55,56,6} for background on model sets. A classic example of a regular model set with eightfold symmetry in the plane is illustrated in Figure 1.

Note that the diffraction spectrum of a general Meyer set (in contrast to that of a lattice or a regular model set) may be mixed, but that they always have a pure point part that is uniformly spread out, and that an analogous property holds for a continuous component; see \cite{69,70} and references therein for details. If a Meyer set happens to be a model set, the data for its description are intrinsic and can be constructed from the set, as explained in \cite{13}.

There is a natural topology on the set of all Delone sets in Euclidean space. This topology can be introduced in various ways. A structural way is to identify a Delone set $\Lambda$ with a measure by considering its \textit{Dirac comb}

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

where $\delta_x$ is the normalised point measure (or Dirac measure) at $x$. Clearly, different Delone sets correspond to different measures. The vague topology on the measures then induces a topology on the Delone sets \cite{9}. To identify Delone sets with measures is more than a convenient mathematical trick. It is of great unifying power as it allows us to treat sets, functions and measures on the same footing. We will have more to say about this later.
Figure 1. A central patch of the eightfold symmetric Ammann–Beenker tiling of the plane, which can be generated by an inflation rule and is thus a self-similar tiling; see [6, Sec. 6.1] for details. The set of its vertex points is an example of a Meyer set, hence it is also an FLC Delone set. Moreover, it is a regular model set, as described in detail in [6, Ex. 7.8].

At this point, we note that the topology on the Delone sets can be generated by a metric as follows [48]. Let

\[ j : S^d \to \mathbb{R}^d \cup \{\infty\} \]

be the stereographic projection. Here, \( S^d \) denotes the \( d \)-dimensional sphere in \( \mathbb{R}^{d+1} \) and the point \( \infty \) denotes the additional point in the one-point compactification of \( \mathbb{R}^d \). The point \( \infty \) is then the image of the ‘north pole’ under \( j \). Let \( d_H \) be the Hausdorff metric on the set of compact subsets of \( S^d \). Then, for any Delone set \( \Lambda \subset \mathbb{R}^d \), the set \( j^{-1}(\Lambda \cup \{\infty\}) \) is a closed and hence compact subset of \( S^d \). Thus, via

\[ d_{\text{loc}}(\Lambda_1, \Lambda_2) := d_H(j^{-1}(\Lambda_1 \cup \{\infty\}), j^{-1}(\Lambda_2 \cup \{\infty\})) \]

we obtain a topology on the set of all Delone sets. It can be shown that this is the same topology as the one discussed above. In this topology, for any fixed \( R > r > 0 \), the set of all \((r, R)\)-Delone sets is compact [9] [43].

There is a canonical action of \( \mathbb{R}^d \) on the set of all Delone sets by translations via

\[ \mathbb{R}^d \times \text{Delone sets} \to \text{Delone sets}, \quad (t, \Lambda) \mapsto t + \Lambda. \]
Clearly, this action is continuous.

Let us fix $R > r > 0$. For any $(r, R)$-Delone set $A$, its hull

$$\mathcal{X}(A) := \{t + A \mid t \in \mathbb{R}^d\}$$

is a closed and hence compact subset of the $(r, R)$-Delone sets. By construction, the hull is invariant under the translation action of $\mathbb{R}^d$. Thus, the pair consisting of the compact hull $\mathcal{X}(A)$ and the restriction of the translation action of $\mathbb{R}^d$ on this hull is a topological dynamical system, which we denote by $(\mathcal{X}(A), \mathbb{R}^d)$. As usual, this dynamical system is called minimal if the translation orbit of $A'$, which is given by $\{t + A' \mid t \in \mathbb{R}^d\}$, is dense for every $A' \in \mathcal{X}(A)$, and it is called uniquely ergodic if it possesses exactly one probability measure $\mu$ that is invariant under the translation action; see [57] and references therein for background and an extension of these context to coloured point sets. In general, there might be several invariant probability measures. A triple such as $(\mathcal{X}(A), \mathbb{R}^d, \mu)$ is called a measure-theoretic dynamical system.

The convolution $\varphi \ast \psi$ of $\varphi, \psi \in C_c(\mathbb{R}^d)$ is an element of $C_c(\mathbb{R}^d)$ with

$$(\varphi \ast \psi)(x) := \int_{\mathbb{R}^d} \varphi(x - y) \psi(y) \, dy$$

for all $x \in \mathbb{R}^d$. We will identify measures on $\mathbb{R}^d$ with linear functionals on $C_c(\mathbb{R}^d)$ by means of the Riesz–Markov theorem. By the convolution of a measure $\nu$ with a function $\varphi \in C_c(\mathbb{R}^d)$, we mean the continuous function $\nu \ast \varphi$ defined by

$$(\nu \ast \varphi)(x) = \int_{\mathbb{R}^d} \varphi(x - y) \, d\nu(y).$$

A particular role will be played by positive definite measures, which are measures $\nu$ with

$$(\nu \ast \varphi \ast \varphi)(x) \geq 0$$

for all $\varphi \in C_c(\mathbb{R}^d)$, where $\varphi$ is defined by $\varphi(x) = \varphi(-x)$. Note that the last condition is equivalent to demanding $\nu(\varphi \ast \varphi) > 0$ for all $\varphi \in C_c(\mathbb{R}^d)$, which is also frequently used in the literature. Often, the measure $\nu$ at hand will also be positive, which means that $\nu(\varphi) \geq 0$ for all non-negative $\varphi \in C_c(\mathbb{R}^d)$. Any positive and positive definite measure is translation bounded, meaning that $\nu \ast \varphi$ is a bounded function for all $\varphi \in C_c(\mathbb{R}^d)$; see [17] Prop. 4.4 for details. For the convolution of measures, one starts with

$$(\mu \ast \nu)(\varphi) := \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \varphi(x + y) \, d\mu(x) \, d\nu(y)$$

for finite measures $\mu, \nu$ and then extends this definition step by step, for instance to $\mu$ finite and $\nu$ translation bounded; we refer to [63] [17] [4] for standard background material.

We will also need the Fourier transform of functions, measures and distributions. For a complex-valued function $f$ on $\mathbb{R}^d$ that is integrable with respect to Lebesgue measure, so $f \in L^1(\mathbb{R}^d)$, we define its Fourier transform $\hat{f}$ as the complex-valued function given by

$$\hat{f}(k) := \int_{\mathbb{R}^d} e^{-2\pi ikx} f(x) \, dx.$$ 

Clearly, this definition can be extended to finite measures; see [63] or [4] Ch. 8 and references therein for details. It turns out that it can also be extended to various other classes of objects, including tempered distributions [64]. This approach, which is also explained in many textbooks, will be sufficient for large parts of this survey.
A little more delicate is the extension to unbounded measures, where we refer to [17] for background; see also [1, 31]. In particular, we note that the Fourier transform of a positive definite measure exists and is a positive measure [6, Prop. 8.6]. Moreover, Fourier transform is a continuous map from the cone of positive and positive definite measures into itself, which is an important property for many arguments.

3. Diffraction of individual objects. Let us begin by considering a single Delone set $\Lambda \subset \mathbb{R}^d$, where we first recall a spectral notion from the pioneering paper [36], which is known as the diffraction measure of $\Lambda$; compare [6, Sec. 9.1] for a more detailed account and [14] for further connections and questions. In order to put our approach in the general perspective of mathematical diffraction theory, we will identify a Delone set $\Lambda$ with its Dirac comb $\delta_\Lambda = \sum_{x \in \Lambda} \delta_x$. In our setting, the diffraction measure emerges as the Fourier transform of the (natural) autocorrelation measure, in extension of the classic Wiener diagram for integrable functions; compare [6, Sec. 9.1.2]. Since $\delta_\Lambda$ is an infinite measure, it cannot be convolved with itself, wherefore one needs to proceed via restrictions to balls (or, more generally, to elements of a general van Hove sequence [6, Def. 2.9]). Setting $\delta^R_\Lambda := \delta_{\Lambda \cap B_R(0)}$, we consider

$$
\gamma^R_\Lambda := \frac{\delta^R_\Lambda \ast \delta^R_\Lambda}{\text{vol}(B_R(0))}
$$

where $\tilde{\mu}$ is the ‘flipped-over’ version of a measure $\mu$, defined by $\tilde{\mu}(g) = \mu(\tilde{g})$ for $g \in C_c(\mathbb{R}^d)$ and $\tilde{g}$ as above. Complex conjugation is not relevant in our point set situation, but is needed for any extension to (complex) weighted Dirac combs and general measures.

Every accumulation point of the family $\{\gamma^R_\Lambda | R > 0\}$ in the vague topology, as $R \to \infty$, is called an autocorrelation of the Delone set $\Lambda$. By standard arguments, compare [6, Prop. 9.1], any Delone set possesses at least one autocorrelation, and any autocorrelation is translation bounded. If only one accumulation point exists, the autocorrelation measure

$$
\gamma_\Lambda = \lim_{R \to \infty} \gamma^R_\Lambda
$$

is well-defined (we will only consider this situation later), and called the natural autocorrelation. Here, the term ‘natural’ refers to the use of balls as averaging objects, as they are closest to the typical situation met in the physical process of diffraction. In ‘nice’ situations, the autocorrelation will not depend on the choice of averaging sequences, as long as they are of van Hove type (where, roughly stating for the case of $\mathbb{R}^d$ at hand, the surface to volume ratio vanishes in the infinite volume limit). Note that a van Hove sequence is a special type of Følner sequence. The volume-averaged convolution in the definition of $\gamma_\Lambda$ is also called the Eberlein convolution of $\delta_\Lambda$ with its flipped-over version, written as

$$
\gamma_\Lambda = \delta_\Lambda \otimes \tilde{\delta}_\Lambda.
$$

We refer to [6, Sec. 8.8] for some basic properties and examples.

A particularly nice situation emerges when $\Lambda$ is an FLC set, so $\Lambda - \Lambda$ is locally finite. Then, assuming the natural autocorrelation to exist, a short calculation shows that

$$
\gamma_\Lambda = \sum_{z \in \Lambda - \Lambda} \eta(z) \delta_z \quad \text{with} \quad \eta(z) = \lim_{R \to \infty} \frac{\text{card}(A_R \cap (A_R - z))}{\text{vol}(B_R(0))}.
$$
According to its definition, \( \eta(z) \) can be seen as the frequency (within \( \Lambda \)) of the vector \( z \) from the difference set \( \Lambda - \Lambda \). Thus, the autocorrelation of \( \Lambda \) stores information on the set of difference vectors of \( \Lambda \) and their frequencies. Note that \( \gamma_\Lambda \) in this case is a pure point measure on \( \mathbb{R}^d \).

By construction, the autocorrelation of any Delone set \( \Lambda \) is a positive measure, which is also positive definite. As a consequence, its Fourier transform, denoted by \( \hat{\gamma}_\Lambda \), exists, and is a positive (and positive definite) measure. This measure describes the outcome of a scattering (or diffraction) experiment with our ‘idealised solid’ when put into a coherent light or particle source; see [23] for background. By continuity of the Fourier transform, we have

\[
\hat{\gamma}_\Lambda = \lim_{R \to \infty} \hat{\gamma}_R = \lim_{R \to \infty} \frac{1}{\text{vol}(B_R(0))} \sum_{x,y \in \Lambda \cap B_R(0)} e^{2\pi i (x-y) \cdot (\cdot)}.
\]

Here, the function on the right hand side is considered as a measure (namely the measure which has the function as its density with respect to Lebesgue measure), and the limit is taken in the sense of vague convergence of measures.

Given the interpretation of the diffraction measure as the outcome of a diffraction experiment, it is natural that special attention is paid to the set

\[
\mathcal{B} := \{ k \in \mathbb{R}^d \mid \hat{\gamma}_\Lambda(\{k\}) > 0 \}.
\]

This set is denoted as the Bragg spectrum (after the fundamental contributions to structure analysis of crystals via diffractions of the Braggs, father and son, which was honoured with the Noble Prize in Physics in 1914). The point measures of \( \hat{\gamma}_\Lambda \) on the Bragg spectrum are known as Bragg peaks, and for any \( k \in \mathcal{B} \), the value \( \hat{\gamma}_\Lambda(\{k\}) \) is called the intensity of the Bragg peak. In this context, there is the idea around that one should have

\[
\hat{\gamma}_\Lambda(\{k\}) = \lim_{R \to \infty} \left| \frac{1}{\text{vol}(B_R(0))} \sum_{x \in \Lambda \cap B_R(0)} e^{2\pi i kx} \right|^2.
\]

Indeed, this formula is quite reasonable as it says that the intensity of the diffraction at \( k \) is given as a square of a mean Fourier coefficient. We will have more to say about its validity as we go along.

**Remark 1.** The validity of such a formula is discussed in [36] with reference to work of Bombieri and Taylor [19, 18], who used the formula without justification for certain systems coming from primitive substitutions. This was later justified in [30]. For regular model sets, the formula was shown in [65], but is also contained in [51]; see [6, Prop. 9.9] as well. In both cases, the special structure at hand is used. A structural approach is given in [47] and will be discussed in Section 9. More recently, the approach via amplitudes in the form of averaged exponential sums was extended to weak model sets of extremal density, where different methods have to be used; see [5, Prop. 8] for details. We shall come back to this topic later.

From now on, whenever the meaning is unambiguous, we will drop the Delone set index and simply write \( \gamma \) and \( \hat{\gamma} \) for the autocorrelation and diffraction of \( \Lambda \). Our approach is not restricted to Delone sets (see various remarks below), though we will mainly consider this case for ease of presentation.

**Example 1.** The set \( \mathbb{Z} \) of integers, in our formulation, is described by the Dirac comb \( \delta_\mathbb{Z} \), and possesses the natural autocorrelation \( \gamma = \delta_\mathbb{Z} \), as follows from a straightforward Eberlein convolution; compare [6, Ex. 8.10]. Its Fourier transform
is then given by $\hat{\gamma} = \delta_2$, as a consequence of the Poisson summation formula (PSF); see [6, Ch. 9.2.2] for details.

More generally, given a crystallographic (or fully periodic) Delone set $\Lambda \subset \mathbb{R}^d$, its Dirac comb is of the form $\delta_\Lambda = \delta_S * \delta_T$ where $\Gamma = \{ t \in \mathbb{R}^d \mid t + \Lambda = \Lambda \}$ is the lattice of periods of $\Lambda$ and $S$ is a finite point set that is obtained by the restriction of $\Lambda$ to a (true) fundamental domain of $\Gamma$; compare [6, Prop. 3.1]. Note that such a domain will not be a closed set. Now, a simple calculation gives the natural autocorrelation

$$\gamma = \text{dens}(\Gamma)(\delta_S * \delta_S) * \delta_T,$$

which is easily Fourier transformable by an application of the convolution theorem together with the general PSF in the form $\delta_\Gamma = \text{dens}(\Gamma) \delta_{\Gamma^*}$. Here, $\Gamma^*$ is the dual lattice of $\Gamma$, which means $\Gamma^* = \{ x \in \mathbb{R}^d \mid x \cdot y \in \mathbb{Z} \}$ where $x \cdot y$ denotes the standard inner product of $\mathbb{R}^d$. The result is the diffraction measure

$$\hat{\gamma} = (\text{dens}(\Gamma))^2 |h|^2 \delta_{\Gamma^*} = (\text{dens}(\Gamma))^2 \sum_{k \in \Gamma^*} |h(k)|^2 \delta_k,$$

where $h = \tilde{\delta}_2$ is a bounded continuous function on $\mathbb{R}^d$; see [6, Sec. 9.2.4] for further details. We thus see that the diffraction measure is a pure point measure that is concentrated on the points of the dual lattice, with intensity $I(k) = (\text{dens}(\Gamma))^2 |h(k)|^2$ for $k \in \Gamma^*$.

It is perhaps worth noting that the finite set $S$ in the above decomposition of the Dirac comb $\delta_\Lambda$ is not unique, and neither is then the function $h$, because there are infinitely many distinct possibilities to choose a fundamental domain of $\Gamma$. Still, all functions $h$ that emerge this way share the property that the values of $|h|^2$ agree on all points of $\Gamma^*$, so that the formula for the diffraction measure is unique and unambiguous.

**Remark 2.** As is quite obvious from our formulation, the Dirac comb of a Delone set is an example of a translation bounded measure on Euclidean space. This suggests that one can extend the entire setting to general translation bounded measures; compare [17, 36, 9] as well as [6, Chs. 8 and 9]. Given such a measure, $\omega$ say, one then defines its autocorrelation measure as $\gamma_\omega = \omega \circ \tilde{\omega}$, provided this limit exists. It is then a translation bounded, positive definite measure, hence Fourier transformable by standard arguments [17], and $\hat{\gamma}_\omega$ is a translation bounded, positive measure, called the **diffraction measure of $\omega$**. This point of view was first developed in [36], and has been generalised in a number of articles; see [6] and references therein for background, and [49] for a general formulation.

Figure 2 below shows an example of a diffraction measure for an aperiodic point set, namely that of the Ammann–Beenker point set introduced in Figure 1. For the detailed calculation in the context of regular cyclotomic model sets, we refer the reader to [6, Secs. 7.3 and 9.4.2].

Although the notion of a diffraction measure is motivated by the physical process of diffraction, so that this approach looks very natural for Delone sets as mathematical models of atomic positions in a solid, the concept is by no means restricted to Delone sets, or even to measures.

**Example 2.** Let $S(\mathbb{R})$ denote the space of Schwartz functions on $\mathbb{R}$ and $S'(\mathbb{R})$ its dual, the space of tempered distributions; see [66, 73] for general background. In this context, $\delta'_x$ is a distribution with compact support, defined by $(\delta'_x, \varphi) = -\varphi'(x)$, where we follow the widely used convention to write $(T, \varphi)$ for the evaluation of a
distribution $T \in S'(\mathbb{R})$ at a test function $\varphi \in S(\mathbb{R})$. Note that $\delta'_x$ is not a measure. Tempered distributions of compact support are convolvable, and one checks that $\delta'_x * \delta'_y = \delta''_{x+y}$.

Let us now consider $\omega = \delta'_Z := \sum_{z \in \mathbb{Z}} \delta'_z$, which clearly is a tempered distribution. Also, we have $\omega = \delta'_0 * \delta_Z$, so that standard arguments imply the existence of the Eberlein convolution of $\omega$. A simple calculation gives

$$\gamma_\omega = \omega * \tilde{\omega} = \delta''_Z = \delta''_0 * \delta_Z.$$  

This is a tempered distribution of positive type, again, so its Fourier transform is a tempered distribution of positive type again, so its Fourier transform is always a tempered distribution, is then actually a positive 

measure, by an application of the Bochner–Schwartz theorem. Observing that $\hat{\delta}'_0$ is a regular distribution, and thus represented by a smooth function, one can check that

$$\hat{\gamma}_\omega = \hat{\omega} * \hat{\tilde{\omega}} = 4\pi^2 y^2.$$ 

Now, using the convolution theorem together with the PSF, it is routine to check that

$$\hat{\gamma}_\omega = \hat{\delta''_0} = 4\pi^2 (\cdot)^2 \delta_Z = \sum_{y \in \mathbb{Z}} 4\pi^2 y^2 \delta_y.$$ 

This is a positive pure point measure, the (natural) diffraction measure of the tempered distribution $\omega$. In comparison to previous examples, it is not translation bounded, which makes it an interesting extension of the measures in Example 1.

More generally, let us consider a lattice $\Gamma \subset \mathbb{R}^d$. If $p = (p_1, \ldots, p_d)$ denotes a multi-index (so all $p_i \in \mathbb{N}_0$) with $|p| = p_1 + \ldots + p_d$ and $x^p = x_1^{p_1} \cdots x_d^{p_d}$, as well as the differential operator

$$D^p = \frac{\partial^{\left|p\right|}}{\partial x_1^{p_1} \cdots \partial x_d^{p_d}},$$

see [73] for background, we get $\delta^{(p)}_{x^p} * \delta^{(q)}_{y^q} = \delta^{(p+q)}_{x+y}$, where $(\delta^{(p)}_x, \varphi) := (-1)^{|p|} (D^p \varphi)(x)$ as usual. Now, for fixed $p$, consider the lattice-periodic tempered distribution $\omega = \delta^{(p)}_{\Gamma} = \delta^{(p)}_{(0) \ast \delta_{\Gamma}}$. As before, the natural autocorrelation $\gamma_\omega$ exists, and is given by

$$\gamma_\omega = \text{dens}(\Gamma) \delta^{(2p)}_{\Gamma} = \text{dens}(\Gamma) \delta^{(2p)}_{(0) \ast \delta_{\Gamma}}.$$ 

This is a tempered distribution of positive type again, so its Fourier transform is a positive tempered measure. Observing

$$\hat{\delta}^{(2p)}_{(0)}(y) = (4\pi^2)^{|p|} y^{2p}$$

in analogy to above, one can employ the convolution theorem together with the general PSF from Example 1 to calculate the diffraction, which results in

$$\hat{\gamma}_\omega = (4\pi^2)^{|p|} \text{dens}(\Gamma) y^{2p} \delta_{\Gamma} = \text{dens}(\Gamma)^2 (4\pi^2)^{|p|} \sum_{y \in \Gamma^*} y^{2p} \delta_y.$$ 

This measure is only translation bounded for $p = 0$, where it reduces to the diffraction measure of the lattice Dirac comb $\delta_{\Gamma}$ of Example 1 as it must.

By the convolution structure, one can further generalise as follows. Let $\Lambda \subset \mathbb{R}^d$ be a Delone set with natural autocorrelation $\gamma_\Lambda$, let $\nu$ be a tempered distribution of compact support, and consider $\omega = \nu \ast \delta_\Lambda$. Clearly, this is a tempered distribution,
with existing (natural) autocorrelation. The latter is given by
\[ \gamma_\omega = (\nu * \hat{\nu} * \gamma_A) \]
which is of positive type again. Fourier transform then results in the diffraction
\[ \hat{\gamma}_\omega = |\hat{\nu}|^2 \hat{\gamma}_A \]
where \( \hat{\nu} \) is a smooth function on \( \mathbb{R}^d \).

Remark 3. As one can see from the general structure of the volume-averaged convolution, the concept of a diffraction measure can be put to use in a wider context. Let us thus start from a locally convex space \( F \) of functions on \( \mathbb{R}^d \) and let \( F' \) be its dual, the space of continuous linear functionals on \( F \). Examples include \( C_c(\mathbb{R}^d) \), which gives the regular Borel measures with the vague topology, and \( S(\mathbb{R}^d) \), with the space \( S'(\mathbb{R}^d) \) of tempered distributions as its dual, but also the space \( D(\mathbb{R}^d) \) of \( C^\infty \)-functions with compact support, then leading to the space \( D'(\mathbb{R}^d) \) of distributions [66, 73]. Various other combinations will work similarly.

What we need is the concept of a functional of compact support, or a suitable variant of it, and the convolution of two linear functionals \( G, H \) of that kind, as defined by
\[ (G * H, \varphi) := (G \times H, \varphi^\times) \]
where \( \varphi \in F \) and \( \varphi^\times : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C} \) is defined by \( \varphi^\times(x, y) = \varphi(x + y) \). To expand on this, let us assume that a distribution \( F \in D'(\mathbb{R}^d) \) is given. Fix some \( \varepsilon > 0 \) and let \( c_{r, \varepsilon} \in D(\mathbb{R}^d) \) be a non-negative function that is 1 on the ball \( B_r(0) \) and 0 outside the ball \( B_{r+\varepsilon}(0) \). Such functions exist for any \( r > 0 \). Now, consider
\[ \gamma_{F, \varepsilon}^{(r)} := \frac{c_{r, \varepsilon} F * c_{r, \varepsilon} F}{\int_{\mathbb{R}^d} c_{r, \varepsilon}(x) \, dx} \]
which is well-defined, with \( \int_{\mathbb{R}^d} c_{r, \varepsilon}(x) \, dx = \text{vol}(B_r(0)) + O(1/r) \) as \( r \to \infty \). If \( \lim_{r \to \infty} \gamma_{F, \varepsilon}^{(r)} \) exists and is also independent of \( \varepsilon \), which will be the case under some mild assumptions on \( F \), we call the limit \( \gamma_F \), the natural autocorrelation of the distribution \( F \). More generally, one can work with accumulation points as well. If \( \gamma \) happens to be a tempered distribution, we are back in the situation that \( \hat{\gamma}_F \) is a positive measure, called the diffraction measure of the distribution \( F \). This setting provides a versatile generalisation of the diffraction theory of translation bounded measures; see [16, 71] for a detailed account.

4. Diffraction of dynamical systems. The diffraction measure of an individual Delone set is a concept that emerges from the physical situation of a diffraction experiment. It is both well founded and useful. Still, it has a number of shortcomings that are related with the fact that it is not obvious how \( \hat{\gamma} \) ‘behaves’ when one changes the Delone set. Since the mapping between autocorrelation and diffraction is Fourier transform, and thus one-to-one, we can address this issue on the level of the autocorrelation. Let us assume that we have a Delone set \( A \) whose natural autocorrelation exists. Clearly, any translate of the set should have the same autocorrelation, so
\[ \gamma_{t+A} = \gamma_A \quad \text{for all} \quad t \in \mathbb{R}^d, \]
and this is indeed a simple consequence of the van Hove property of the family of balls \( \{ B_R(0) \mid R > 0 \} \). In fact, a proof only uses the (slightly weaker) Følner property of them for single points.

Less obvious is what happens if one goes to the compact hull \( X(A) \) as introduced above. Nevertheless, at least from a dynamical systems point of view, it is very
natural to define an autocorrelation for a dynamical system. Here, one best starts with a measure-theoretic dynamical system \((X, \mathcal{A}, \mathbb{R}^d, \mu)\), where \(\mu\) is an invariant probability measure on \(X\). In the large and relevant subclass of uniquely ergodic Delone dynamical systems with FLC, the unique measure \(\mu\) is the patch frequency measure. Then, any such measure-theoretic dynamical system \((X, \mathcal{A}, \mathbb{R}^d, \mu)\) comes with an autocorrelation \(\gamma_\mu\) associated to it via a closed formula (as opposed to a limit). This is discussed next, where we follow [9]; see [33] as well.

Choose a function \(\chi \in C_c(\mathbb{R}^d)\) and consider the map \(\gamma_{\mu,\chi} : C_c(\mathbb{R}^d) \to \mathbb{C}\) defined by

\[
\varphi \mapsto \int_{\mathcal{A}(\chi)} \sum_{y \in A'} \varphi(x - y) \chi(x) \, d\mu(A') .
\]

Clearly, \(\gamma_{\mu,\chi}\) is a continuous functional on \(C_c(\mathbb{R}^d)\). By the Riesz–Markov theorem, it can then be viewed as a measure. Now, for fixed \(\varphi \in C_c(\mathbb{R}^d)\), the map

\[
C_c(\mathbb{R}^d) \to \mathbb{C}, \quad \chi \mapsto \gamma_{\mu,\chi}(\varphi),
\]

is continuous. Hence, it is a measure as well. Moreover, as \(\mu\) is translation invariant, this measure can easily be seen to be invariant under replacing \(\chi\) by any of its translates. Hence, it must be a multiple of Lebesgue measure. Consequently, it will take the same values for all \(\chi\) that are normalised in the sense that they satisfy \(\int_{\mathbb{R}^d} \chi(t) \, dt = 1\). So, the map \(\gamma_{\mu,\chi}\) will be independent of \(\chi\) provided \(\chi\) is normalised. Thus, we can unambiguously define

\[
\gamma_\mu := \gamma_{\mu,\chi}
\]

for any such normalised \(\chi\). This is then called the autocorrelation of the dynamical system \((X, \mathcal{A}, \mathbb{R}^d, \mu)\).

If \(\mu\) is an ergodic measure, it can be shown that, for \(\mu\)-almost every element \(A'\) in the hull \(\mathcal{A}(\chi)\), the individual autocorrelation \(\gamma_{A'}\) of \(A'\) exists and equals \(\gamma_\mu\). In general, the assessment of equality is difficult, unless one knows that \(A'\) is generic for \(\mu\) in the hull. However, if the dynamical system \((X, \mathbb{R}^d)\) is even uniquely ergodic, the autocorrelation can be shown to exist and to be equal to \(\gamma_\mu\) for every element in the hull. We refer to [9] for further details and references. Important cases include Delone sets derived from primitive substitution rules via their geometric realisations, see [6] Chs. 4 and 9] for details and many examples, and regular model sets in Euclidean space, such as the Ammann–Beenker point set from Figures [1] and [2] compare [6] Chs. 7 and 9] for more.

For any \((X, \mathcal{A}, \mathbb{R}^d, \mu)\), the autocorrelation \(\gamma_\mu\) can be shown to be a positive definite measure. Hence, its Fourier transform exists and is a positive measure. This measure will be called the diffraction measure of the dynamical system, and denoted by \(\hat{\gamma}_\mu\). As in the case of the diffraction of an individual set, we will be particularly interested in the point part of the diffraction measure. The set of atoms of this pure point part is again denoted by \(\mathcal{B}\) and called Bragg spectrum; this is sometimes also called the diffraction spectrum. It is then possible to compute the Bragg spectrum via the following functions defined for each \(k \in \mathbb{R}^d\) by

\[
c_k^{(R)} : \mathcal{X}(\chi) \to \mathbb{C}, \quad c_k^{(R)}(A') := \frac{1}{\text{vol}(B_R(0))} \sum_{x \in A' \cap B_R(0)} e^{2 \pi i k x}.
\]

More specifically, as shown in [25], we have

\[
\hat{\gamma}_\mu(\{k\}) = \lim_{R \to \infty} \|c_k^{(R)}\|_{L^2}^2 ,
\]
Figure 2. Illustration of a central patch of the diffraction measure of the Ammann–Beenker point set of Figure 1, which has pure point diffraction. A Bragg peak of intensity $I$ at $k \in B$ is represented by a disc of an area that is proportional to $I$ and centred at $k$. Here, $B$ is a scaled version of $\mathbb{Z}[e^{\pi i/4}]$, which is a group; compare [4] Sec. 9.4.2 for details. Although $B$ is dense, the figure only shows Bragg peaks beyond a certain threshold. In particular, there are no extinctions in this case. At the same time, this measure is the diffraction measure of the Delone dynamical system defined by the (strictly ergodic) hull of the Ammann–Beenker point set, and $B$ is its dynamical spectrum for the translation action of $\mathbb{R}^2$ on the hull.

where $\| \cdot \|_{L^2}$ denotes the norm of the Hilbert space $L^2(\mathcal{X}(\Lambda), \mu)$, and if the dynamical system is ergodic, we even have

$$\widehat{c}_\mu(k) = \lim_{R \to \infty} \left| c_k^{(R)}(A') \right|^2$$

for $\mu$-almost every $A' \in \mathcal{X}(\Lambda)$. Note that, in these cases, the corresponding limit will vanish for all $k \in \mathbb{R}^d \setminus B$. One may expect that convergence holds for all $A' \in \mathcal{X}(\Lambda)$ in the uniquely ergodic case. However, this is not clear at present. We will have more to say about this in Section 9.
Remark 4. In the preceding discussion, ergodicity of the measure on the hull has played some role. Thus, one may wonder about what happens for general measures. So, let $\nu$ be an arbitrary invariant probability measure on the hull that can be written as a convex combination $\nu = \sum_{i \in I} \alpha_i \mu_i$ of other invariant probability measures on the hull, hence $\alpha_i > 0$ and $\sum_{i \in I} \alpha_i = 1$. Then, using the same function $\chi$ for all autocorrelations, one sees that

$$\gamma_\nu = \sum_{i \in I} \alpha_i \gamma_{\mu_i}.$$  

Invoking Choquet’s theorem, compare [58] for background, one can thus see that the analysis of the autocorrelations of extremal and thus ergodic invariant probability measures on the hull is the essential step in the diffraction analysis of a Delone dynamical system.

Remark 5. At this point, we have discussed two ways of defining an autocorrelation, namely via a limiting procedure for individual Delone sets and via integration for hulls of Delone sets. While these may seem very different procedures at first, we would like to stress that both have in common that they involve some form of averaging. Indeed, in the limiting procedure, this is an average over $\mathbb{R}^d$, while in the closed formula given above, it is an average over the hull. The connection between these two averages is then made by an ergodic theorem.

5. The dynamical spectrum. In the preceding section, we have seen that any Delone dynamical system $(X(A), \mathbb{R}^d, \mu)$ comes with an autocorrelation measure $\gamma_\mu$ (and thus also with a diffraction measure $\gamma_\mu^d$). We have also seen that this autocorrelation measure agrees, for a (typical) element of the hull, with the individual autocorrelation of this element if the measure $\mu$ is ergodic. This suggests that there is a close connection between properties of the dynamical system and the diffraction. As was realised by Dworkin [26], this is indeed the case. This is discussed in this section. In order to do so properly, we will first have to introduce the spectral theory of a dynamical system. This is the spectral theory of what we call (in line with various other people) the Koopman representation of the dynamical system, in recognition of Koopman’s pioneering work [41].

A Delone dynamical system $(X(A), \mathbb{R}^d, \mu)$ gives rise to a unitary representation $T$ of $\mathbb{R}^d$ on the Hilbert space $L^2(X(A), \mu)$ via

$$T: \mathbb{R}^d \rightarrow \text{unitary operators on } L^2(X(A), \mu), \ t \mapsto T_t,$$

with

$$T_t f = f(\cdot - t).$$

Indeed, we obviously have $T_{t+s} = T_t T_s$ for any $t, s \in \mathbb{R}^d$ as well as $T_0 = 1$. So, $T$ is a representation of $\mathbb{R}^d$. Also, as the measure $\mu$ is invariant, any $T_t$, with $t \in \mathbb{R}^d$, is isometric and, clearly, $T_{-t}$ is the inverse to $T_t$. Thus, any $T_t$ is isometric and invertible and thus unitary. Moreover, it is not hard to see that $T$ is strongly continuous, which means that, for any fixed $f \in L^2(X(A), \mu)$, the map

$$\mathbb{R}^d \rightarrow L^2(X(A), \mu), \ t \mapsto T_t f,$$

is continuous. We call the map $T$ the Koopman representation of the dynamical system. As $T$ is a strongly continuous unitary representation, Stone’s theorem (compare [50]) guarantees the existence of a projection-valued measure

$$E_T: \text{Borel sets on } \mathbb{R}^d \rightarrow \text{projections on } L^2(X(A), \mu)$$
with

\[ \langle f, T_t f \rangle = \int_{\mathbb{R}^d} e^{2\pi i tk} d\rho_f(k) = \hat{\rho}_f(-t), \]

for all \( t \in \mathbb{R}^d \), where \( \rho_f \) is the measure on \( \mathbb{R}^d \) defined by

\[ \rho_f(B) := \langle f, E_T(B) f \rangle. \]

The measure \( \rho_f \) is known as the spectral measure of \( f \) (with respect to \( T \)). It is the unique measure on \( \mathbb{R}^d \) with \( \langle f, T_t f \rangle = \hat{\rho}_f(-t) \) for all \( t \in \mathbb{R}^d \). The study of the properties of the spectral measures is then known as the spectral theory of the dynamical system; see [59] for a general exposition in the one-dimensional case.

In particular, the spectrum of the dynamical system is given as the support of \( E_T \) defined by

\[ \{ k \in \mathbb{R}^d \mid E_T(B_\varepsilon(k)) \neq 0 \text{ for all } \varepsilon > 0 \}. \]

Of course, the spectrum is a set and as such does not carry any information on the type of the spectral measures. For this reason, one is mostly not interested in the spectrum alone, but also in determining a spectral measure of maximal type (thus a spectral measure having the same zero sets as \( E_T \)). We discuss a substitution-based system with mixed spectrum below in Example 3. For us, the following subset of the spectrum will be particularly relevant. The point spectrum of the dynamical system is given as

\[ \{ k \in \mathbb{R}^d \mid E_T(\{k\}) \neq 0 \}. \]

A short consideration reveals that \( k \in \mathbb{R}^d \) belongs to the point spectrum if and only if it is an eigenvalue of \( T \). Here, an \( f \neq 0 \) with \( f \in L^2(\mathcal{X}(\Lambda), \mu) \) is called an eigenfunction to the eigenvalue \( k \in \mathbb{R}^d \) if

\[ T_t f = e^{2\pi i k t} f \]

holds for all \( t \in \mathbb{R}^d \). Note that, following common practice, we call \( k \) (rather than \( e^{2\pi i k x} \)) the eigenvalue, as this matches nicely with the structure of the translation group as well as its dual (the latter written additively).

If our dynamical system is ergodic, the modulus of any eigenfunction must be constant (as it is an invariant function). So, in this case, all eigenfunctions are bounded. If the system fails to be ergodic, eigenfunctions need not be bounded. However, by suitable cut-off procedures, one can always find a bounded eigenfunction to each eigenvalue; compare [9] for a recent discussion. It is not hard to see that the eigenvalues form a group. Indeed,

- the constant function is an eigenfunction to eigenvalue 0,
- whenever \( f \) is an eigenfunction to \( k \), then \( T \) is an eigenfunction to \( -k \), and
- whenever \( f \) and \( g \) are bounded eigenfunctions to \( k \) and \( \ell \), respectively, the product \( fg \) is an eigenfunction to \( k + \ell \).

We denote this group of eigenvalues by \( \mathcal{E}(\mu) \). Standard reasoning also shows that eigenfunctions to different eigenvalues are orthogonal. We will have more to say on eigenvalues and eigenfunctions later.

6. Connections between dynamical and diffraction spectrum. Having introduced the dynamical spectrum, we now turn to the connection with diffraction. The crucial ingredient is that the Schwartz space \( \mathcal{S}(\mathbb{R}^d) \) can be embedded into \( C(\mathcal{X}(\Lambda)) \) via

\[ f : \mathcal{S}(\mathbb{R}^d) \longrightarrow C(\mathcal{X}(\Lambda)), \quad \varphi \mapsto f_{\varphi}, \]
with
\[ f_\varphi(A') := (\varphi * \delta_{A'})(0) = \sum_{x \in A'} \varphi(-x). \]

**Remark 6.** We could also work with the corresponding embedding of \(C_c(\mathbb{R}^d)\) into \(C(\mathcal{X}(\Lambda))\), and indeed this is often done. Note also that the existence of such embeddings will not be true for general dynamical systems, but rather requires the possibility of a ‘pairing’ between the elements of the dynamical system and functions. Indeed, it is possible to extend (some of) the considerations below whenever such a pairing is possible \([16, 71, 46]\).

Based on this embedding, one can provide the connection between diffraction and dynamical spectrum. Here, we follow \([25]\) (see \([46]\) as well), to which we refer for further details and proofs. The key formula emphasised in \([26]\) is
\[ (\gamma_\mu * \tilde{\varphi} * \varphi)(0) = \langle f_\varphi, f_\varphi \rangle \]
for \(\varphi \in \mathcal{S}(\mathbb{R}^d)\). This result was quite influential in the field, as it highlighted a connection that was implicitly also known in point process theory, compare \([24]\) as well as \([32]\), but had not been observed in the diffraction context. Taking Fourier transforms and using the denseness of \(\mathcal{S}(\mathbb{R}^d)\) in \(L^2(\mathbb{R}^d)\), one can use this formula to obtain a (unique) isometric map
\[ \Theta: L^2(\mathbb{R}^d, \gamma_\mu) \rightarrow L^2(\mathcal{X}(\Lambda), \mu), \quad \text{with } \Theta(\tilde{\varphi}) = f_\varphi \]
for all \(\varphi \in \mathcal{S}(\mathbb{R}^d)\). Now, both \(L^2\)-spaces in question admit a unitary representation of \(\mathbb{R}^d\). Indeed, we have already met the Koopman representation \(T\). Moreover, for any \(t \in \mathbb{R}^d\), we have a unitary map
\[ S_t: L^2(\mathbb{R}^d, \gamma_\mu) \rightarrow L^2(\mathbb{R}^d, \gamma_\mu), \quad S_t h = e^{2\pi i t \cdot h}, \]
and these maps yield a representation \(S\) of \(\mathbb{R}^d\) on the Hilbert space \(L^2(\mathbb{R}^d, \gamma_\mu)\). Then, it is not hard to see that \(\Theta\) intertwines \(S\) and \(T\), which means that
\[ \Theta S_t = T_t \Theta \]
holds for all \(t \in \mathbb{R}^d\). In fact, this is clear when applying both sides to functions of the form \(\tilde{\varphi}\) for \(\varphi \in \mathcal{S}(\mathbb{R}^d)\) and then follows by a denseness argument in the general case. Consider now
\[ \mathcal{U} := \Theta(L^2(\mathbb{R}^d, \gamma_\mu)) = \overline{\operatorname{Lin}}\{ f_\varphi : \varphi \in \mathcal{S}(\mathbb{R}^d) \} \subset L^2(\mathcal{X}(\Lambda), \mu), \]
where the closure is taken in \(L^2(\mathcal{X}(\Lambda), \mu)\). Then, \(\mathcal{U}\) is a subspace. As \(\Theta\) intertwines \(S\) and \(T\) and is an isometry, this subspace is invariant under \(T\) and the action of \(S\) is equivalent to the restriction of \(T\) to this subspace. In this sense, the diffraction measure completely ‘controls’ a subrepresentation of \(T\). This is the fundamental connection between diffraction and dynamics.

Using the map \(\Theta\), we can easily provide a closed formula for the pure point part of the diffraction measure. Any \(k \in \mathcal{B}\) is an eigenvalue of \(S\) (with the characteristic function \(1_{\{k\}}\) being an eigenfunction). Hence, any \(k \in \mathcal{B}\) is an eigenvalue of \(T\) with eigenfunction
\[ c_k := \Theta(1_{\{k\}}). \]
So, for any Bragg peak, there exists a canonical eigenfunction. This is quite remarkable as eigenfunctions are usually only determined up to some phase. The function \(c_k\) is not normalised in \(L^2\). Instead, using that \(\Theta\) is an isometry, we obtain
\[ \langle c_k, c_k \rangle_{L^2(\mathcal{X}(\Lambda), \mu)} = \langle \Theta(1_{\{k\}}), \Theta(1_{\{k\}}) \rangle_{L^2(\mathcal{X}(\Lambda), \mu)} \]
\[ = \langle 1_k, 1_k \rangle_{L^2(\mathbb{R}^d, \gamma_\mu)} = \vec{\gamma}_\mu(\{k\}). \]

For the pure point part of the diffraction, we thus get
\[
(\vec{\gamma}_\mu)_{pp} = \sum_{k \in B} \|c_k\|^2 \delta_k.
\]

For a given Delone set \( \Lambda \), we have now considered two procedures to investigate the associated diffraction, one via a limiting procedure and one via considering the hull. A short summary on how these two compare may be given as follows:

- **point set \( \Lambda \)** \( \leftrightarrow \) **dynamical system** \((X(\Lambda), \mathbb{R}^d, \mu)\)
- \( \gamma \) as a limit \( \leftrightarrow \) closed formula for \( \gamma \)
- \( S \) on \( L^2(\mathbb{R}^d, \vec{\gamma}) \) \( \leftrightarrow \) restriction of \( T \) to \( \mathcal{U} \)
- Bragg spectrum \( \mathcal{B} \) \( \rightarrow \) group of eigenvalues \( \mathcal{E} \)
- Intensity \( \vec{\gamma}(\{k\}) \) \( \leftrightarrow \) norm \( \|c_k\|^2 \).

There is more to be said about the connection between the group of eigenvalues and the Bragg spectrum, as we shall see later.

### 7. Pure point diffraction and expansion in eigenfunctions.

The phenomenon of (pure) point diffraction lies at the heart of aperiodic order, both in terms of physical experiments and in terms of mathematical investigations. In this section, we take a closer look at it.

We consider an ergodic Delone dynamical system \((X(\Lambda), \mathbb{R}^d, \mu)\). This system comes with a unitary representation \( T \) of \( \mathbb{R}^d \) and a diffraction measure \( \vec{\gamma}_\mu \). It is said to have pure point diffraction if this measure is a pure point measure. It is said to have pure point dynamical spectrum if there exists an orthonormal basis of \( L^2(X(\Lambda), \mu) \) consisting of eigenfunctions.

We have already seen in the previous section that and how the diffraction measure controls a subspace of the whole \( L^2(X(\Lambda), \mu) \). Accordingly, it should not come as a surprise that any \( k \in B \) is an eigenvalue of \( T \) and pure point dynamical spectrum implies pure point diffraction spectrum. Somewhat surprisingly it turns out that the converse also holds. So, the Delone dynamical system \((X(\Lambda), \mathbb{R}^d, \mu)\) has pure point diffraction if and only if it has pure point dynamical spectrum. Thus, the two notions of pure pointedness are equivalent.

Following [9], we can sketch a proof as follows: The diffraction is pure point if \( \vec{\gamma} \) is a pure point measure. By the discussion above, this is the case if and only if the subrepresentation of \( T \) coming from the restriction to \( \mathcal{U} \) has pure point spectrum. Clearly, if \( T \) has pure point spectrum, then this must be true of any subrepresentation as well and pure point diffraction follows. To show the converse, note that pure point diffraction implies that all spectral measures \( \varrho_{f,\varphi} \), with arbitrary \( \varphi \in \mathcal{S}(\mathbb{R}^d) \), are pure point measures (as these are equivalent to the spectral measures of \( \phi \) with respect to \( S \)). We have to show that then all spectral measures \( \varrho_f \), with \( f \in L^2(X(\Lambda), \mu) \), are pure point measures. Consider

\[ \mathcal{A} := \{ f \in C(X(\Lambda)) \mid \varrho_f \text{ is a pure point measure} \}. \]

Then, \( \mathcal{A} \) is a vector space with the following properties.

- It is an algebra. (This ultimately follows as the product of eigenfunctions is an eigenfunction.)
• It is closed under complex conjugation. (This ultimately follows as the complex conjugate of an eigenfunction is an eigenfunction.)
• It contains all constant functions (as these are continuous eigenfunctions to the eigenvalue 0).
• It contains all functions of the form \( f_{\varphi} \) (as has just been discussed) and these functions clearly separate the points of \( X(\Lambda) \).

Given these properties of \( \mathcal{A} \), we can apply the (complex) Stone–Weierstrass theorem to conclude that \( \mathcal{A} \) is dense in \( C(X(\Lambda)) \) with respect to the supremum norm. Hence, \( \mathcal{A} \) is also dense in \( L^2(X(\Lambda), \mu) \) with respect to the Hilbert space norm, and the desired statement follows.

A closer inspection of the proof also shows that the group \( \mathcal{E}(\mu) \) of eigenvalues is generated by the Bragg spectrum \( \mathcal{B} \) if the system has pure point diffraction spectrum. Note that the Bragg spectrum itself need not to be a group. The eigenvalues of \( T \) which are not Bragg peaks are called extinctions. We refer to [6, Rem. 9.10] for an explicit example. However, it is an interesting observation in this context that \( \mathcal{B} \), in many examples, actually is a group, in which case one has identified the pure point part of the dynamical spectrum as well. This is the case for the Ammann–Beenker point set, so that Figure 2 also serves as an illustration of the dynamical spectrum.

In the case of pure point diffraction, the diffraction agrees with its pure point part and the corresponding formula from the previous section gives \( \hat{\gamma}_\mu = \sum_{k \in \mathcal{B}} \| c_k \|^2 \delta_k \) with \( c_k = \Theta(1_{\{k\}}) \). This way, the diffraction measure can actually be used very efficiently to calculate the dynamical spectrum (in additive formulation, as we use it here).

**Remark 7.** The result on the equivalence of the two types of pure point spectrum has quite some history. As mentioned above, the work of Dworkin [26] provides the basic connection between the diffraction and the dynamical spectrum and gives in particular that pure point dynamical spectrum implies pure point diffraction spectrum; see [36, 65] for a discussion as well. In fact, for quite a while this was the main tool to show pure point diffraction spectrum [61, 67]. For uniquely ergodic Delone dynamical systems with FLC, the equivalence between the two notions of pure pointedness was then shown in [44]. These considerations are modeled after a treatment of a related result for one-dimensional subshifts given in [59].

A different proof (sketched above), which permits a generalisation to arbitrary dynamical systems consisting of translation bounded measures, was then given in [9]. There, one can also find the statement that the Bragg spectrum generates the group of eigenvalues. The setting of [9] does not require any form of ergodicity and applies to all Delone dynamical systems (irrespective of whether they are FLC or not), though it might be difficult then to actually determine the autocorrelation explicitly, despite the closed formula given in Section 4.

A generalisation of [44] to a large class of point processes was given in [33]. This work applies to all Delone dynamical systems and requires neither ergodicity nor the FLC property. In fact, it does not even require translation boundedness of the point process, but the weaker condition of existence of a second moment. A treatment containing both the setting of [33] and [9] was then provided in [49] and, in a slightly different form, in [46]. These are the most general results up to date. The statement on the intensity of a Bragg peak being given by the square of an \( L^2 \)-norm and the formula for \( \hat{\gamma}_\mu \) can be found in [45].
It is worth noting that the equivalence between the dynamical spectrum and the diffraction spectrum only holds in the pure point case and does not extend to other spectral types, as follows from corresponding examples in [28]; compare Section 8 as well. It turns out, however, that — under suitable assumptions — the dynamical spectrum is equivalent to a family of diffraction spectra [12]. Details will be discussed in Section 8.

We finish this section with a short discussion how pure point spectrum can be thought of as providing a ‘Fourier expansion for the underlying Delone sets’. To achieve this, we will need a (canonically) normalised version of the $c_k$, with $k \in B$, which is given by

$$\tilde{c}_k := \frac{c_k}{\gamma_\mu(\{k\})^{1/2}}.$$ 

As $\Theta$ is an isometry, we obtain from the very definition of $c_k$ that

$$\langle f_\varphi, c_k \rangle = \langle \Theta(\hat{\varphi}), \Theta(1_{\{k\}}) \rangle = \langle \hat{\varphi}, 1_{\{k\}} \rangle = \gamma_\mu(\{k\})^{1/2} \hat{\varphi}(k)$$

holds for any $k \in B$ and any $\varphi \in \mathcal{S}(\mathbb{R}^d)$. This in particular implies the relation

$$\langle f_\varphi, \tilde{c}_k \rangle \tilde{c}_k = \hat{\varphi}(k) c_k.$$ (1)

This formula can be found in [45] (with a different proof). It will be used shortly.

Consider a Delone dynamical system $(X(\Lambda), \mathbb{R}^d, \mu)$ with pure point diffraction and, hence, pure point dynamical spectrum. The basic aim is now to make sense of the ‘naive’ formula

$$\delta_{\Lambda'} = \sum_{k \in B} c_k(\Lambda') \delta_k.$$ 

To do so, we consider this equation in a weak sense. Thus, we pair both sides with $\hat{\varphi}$ for some $\varphi \in \mathcal{S}(\mathbb{R}^d)$. With $\varphi$, defined by $\varphi(x) = \varphi(-x)$, we can then calculate

$$\langle \delta_{\Lambda'}, \hat{\varphi} \rangle = \langle \delta_{\Lambda'}, \hat{\varphi} \rangle = \langle \delta_{\Lambda'}, \hat{\varphi} \rangle = f_\varphi(\Lambda') \stackrel{(!)}{=} \sum_{k \in B} \langle f_\varphi, \tilde{c}_k \rangle \tilde{c}_k(\Lambda')$$

$$= \sum_{k \in B} \hat{\varphi}(k) c_k(\Lambda') = \left( \sum_{x \in B} c_k(\Lambda') \delta_k, \hat{\varphi} \right).$$

Here, the second step follows from the definition of $f_\varphi$, while (!) requires some justification and this justification is missing. Note, however, that (!) does hold in the $L^2$ sense. Indeed, by the definition of pure point diffraction, the $\tilde{c}_k$, with $k \in B$, form an orthonormal basis of $\mathcal{U}$ and hence

$$f_\varphi = \sum_{k \in B} \langle f_\varphi, \tilde{c}_k \rangle \tilde{c}_k$$

is indeed valid. In fact, this is just the expansion of a function in an orthonormal basis. So, the problem in the above reasoning is the pointwise evaluation of the Fourier series at $\Lambda'$. We consider this an intriguing open problem.

Remark 8. Already in the original work of Meyer [51, 52], it was an important point to capture the harmonic properties of point sets via trigonometric approximations. This led to the theory of harmonious sets; see [55, 56] for a detailed summary. More recently, Meyer has revisited the problem [53] and designed new schemes of almost periodicity that should help to come closer to a direct interpretation in the sense of an expansion.
8. Further relations between dynamical and diffraction spectra. Our approach so far was guided by the physical process of diffraction. The latter is usually aimed at the determination (in our terminology) of the Delone set, or as much as possible about it, from the diffraction measure. This is a hard inverse problem, generally without a unique solution. As mentioned before, diffraction is thus tailored to one set, or to one dynamical system, and not invariant under (metric) isomorphism of dynamical systems. This is probably the reason why, from a mathematical perspective, it has not received the attention it certainly deserves.

If one comes from dynamical systems theory, which has a huge body of literature on spectral properties, it appears more natural to define a spectrum in such a way that invariance under metric isomorphism is automatic, and this was achieved by Koopman [41], and later systematically explored by von Neumann [72]. One celebrated result in this context then is the Halmos–von Neumann theorem which states that two ergodic dynamical systems with pure point spectrum are (metrically) isomorphic if and only if they have the same spectrum, and that any such system has a representative in the form of an ergodic group addition on a compact Abelian group [72, 34, 22]. This is well in line with the discussion of pure point diffraction in the previous section (see [46] as well). There, we have seen that pure point diffraction and pure point dynamical spectrum are equivalent. So, in this case, the diffraction essentially captures the whole spectral theory. A priori, it is not clear what diffraction has to say on Delone dynamical systems with mixed spectra, and the situation is indeed more complex then.

Example 3. As was observed in [28], the subshift \( X_{\text{TM}} \) defined by the Thue–Morse (TM) substitution

\[
\sigma_{\text{TM}} : a \mapsto ab, \ b \mapsto ba,
\]

has a mixed dynamical spectrum that is not captured by the diffraction measure of the system; see also [6, Secs. 4.6 and 10.1] for a detailed discussion. Note that we use a formulation via substitutions here, but that one can easily obtain a Delone set as well, for instance via using the positions of all letters of type \( a \) in a bi-infinite TM sequence (letters correspond to unit intervals this way). To expand on the structure, the dynamical spectrum consists of the pure point part \( \mathbb{Z} \left[ \frac{1}{2} \right] \) together with a singular continuous part that can be represented by a spectral measure in Riesz product form,

\[
\vartheta_{\text{TM}} = \prod_{\ell=0}^{\infty} \left( 1 - \cos(2^{\ell+1} \pi x) \right),
\]

where convergence is understood in the vague topology (not pointwise); compare [74, 59] for background. More precisely, in line with the common practice for Riesz products, the right-hand side is to be read as the vague limit of a sequence of (continuous) Radon–Nikodym densities, each representing an absolutely continuous measure (either on the unit interval, or on the entire real line). The limit is a singular continuous measure. For this system, \( \vartheta_{\text{TM}} \) is a spectral measure of maximal type in the ortho-complement of the pure point sector.

Now, the diffraction measure picks up \( \vartheta_{\text{TM}} \) completely, but only the trivial part of the point spectrum, which is \( \mathbb{Z} \) in this case. Nevertheless, there is a single factor, the so-called period doubling subshift (as defined by the primitive period doubling substitution \( \sigma_{\text{pd}} : a \mapsto ab, \ b \mapsto aa \)), which has pure point spectrum (both diffraction and dynamical). Via the equivalence in this case, one picks up the entire
point spectrum, namely $\mathbb{Z}^{[1, T]}$. The period doubling subshift emerges from the TM subshift via a simple sliding block map; see [6] Sec. 4.6 for details.

In fact, it is possible to replace the TM system by a topologically conjugate one, also based upon a primitive substitution rule (hence locally equivalent in the sense of mutual local derivability), with the property that one restores the equivalence of the two spectral types for this system. The simplest such possibility emerges via the induced substitution for legal words of length 2; see [59] Sec. 5.4.1 or [6] Sec. 4.8.3 for details on this construction. Here, this leads to a primitive substitution rule of constant length over a 4-letter alphabet. Similar situations also emerge for higher-dimensional analogues; see [29] [7] for examples.

It turns out [12] that even in the case of mixed diffraction one can capture the whole dynamical spectrum via diffraction (at least in the case of FLC systems). However, to do so properly, one generally will have to consider not only the diffraction of the original system (which is not an isomorphism invariant) but also the diffraction of a suitable set of factors (which, when taken together, provides an isomorphism invariant). This is discussed in this section, where we follow [12].

Let $(\mathcal{X}(\mathcal{A}), \mathbb{R}^d, \mu)$ be a Delone dynamical system with FLC. Let $T$ be the associated Koopman representation and $E_T$ the corresponding projection valued measure. A family $\{\sigma_i\}$ of measures on $\mathbb{R}^d$ (with $i$ in some index set $J$) is called a complete spectral invariant when $E_T(A) = 0$ holds for a Borel set $A \subset \mathbb{R}^d$ if and only if $\sigma_i(A) = 0$ holds for all $i \in J$.

An example for a complete spectral invariant is given by the family of all spectral measures $\mathcal{E}_f$, with $f \in L^2(\mathcal{X}(\mathcal{A}), \mu)$. We will meet another spectral invariant shortly. Recall that a topological dynamical system $(Y, \mathbb{R}^d)$ (meaning a compact space $Y$ with a continuous action of $\mathbb{R}^d$) is called a factor of $(\mathcal{X}(\mathcal{A}), \mathbb{R}^d)$ if there exists a surjective continuous map

$$\Phi: \mathcal{X}(\mathcal{A}) \to Y$$

which intertwines the respective actions of $\mathbb{R}^d$. In our context, the dynamical systems will naturally be equipped with measures and we will require additionally that the factor map sends the measure on $\mathcal{X}(\mathcal{A})$ onto the measure on $Y$; see [10] for background and further details.

If $\mathcal{Y}$ is the hull of an FLC Delone set, then $(\mathcal{Y}, \mathbb{R}^d, \nu)$ is called an FLC Delone factor. Of course, any FLC Delone factor comes with an autocorrelation $\gamma_{(\mathcal{Y}, \mathbb{R}^d, \nu)}$ and a diffraction $\hat{\gamma}_{(\mathcal{Y}, \mathbb{R}^d, \nu)}$. The main abstract result of [12] then states that the family $\hat{\gamma}_{(\mathcal{Y}, \mathbb{R}^d, \nu)}$, where $(\mathcal{Y}, \mathbb{R}^d, \nu)$ runs over all FLC Delone factors of $(\mathcal{X}(\mathcal{A}), \mathbb{R}^d, \mu)$, is a complete spectral invariant for $T$. In fact, it is not even necessary to know the diffraction of all such factors. It suffices to know the diffraction of so-called derived factors that arise as follows.

Let $P$ be a $K$-cluster of $A$. For any $A' \in \mathcal{X}(\mathcal{A})$, the set of $K$-clusters of $A'$ is a subset of the $K$-clusters of $A$, as a consequence of the construction of the hull $\mathcal{X}(\mathcal{A})$. We may thus define the locator set

$$T_{K,P}(A') = \{t \in \mathbb{R}^d \mid (A' - t) \cap K = P\} = \{t \in A' \mid (A' - t) \cap K = P\} \subset A',$$

which contains the cluster reference points of all occurrences of $P$ in $A'$. Then, any $K$-cluster $P$ of $A$ gives rise to a factor

$$\mathcal{Y} = \mathcal{Y}_{K,P} := \{T_{K,P}(A') \mid A' \in \mathcal{X}(\mathcal{A})\}$$
with factor map
\[ \Phi = \Phi_{K,P} : X \to Y, \quad X \mapsto T_{K,P}(X). \]
This factor will be called the factor derived from \((X, \mathbb{R}^d)\) via the \(K\)-cluster \(P\) of \(\Lambda\). It is the diffraction of these factors (for all clusters) that is a complete spectral invariant.

This result is relevant on many levels. On the abstract level, it shows that the diffraction spectrum and dynamical spectrum are equivalent in a certain sense. This may then be used to gather information on the dynamical spectrum via diffraction (and thus Fourier) methods. On the concrete level, the result may even be relevant in suitably devised experimental setups; see [28, 12, 6] and references therein for more.

The considerations presented in this section naturally raise various questions and problems. For instance, it seems that, in concrete examples, often finitely many factors suffice. Thus, it would be of interest to find criteria when this happens. Also, it is not unreasonable to expect that in such situations also the diffraction of one factor (or rather of one topologically conjugate system) suffices. Finally, it would certainly be of interest to extend the considerations to situations where FLC does not hold.

9. Continuous eigenfunctions and the maximal equicontinuous factor. Let \(\Lambda\) be a Delone set with hull \(\mathbb{X}(\Lambda)\). Then, there is natural embedding
\[ \mathbb{R}^d \to \mathbb{X}(\Lambda), \quad t \mapsto t + \Lambda, \]
with dense range. In this way, the hull can be seen as a compactification of \(\mathbb{R}^d\). As \(\mathbb{R}^d\) is an Abelian group, it is then a natural question whether the hull carries a group structure such that this natural embedding becomes a group homomorphism. In general, this will not be the case. Indeed, as shown in [39] for an FLC Delone set \(\Lambda\), such a group structure on the hull \(\mathbb{X}(\Lambda)\) will exist if and only if \(\Lambda\) is crystallographic (or fully periodic), which means that \(\Lambda = F + \Gamma\) with a lattice \(\Gamma\) and a finite set \(F\); compare [6, Prop. 3.1]. So, the general question then becomes how close the hull is to being a group. An equivalent formulation would be how much the metric on the hull differs from being translation invariant. The concept of the maximal equicontinuous factor (which we will recall shortly) allows one to deal with these questions. This concept is not specific to Delone dynamical systems. It can be defined for arbitrary dynamical systems and this is how we will introduce it.

Throughout this section, we will assume that the occurring dynamical systems are minimal (meaning that each orbit is dense). This is a rather natural assumption as we want to compare the dynamical systems to certain dynamical systems on groups, which turn out to be minimal.

A dynamical system \((T, \mathbb{R}^d)\) is called a rotation on a compact group if \(T\) is a compact group and there exists a group homomorphism
\[ \xi : \mathbb{R}^d \to T \]
with dense range that induces an action of \(\mathbb{R}^d\) on \(T\) via
\[ t \cdot u := \xi(t)u \]
for all \(u \in T\) and \(t \in \mathbb{R}^d\). (Here, \(\xi(t)u\) denotes the product in the group \(T\) of the two elements \(\xi(t)\) and \(u\).) As \(\xi\) has dense range, the group \(T\) must necessarily be Abelian. It is well known (compare [3] for a recent discussion) that any such rotation on a compact group is strictly ergodic (meaning uniquely ergodic and minimal) and
has pure point dynamical spectrum with only continuous eigenfunctions (and the
eigenvalues are just given by the dual of the group \( \mathbb{T} \)).

The maximal equicontinuous factor (MEF) of a minimal dynamical system, say
\((X, \mathbb{R}^d)\), is then the largest rotation on a compact group \((\mathbb{T}, \mathbb{R}^d)\) which is a factor
of \((X, \mathbb{R}^d)\). It will be denoted as \((X_{\text{mef}}, \mathbb{R}^d)\), and the factor map will be denoted as
\[
\Psi_{\text{mef}} : X \rightarrow X_{\text{mef}}.
\]

With this factor map at our disposal, the question of how close \(X\) is to being a

### Remark 9.

Indeed, quite a substantial part of the general theory of the MEF
is devoted to studying these three regimes [1]. However, various other cases have
been considered as well. In particular, this concerns situations where the condition
of being one-to-one is replaced by being \(m\)-to-one with a fixed integer \(m\). In this
context, there is an emerging theory centred around the notion of the coincidence
rank; see [3] for a recent survey. In the special case \(m = 2\), which occurs for instance
for the TM subshift of Example 3 or for the twisted silver mean chain [5], interesting
and strong results are possible because such an index-2 extension is quite restrictive;
compare [35] and [59, Sec. 3.6] for background.

Here, we are concerned with the situation that \(X = \mathbb{X}(\Lambda)\) is the hull of a Delone
set \(\Lambda\). Then, particular attention has been paid to the case that \(\Lambda\) is a Meyer
set. In this case, the corresponding parts of [2, 11, 40] can be summarised as
giving that these three regimes above (namely \(\Psi_{\text{mef}}\) one-to-one everywhere, almost
everywhere, or in one point, respectively) correspond exactly to the situation that
\(\Lambda\) is crystallographic, a regular model set, or a model set, respectively. We refrain
from giving precise definitions or proofs but rather refer the reader to [3] for a recent
discussion; see [38] as well.

Next, we will provide an explicit description of the MEF for Delone dynamical
systems. In fact, it is not hard to see that a similar description can be given for
rather general dynamical systems as well. For further details and further references,
we refer the reader to [3] or [11]. Let \(\mathcal{E}_{\text{top}}\) be the set of continuous eigenvalues
of \((\mathbb{X}(\Lambda), \mathbb{R}^d)\). Here, an eigenvalue \(k \in \mathbb{R}^d\) is called a continuous eigenvalue of
\((\mathbb{X}(\Lambda), \mathbb{R}^d)\) if there exists a continuous non-vanishing function \(f : \mathbb{X}(\Lambda) \rightarrow \mathbb{C}\) with
\[
f(t + A') = e^{2\pi i k t} f(A')
\]
for all \(t \in \mathbb{R}^d\) and \(A' \in \mathbb{X}(\Lambda)\). It is not hard to see that the set of continuous eigen-
values is an (Abelian) group. We equip this set with the discrete topology. Then,
the Pontryagin dual $\hat{E}_{\text{top}}$ of this group, which is the set of all group homomorphisms
$$E_{\text{top}} \longrightarrow S^1 = \{ z \in \mathbb{C} \mid |z| = 1 \},$$
will be a compact group, which we denote by $T$. There is a natural group homomorphism
$$\xi: \mathbb{R}^d \longrightarrow T \quad \text{with} \quad \xi(t)(k) := e^{2\pi i tk}$$
for all $t \in \mathbb{R}^d$ and $k \in E_{\text{top}}$. In this way, $(T, \mathbb{R}^d)$ becomes a rotation on a compact Abelian group. Also, $(T, \mathbb{R}^d)$ is a factor of $(X(\Lambda), \mathbb{R}^d)$. Indeed, choose for each $k \in E_{\text{top}}$ the unique continuous eigenfunction $f_k$ with $f_k(\Lambda) = 1$. Then, the map
$$X(\Lambda) \longrightarrow T = \hat{E}_{\text{top}}, \quad \Lambda' \mapsto (k \mapsto f_k(\Lambda')),$$
can easily be seen to be a factor map. Via this factor map, the dynamical system $(T, \mathbb{R}^d)$ is the MEF of $(X(\Lambda), \mathbb{R}^d)$.

The preceding considerations show that there is a strong connection between continuous eigenfunctions and the MEF. Somewhat loosely speaking, one may say that the MEF stores all information on continuous eigenvalues.

In this context, dynamical systems coming from Meyer sets $\Lambda$ play a special role. Indeed, this could already be seen from the discussion above that relates a hierarchy of Meyer sets to injectivity properties of the factor map $\Psi_{\text{mf}}$. It is also visible in recent results in [40] showing that the dynamical system $(X(\Lambda), \mathbb{R}^d)$ coming from a Delone set with FLC has $d$ linearly independent continuous eigenvalues if and only if it is conjugate to a dynamical system $(X(\tilde{\Lambda}), \mathbb{R}^d)$ with $\tilde{\Lambda}$ a Meyer set. In this sense, Delone dynamical systems with FLC and ‘many’ continuous eigenvalues are systems coming from Meyer sets.

Continuous eigenvalues also play a role in diffraction theory, as we discuss next. In Section 4, we have seen how the autocorrelation of $(X(\Lambda), \mathbb{R}^d, \mu)$ can be computed by a limiting procedure for $\mu$-almost every element $\Lambda' \in X(\Lambda)$ if $\mu$ is ergodic, and for all $\Lambda' \in X(\Lambda)$ if the system is uniquely ergodic. In this context, we have also discussed the validity of the formula
$$\hat{\gamma}((k)) = \lim_{R \to \infty} \frac{1}{\text{vol}(B_R(0))} \sum_{x \in \Lambda' \cap B_R(0)} e^{2\pi i k x}$$
for almost every $\Lambda'$ in the ergodic case. Now, in the uniquely ergodic case, this formula can be shown to even hold for all $\Lambda'$ provided the eigenvalue $k$ is continuous [45]; see [60] for related earlier work as well.

**Remark 10.** As discussed in Remark 1, the validity of such a formula is known for sets coming from primitive substitutions as well as for regular model sets. In both cases, the associated Delone dynamical system is uniquely ergodic with only continuous eigenvalues. So, the mentioned work [45] provides a unified structural treatment.

It is an interesting open problem to which extent such a formula is valid beyond the case of continuous eigenfunctions. For example, it is shown in [45] that such a formula holds for all linearly repetitive systems even though such systems may have discontinuous eigenfunctions [20]. Also, the formula can be shown for weak model sets of extremal density [8, Prop. 6], where continuity of eigenfunctions generally fails. It then also holds for generic elements in the corresponding hull, equipped with a natural patch frequency measure. Moreover, nonperiodic measures with locally finite support and spectrum, as recently constructed in [54], are further examples.
with well-defined amplitudes. So, there is room for generalisation, and hence work to be done to clarify the situation.

10. **Quasicrystals and hulls of quasiperiodic functions.** So far, we have (mostly) considered the dynamical system \((X(\Lambda), \mathbb{R}^d)\) arising from a Delone set \(\Lambda\). Special emphasis has been paid to the case that this system is minimal and uniquely ergodic with pure point dynamical spectrum and only continuous eigenfunctions. Indeed, these are the systems to which all results of the preceding four sections apply. In particular, these systems have pure point diffraction and the set of (continuous) eigenvalues is a group generated by the Bragg spectrum. Moreover,

\[
\Psi_{\text{mf}} : X(\Lambda) \longrightarrow T
\]

is the factor map to its MEF, where \(T\) is given as the dual of the group of eigenvalues. While it is not clear at present what a mathematical definition for a quasicrystal should be, it seems reasonable that such systems should fall into the class of quasicrystals. For an extensive exposition of cut-and-project sets and model sets, we refer to [6] and references therein. At the same time, certain quasiperiodic functions are also sometimes treated under the label of quasicrystals [15]. In this section, we compare these two approaches and also compute the diffraction of a quasiperiodic function. This will actually show an important structural difference in the diffraction measure which seems to favour Delone sets as mathematical models for quasicrystals over a description via quasiperiodic functions.

Let \(C\) be a countable subset of \(\mathbb{R}^d\). Let \(a_k, k \in C\), be non-vanishing complex numbers that satisfy the summability condition

\[
\sum_{k \in C} |a_k| < \infty.
\]

Denote the subgroup of \(\mathbb{R}^d\) generated by \(C\) by \(E'\), so \(E' = \langle C \rangle\). Define

\[
u : \mathbb{R}^d \longrightarrow \mathbb{C}, \quad u(x) = \sum_{k \in C} a_k e^{2\pi ikx}.
\]

By the summability condition, the sum is absolutely convergent and the function is continuous and bounded. In fact, such functions form a subclass of the *almost periodic functions* in the sense of Bohr; see [21, 37], or [6, Sec. 8.2] for a short summary. An almost periodic function is called *quasiperiodic* when \(C \subset \bigcup_{j \in J} k_j \mathbb{Z}^d\) for \(J\) a finite set. Note that our considerations below can actually be extended to all Bohr almost periodic functions (with a little more effort). In this case, one ends up with numbers \(a_k, k \in C\), that need not be summable, but are still square-summable.

Clearly, we can view a bounded continuous function \(f\) as a Radon–Nikodym density relative to Lebesgue measure, and then identify \(f\) with the translation bounded measure defined that way. Consequently, we can equip the set of such functions with the vague topology induced from measures. In particular, we can consider the *hull* of \(f\) defined by

\[
X(f) := \{f(\cdot - t) \mid t \in \mathbb{R}^d\},
\]

where the closure is taken in the vague topology on measures. Then, \(X(f)\) is compact and \(\mathbb{R}^d\) acts continuously via translations on it (compare [6]). Thus, we are given a dynamical system \((X(f), \mathbb{R}^d)\). Assume now that \(f = u\) is the quasiperiodic function
introduced above. Then, the closure $X(u)$ actually agrees with the closure of the translates of $u$ in the topology of uniform convergence, so

$$X(u) = \overline{\{u(\cdot - t) \mid t \in \mathbb{R}^d\}}_{\text{\|\cdot\|}_\infty}.$$

In particular, all elements in $X(u)$ (which, a priori, are only measures) are continuous, bounded functions. Moreover, by standard theory of almost periodic functions, compare [50] or [6, Sec. 8.2] and references given there, this closure has the structure of an Abelian group. More specifically, define

$$\xi: \mathbb{R}^d \rightarrow X(u), \quad t \mapsto u(\cdot - t).$$

Then, there exists a unique group structure on $X(u)$ that makes $\xi$ a homomorphism of Abelian groups (see [47] as well for a recent discussion). This homomorphism has dense range and the translation action of $\mathbb{R}^d$ on $X(u)$ is given by

$$\mathbb{R}^d \times X(u) \rightarrow X(u), \quad (t, v) \mapsto v(\cdot - t) = \xi(t) \cdot v.$$

Thus, $(X(u), \mathbb{R}^d)$ is a rotation on a compact group (in the notation of Section 9). In particular, it is strictly ergodic and has pure point dynamical spectrum with only continuous eigenfunctions. Now, it is not hard to see that

$$C = \left\{ k \in \mathbb{R}^d \mid \lim_{R \to \infty} \frac{\int_{B_R(0)} u(x) e^{-2\pi i kx} \, dx}{\operatorname{vol}(B_R(0))} \neq 0 \right\}.$$

So, by standard theory of almost periodic functions, we infer

$$E' = \langle C \rangle = \hat{X}(u).$$

Dualising once more, we infer

$$X(u) = \hat{E'}.$$

Assume now that the group $E'$ is the group of eigenvalues of the strictly ergodic system $(X(\Lambda), \mathbb{R}^d)$ with pure point spectrum, which has only continuous eigenfunctions. Then, its dual group $\hat{E'}$ is the MEF of $(X(\Lambda), \mathbb{R}^d)$, as discussed at the beginning of this section. Moreover, as just derived, this dual group is isomorphic to $X(u)$. Putting this together, we see that the map $\Psi_{\text{mef}}$ can be considered as a map

$$\Psi_{\text{mef}}: X(\Lambda) \rightarrow X(u).$$

In terms of the associated dynamical systems, we thus find a precise relationship between the hulls of $\Lambda$ and of $u$: One is a factor of the other and, in fact, a special one via the connection with the MEF.

These considerations can be slightly generalised as follows. Let $(X(\Lambda), \mathbb{R}^d)$ be uniquely ergodic with pure point spectrum, and only continuous eigenfunctions and group of eigenvalues $E$. If the group $E' = \langle C \rangle$ is only a subgroup of $E$, we would still get a factor map

$$\Psi: X(\Lambda) \rightarrow X(u),$$

as, in this case, the dual of the group $E'$ can easily be seen to be a factor of $\hat{E}$.

**Remark 11.** The preceding considerations naturally raise the question whether, to any countable set $C$ and the induced group $E'$, one can find a strictly ergodic Delone dynamical system with pure point spectrum, only continuous eigenvalues and dynamical spectrum $E'$. The answer to this question is positive. In fact, it is even possible to find a Meyer set $\Lambda$ such that its hull $X(\Lambda)$ has the desired properties. Indeed, the work of Robinson [60] gives that, for any countable subgroup of $\mathbb{R}^d$, one can find a cut and project scheme whose torus is just the dual of the subgroup.
Then, any model set arising from a regular window (in a suitable position) from this cut and project scheme will be such a Meyer set \[65\].

It is possible to set up a diffraction theory for the elements of \(X(u)\) along the same lines as for \(X(\Lambda)\). Indeed, if both \(u\) and \(\Lambda\) are considered as translation bounded measures, there is virtually no difference in the framework and this is the point of view proposed in \[9\]. As it is instructive, let us discuss the diffraction theory of \(u\). As before, we consider \(u\) as a measure by viewing it as a Radon–Nikodym density relative to Lebesgue measure \(\lambda\). Then, the measure \(\widetilde{u}\lambda\) is given by \(\widetilde{u}\). Consequently, the autocorrelation of \(u\) can then simply be written as

\[
\gamma_u := \lim_{R \to \infty} \frac{u_R * \widetilde{u}_R}{\text{vol}(B_R(0))},
\]

where we use the shorthand \(u_R = u|_{B_R(0)}\) for the restriction of \(u\) to the open ball of radius \(R\) around 0. Of course, the existence of the limit has still to be established. Before we do this, via an explicit calculation, let us pause for a very simple special case.

**Example 4.** Consider \(u \equiv 1\), hence Lebesgue measure itself. A simple calculation with the volume-averaged convolution, compare \[6\, \text{Ex. 8.10}\], now gives \(\gamma_u = \lambda\), and thus diffraction \(\hat{\gamma}_u = \delta_0\), which is a finite pure point measure. Indeed, as we shall see later, this is an important distinction to the diffraction of a Delone set.

To proceed with the general case, we will need two ingredients:

- One of the characteristic functions can be removed in the definition of \(\gamma_u\). In particular, assuming existence of the limit, we have

\[
\gamma_u := \lim_{R \to \infty} \frac{u_R * \widetilde{u}}{\text{vol}(B_R(0))},
\]

(This is well-known and can be seen by a direct computation; compare \[65, 9\]).

- For any \(k \in \mathbb{R}^d\), the limit

\[
\lim_{R \to \infty} \frac{1}{\text{vol}(B_R(0))} \int_{B_R(0)} e^{-2\pi i k x} u(x) \, dx
\]

exists. It is \(a_k\) if \(k \in \mathcal{C}\) and 0 otherwise. (This is the formula for the Fourier–Bohr coefficient of \(u\). It is easy to see by direct computation and well-known in the theory of Bohr almost periodic functions; see \[21, 67\] or \[6\, \text{Thm. 8.2}\].)

Equipped with these two pieces of preparation, we are now going to compute \(\gamma_u\). Let \(g \in \mathcal{S}\) be arbitrary. Using the first ingredient, we find

\[
\gamma_u(g) = \lim_{R \to \infty} \frac{(u_R * \widetilde{u})(g)}{\text{vol}(B_R(0))}.
\]

Direct computations then give

\[
(u_R * \widetilde{u})(g) = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} u_R(y) \overline{u}(y-x) g(x) \, dy \, dx
\]

\[
= \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} u_R(y) \sum_{k \in \mathcal{C}} a_k e^{-2\pi i k y} g(x) \, dy \, dx
\]

\[
= \sum_{k \in \mathcal{C}} a_k \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} u_R(y) e^{-2\pi i k y} e^{2\pi i k x} g(x) \, dy \, dx
\]
\[ \gamma_u(g) = \sum_{k \in \mathcal{C}} |a_k|^2 F^{-1}(g)(k). \]

As this holds for all \( g \in \mathcal{S} \), we obtain

\[ \gamma_u = \left( \sum_{k \in \mathcal{C}} |a_k|^2 \delta_k \right) \circ F^{-1}. \]

Taking one more Fourier transform, and recalling \((\hat{T}, g) = (T, \hat{g})\) for distributions \( T \), we then find

\[ \hat{\gamma}_u = \sum_{k \in \mathcal{C}} |a_k|^2 \delta_k. \]

So, \( \hat{\gamma}_u \) is a pure point measure with its Bragg spectrum being given by \( \mathcal{C} \).

**Remark 12.** Due to the summability of the \( (a_k) \), the \( |a_k|^2 \) are also summable, and the pure point measure \( \hat{\gamma}_u \) is finite, thus generalising the finding of Example 4. In fact, one has the relation

\[ \sum_{k \in \mathcal{C}} |a_k|^2 = \lim_{R \to \infty} \frac{1}{\text{vol}(B_R(0))} \int_{B_R(0)} |u(x)|^2 \, dx. \]

This formula, which is not hard to derive from our above considerations, is nothing but Parseval’s identity for Bohr almost periodic functions [21, Thm. I.1.18]. This way, one can see immediately why the diffraction measure \( \hat{\gamma}_u \) must be a finite measure. This is an important structural difference to the case of Delone sets. ♦

Let us add the comment that this innocent-looking observation, with hindsight, sheds some light on the old dispute about the ‘right’ model for the description of quasicrystals between the quasiperiodic function approach and the tiling or Delone set approach. While the former leads to finite diffraction measures, the latter does not; compare [6] Rem. 9.11 for a simple argument in the context of cut and project sets, and [69] as well as [6] Rem. 9.12 for an argument in the more general situation of Meyer sets. In particular, for a typical model set, there are series of Bragg peaks (which lie on outgoing rays from the origin) that have intensities which converge against the central intensity, such as those described in [6, Rem. 9.11]. Now, the experimental findings, see [68] and references therein, seem to indicate the existence of such series of Bragg peaks with growing \( k \) and converging intensity, which is not compatible with a finite diffraction measure in the infinite volume limit.

Clearly, the interpretation of the experimental situation is subtle, but the least one can say is that Delone sets are a valid idealisation of the set of atomic positions. It is conceivable that both notions are useful, possibly for different aspects. In any case, the most natural way to resolve the underlying dispute is to use a setting that
can easily accommodate both points of view — and that is provided by the use of translation bounded measures as models, because they comprise both scenarios as special cases.

**Remark 13.** The Fourier–Bohr coefficients $a_k$ as volume-averaged integrals can once again be interpreted as *amplitudes* in our above sense, and it is then no surprise that the intensities of the Bragg peaks are once again given as the absolute squares of these amplitudes. This is another indication that there is more to be done in this direction.

**Acknowledgments.** The authors would like to thank the organizers of the 3rd Bremen Winter School and Symposium: Diffusion on Fractals and Nonlinear Dynamics (2015) for setting up a most stimulating event inspiring in particular the material presented in Section 10. We also thank two anonymous reviewers for their careful comments, which helped to improve the manuscript. This work was supported by the German Research Foundation (DFG), within the CRC 701.

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Received January 2016; revised November 2016.

E-mail address: mbaake@math.uni-bielefeld.de
E-mail address: daniel.lenz@uni-jena.de