Mathematical Quasicrystals and the Problem of Diffraction

Jeffrey C. Lagarias

Abstract. This paper studies three mathematical idealizations of quasicrystals which embody a notion of perfectly sharp diffraction spectrum. These idealizations consist of Delone sets that satisfy additional conditions. The first concept (Patterson set) is based on having a pure point diffraction spectrum. To each Patterson set which is a Delone set of finite type there corresponds a summation formula, which can be viewed as generalizing the Poisson summation formula. The second and third concepts (Bohr almost periodic Delone set and Besicovitch almost periodic Delone set) are based on almost-periodicity conditions imposed on their Fourier transform. The latter two concepts are proposed to extract "phase information" for quasicrystals. The paper concludes with a list of open problems.

1. Introduction

The discovery of quasicrystalline materials in 1982 by Schechtman (published two years later, [**SBGC**]) led to extensive theoretical and empirical efforts to understand their structure, see [**Jan**],[**Sen**]. The intuitive notion of a quasicrystal is a (very large) discrete set of atoms in space whose X-ray diffraction pattern exhibits sharp spots. This condition requires that the interatomic distance vectors exhibit long-range order under translations, in a statistical sense. This paper considers mathematical idealizations of such structures which are infinite discrete sets which have perfect diffraction patterns (pure delta functions), rather than the slightly diffuse spots of actual X-ray diffraction patterns. These structures could model pure point diffractive quasicrystalline materials. In this framework we view ideal crystals as a special kind of pure point diffractive quasicrystal.

The basic mathematical object is a set in $\mathbb{R}^n$ which models an infinite limit of a physical structure consisting of a discrete set of atoms.

Definition 1.1. A *Delone set* Λ in $\mathbb{R}^n$ is a set with the properties:

(1) *Uniform Discreteness.* There is $r > 0$ such that each ball of radius r contains at most one element of Λ.
(2) *Relative Denseness.* There is $R > 0$ such that each ball of radius R contains at least one element of Λ.

Such sets are sometimes called *(r,R)-sets.* These sets are named after the Russian crystallographer and number theorist B. N. Delone [**D**].

We consider Delone sets that usually satisfy additional conditions. Recently Lagarias [**La99a**] formulated the notion of Delone set of finite type as a model for Delone sets having weak translational order.

DEFINITION 1.2. (i) A *Delone set of finite type* is a Delone set Λ such that $\Lambda - \Lambda$ is a closed discrete set.

(ii) A *Meyer set* is a a Delone set Λ such that $\Lambda - \Lambda$ is a Delone set.

Delone sets of finite type are exactly those Delone sets that have a "finite number of local patterns", see [**La99a**, Thm. 2.2]. This property is also called 'finite local complexity" , see [**BH**],[**S99**]. Meyer sets are an important subclass of these sets, introduced much earlier, whose properties are given in detail in Moody [**Mo97**]. They have several equivalent definitions, the one above being formulated in [**La95**].

DEFINITION 1.3. An *ideal crystal* (or *perfect crystal*) in $\mathbb{R}^n$ is any set Λ that consists of a finite number of translates of a full rank lattice L in $\mathbb{R}^n$. That is $\Lambda = L + F$, where F is a finite set.

Note that ideal crystals are Meyer sets, and we view them as a special kind of quasicrystal.

We consider three different concepts of pure point diffractive quasicrystal, all for Delone sets. The first concept, of Patterson set, is based on a mathematical analogue of X-ray diffraction developed by Hof ([**H92**]–[**H97**]). The second and third concepts, of Bohr almost periodic set and its extension to the concept of Besicovitch almost periodic set, are based on Fourier analysis, and each gives a notion of "spectrum" assigned to the Fourier transform of point masses at the points of Λ. These two concepts add "phase information" to the X-ray diffraction data.

The concept of *Patterson set* is studied in §2. It is based on the notion of autocorrelation measure (or Patterson function) associated to the difference set $\Lambda - \Lambda$ of the set Λ. The diffraction measure is the Fourier transform of the autocorrelation measure, and a Patterson set is a Delone set which has a unique diffraction measure which is a pure discrete measure. Our main new observation in §2 is to show that this concept has a precise relation with summation formulae in Fourier analysis (Theorem 2.9).

There are two general constructions of Delone sets of finite type Λ that are known to yield Patterson sets in special cases: model sets, which include as a special case cut-and-project sets, and certain Delone sets defined by self-similarity properties, which we call self-replicating Delone sets. A general method of proof that certain such sets are Patterson sets uses dynamical system methods described at the end of §2.

Cut and project sets are Delone sets in $\mathbb{R}^n$ constructed from a full rank lattice L in $\mathbb{R}^{n+m}$ for some $m \geq 0$, together with a compact set B in $\mathbb{R}^m$ which has nonempty interior. The space $\mathbb{R}^m$ is the "internal space" of the construction, and the set B in the "internal space" is called a mask or window. View $\mathbb{R}^{n+m} = \mathbb{R}^n \times \mathbb{R}^m$ with orthogonal projections $\pi_{||}$ and $\pi_{\perp}$ onto the first n coordinates and last m coordinates, respectively. The *cut and project set* $\Lambda = \Lambda(B, L)$ is defined by

$$\Lambda := \{\pi_{||}(\boldsymbol{y}) : \boldsymbol{y} \in L \quad \text{and} \quad \pi_{\perp}(\boldsymbol{y}) \in B\} \ . \tag{1.1}$$

Cut-and-project sets are always Meyer sets. Whenever a cut-and-project set is a Patterson set, its spectrum is contained in a finitely-generated $\mathbb{Z}$-module in $\mathbb{R}^n$, related to the dual lattice L^* of L.

Model Sets are Delone sets in $\mathbb{R}^n$ which generalize cut-and-project sets, and include them as a special case. The concept of model set was introduced in 1972 by Y. Meyer [**Me72**, p. 48]. They are produced by a similar construction in which the "internal space" is allowed to be an arbitrary locally compact Abelian group, see Schlottmann [**S98**] and Moody [**Mo99**]. The window set B is required to be a compact set with nonempty interior. A model set is said to be *regular* if the window B has a boundary $\partial B := B \backslash Int(B)$ of (Haar) measure zero. Schlottmann [**S99**] shows that regular model sets have a well-defined pure point diffraction measure. Model sets using a p-adic internal space occur in certain self-similar tiling constructions, see Baake, Moody and Schlottmann [**BMS**] and Lee and Moody [**LM**]. Model sets are always Meyer sets. The spectrum of a regular model set is not always contained in a finitely-generated $\mathbb{Z}$-module, as indicated by the example studied in [**BMS**].

Self-replicating Delone sets describe "control points" of associated self-affine tilings, see Gähler and Klitzing [**GK**] and Solomyak [**So97**, Sec. 5]. These sets are studied in Lagarias and Wang [**LaWa3**], and have a theory analogous to that for self-replicating tilings. At this point we observe only that such sets are Delone sets Λ that have a partition $\Lambda = \cup_{i=1}^{m} \Lambda_i$ in which the subsets Λ_i satisfy a system of functional equations

$$\Lambda_i = \bigcup_{j=1}^{m} (\phi(\Lambda_j) + \mathcal{D}_{ji}), \quad 1 \le i \le m \ , \tag{1.2}$$

in which

$$\phi(\boldsymbol{x}) = A\boldsymbol{x} + \mathbf{b} \tag{1.3}$$

is an expanding affine map , i.e. the matrix A has all eigenvalues $|\lambda| > 1$, and the *digit sets* $\mathcal{D}_{ij}$ are finite sets. The matrix A is called the *inflation matrix.* Associated to the functional equation (1.2) is a *substitution matrix* S which is a nonnegative integer matrix defined by

$$S_{ij} := |\mathcal{D}_{ij}|, \quad 1 \le i, j \le m \ . \tag{1.4}$$

We suppose that the substitution matrix is *primitive*, which means that some power S^k has strictly positive entries. Only special choices of the data $\{\phi, \mathcal{D}_{ij}\}$ yield functional equations (1.2) that have solutions which are self-replicating Delone sets of finite type. For example, the real matrix A must have algebraic integer eigenvalues, and if S is primitive then the largest eigenvalue of S must equal $|\det A|$. There exist self-replicating Delone sets which are Delone sets of finite type but are not Meyer sets. Some self-replicating Delone sets are Patterson sets, while others are not. All known examples of primitive self-replicating Delone sets that have been proved to have pure point diffraction spectrum are Meyer sets. The diffraction spectrum results in the literature are generally proved for the associated tiling models, as in Solomyak [**So97**], but Delone sets are explicitly considered in Solomyak [**So98b**]. For various results concerning self-affine and self-replicating tilings, see Gröchenig, Haas and Raugi [**GHR**], Kenyon[**Ke92**]-[**Ke96**], Lagarias and Wang [**LaWa1**], [**LaWa2**], Solomyak [**So97**], [**So98a**] and Vince [**Vin1**], [**Vin2**].

The concepts of *Bohr almost periodic set* and *Besicovitch almost periodic set* are presented in §3. We view these concepts as supplying "phase information" about f_Λ

which is lost in passing to the autocorrelation measure. We associate to a Delone set Λ the Radon measure whose density function f_Λ consists of delta functions at the points of Λ. A Bohr almost periodic set is defined to be a distribution f_Λ whose Fourier transform is in a suitable weak sense a countable set of weighted delta functions. We formalize this concept using uniformly almost periodic functions and distributions, see Appendix B. However the concept of Bohr almost periodic set seems too narrow to include many sets regarded as quasicrystalline (including most cut-and-project sets), so we formulate a relaxed concept of *Besicovitch almost periodic set*, whose definition uses a wider class of almost periodic functions. This concept is expected to include cut-and-project sets; see the open problems in §4. We define more generally *$\mathcal{B}$-almost periodic sets*, where $\mathcal{B}$ is a suitable class of almost periodic distributions, and it remains to determine a good class $\mathcal{B}$ that gives a reasonable theory.

The inclusion relations between these three concepts of pure point diffraction quasicrystal are not known, except that Bohr almost periodic sets are Besicovitch almost periodic sets, which follows from the definition. It is natural to hope that a suitable class of $\mathcal{B}$-Besicovitch almost periodic sets will all be Patterson sets and have the consistent phase property given in (3.9), but this is an open question.

It is known that the information contained in the diffraction spectrum is not sufficient to reconstruct the set, up to translation. If Λ is a Patterson set and $\tilde{\Lambda}$ is a Delone set such that the symmetric difference

$$\Lambda \,\Delta\, \tilde{\Lambda} := (\Lambda/\Lambda') \cup (\Lambda'/\Lambda)$$

is a set of density zero, then $\tilde{\Lambda}$ is a Patterson set with the same spectrum. For similar reasons, the " phase information" obtained in a Besicovitch almost periodic set (of type B^2) is generally insufficient to reconstruct the set, because the "Fourier coefficients" are also unchanged by sets of density zero, see §3. However the narrower class of Bohr almost periodic sets (which include ideal crystals) are uniquely reconstructible from the "Fourier coefficients" of their spectrum.

The final section §4 lists a large number of open problems raised by the topics above.

There are several other concepts of mathematical quasicrystal not considered here. The first models proposed for quasicrystalline structures were based on tilings of $\mathbb{R}^n$ using a finite number of different tile shapes, see Duneau and Katz [**DuKa**] and Levine and Steinhardt [**LSt**]. Later Lunnon and Pleasants [**LuP**] introduced a notion of *quasiperiodic tiling* in which $\mathbb{R}^n$ is tiled by tiles of a finite number of shapes $P_1, \ldots, P_k$, all polytopes, with the property that if any set of continuous functions $f_1, f_2, \ldots, f_k$ are assigned to these polytopes, and used to construct a function f on $L^\infty(\mathbb{R}^n)$ by replicating $f_i(\boldsymbol{x}+\boldsymbol{v})$ on each tile $P_i+\boldsymbol{v}$, then the Fourier transform $\hat{f}$ (in a suitable space of distributions) consists entirely of delta functions supported on a finitely-generated additive subgroup of $\mathbb{R}^n$ (a *quasilattice*), see also Le, Piunikhin and Sadov [**LPS**]. There are also notions of quasicrystals as consisting of a collection of an uncountable number of tilings viewed as a dynamical system under the action of the group of translations of $\mathbb{R}^n$. These are called *tiling dynamical* systems. The eigenvalues of the $\mathbb{R}^n$-action of translation on tilings then play a role analogous to diffraction spectra, see Dworkin [**Dw**], and Hof [**H97**, p. 254]. Analogous dynamical systems for Delone sets play a role in proving certain sets are Patterson sets, see Section 2. A discussion of other mathematical concepts related to quasicrystals appears in Cahn and Taylor [**CT**] and Baake [**Ba**].

The final §4 lists a number of open problems.

Notation. The Euclidean inner product on $\mathbb{R}^n$ is

$$\langle \boldsymbol{\xi}, \boldsymbol{x} \rangle = \sum_{i=1}^{n} \xi_i x_i \ .$$

The Schwartz space of rapidly decreasing smooth functions on $\mathbb{R}^n$ is $\mathcal{S}(\mathbb{R}^n)$. The (normalized) Fourier transform $\hat{f}$ of $f \in \mathcal{S}(\mathbb{R}^n)$ is

$$\hat{f}(\boldsymbol{\xi}) := \int_{\mathbb{R}^n} e^{-2\pi i \langle \boldsymbol{\xi}, \boldsymbol{x} \rangle} f(\boldsymbol{x}) d\boldsymbol{x} \ . \tag{1.5}$$

The Fourier transform is defined for tempered distributions $f \in \mathcal{S}'(\mathbb{R}^n)$ in the usual fashion: $\langle \hat{f}, \psi \rangle = \langle f, \hat{\psi} \rangle$ for test functions $\psi \in \mathcal{S}(\mathbb{R}^n)$. The definition of spectrum in this paper removes a factor of 2π from the standard one, due to the 2π appearing in the definition of Fourier transform (1.5), see Appendix B.

2. Patterson Sets and Summation Formulas

The fundamental notion of a "quasicrystal" is a physical structure whose X-ray diffraction measure pattern consists of sharp spots. The concept of Patterson set is based on a mathematical concept of diffraction measure developed by A. Hof ([**H92**], [**H95a**], [**H95b**], [**H97**]).

We will model sets of atoms[1] located at a discrete set Λ by the pure point measure μ_Λ which consists of unit masses at the points of Λ. The measure μ_Λ can be regarded either as a regular Borel measure on $\mathbb{R}^n$, or alternatively as a positive Radon measure (by the Riesz representation theorem). However we shall generally regard it as a distribution, also denoted μ_Λ, and written

$$\mu_\Lambda := \sum_{\boldsymbol{x} \in \Lambda} \delta_{\boldsymbol{x}} \ , \tag{2.1}$$

which is associated to the measure by

$$\langle \mu_\Lambda, g \rangle := \int_{\mathbb{R}^n} g(\boldsymbol{x}) d\mu_\Lambda(\boldsymbol{x}) = \sum_{\boldsymbol{x} \in \Lambda} g(\boldsymbol{x}). \tag{2.2}$$

for test functions g. If Λ is a Delone set, then μ_Λ is a tempered distribution. Given a distribution of the general type

$$g = \sum_{\boldsymbol{x} \in \Lambda} n(\boldsymbol{x}) \delta_{\boldsymbol{x}} \ , \tag{2.3}$$

in which Λ is a discrete set the weights $n(\boldsymbol{x})$ are complex numbers with $|n(\boldsymbol{x})| \le C$, the associated regular Borel measure is uniquely defined via (2.2).

Definition 2.1. A complex-valued regular Borel measure μ on $\mathbb{R}^n$ is called *translation-bounded* if there is a constant C such that

$$|\mu|(\boldsymbol{x} + [0,1]^n) \le C \ , \quad \text{for all} \quad \boldsymbol{x} \in \mathbb{R}^n \ . \tag{2.4}$$

---

[1] An atomic structure may be more accurately represented as a measure obtained by convolving μ_Λ with a compactly supported nonnegative "bump function", see Hof [**H95b**]. Here we are concerned with the perfect idealization.

A. Hof developed a mathematical formalization of a diffraction measure associated to an arbitrary translation-bounded measure μ. To define it we first need the notion of an autocorrelation measure.

DEFINITION 2.2. Given a translation-bounded measure μ an *autocorrelation measure* γ of μ is any measure that is a limit point in the vague topology of a sequence of measures $\{\nu_{j,\boldsymbol{w}_j} : j = 1, 2, 3, \ldots\}$, where

$$\nu_{T,\boldsymbol{w}} := \frac{1}{T^n} \left(\mu\big|_{\boldsymbol{w}+T[0,1]^n} * \tilde{\mu}\big|_{\boldsymbol{w}+T[0,1]^n} \right) , \tag{2.5}$$

in which $\tilde{\mu}$ is the complex-conjugate measure to μ, with the space direction reversed. Here convergence $\nu_j \to \nu$ as $n \to \infty$ in the vague topology means that for each compactly supported continuous function $\phi : \mathbb{R}^n \to \mathbb{C}$ one has $\int_{\mathbb{R}^n} \phi(\boldsymbol{x}) d\nu_j \to \int_{\mathbb{R}^n} \phi(\boldsymbol{x}) d\nu$.

A translation-bounded measure μ has at least one autocorrelation measure; in general it has many autocorrelation measures. We mainly consider cases where μ_Λ has a unique autocorrelation measure.

For a discrete measure μ_Λ an autocorrelation measure encodes information about the "two-point correlation function" of Λ, i.e. the difference set $\Lambda - \Lambda$, with elements counted with multiplicity. The notion of autocorrelation measure is translation-invariant: for each translate $\Lambda + \boldsymbol{x}$ of a set Λ the measure $\mu_\Lambda + \boldsymbol{x}$ has the same autocorrelation measures as μ_Λ.

LEMMA 2.3. *Let μ be a positive measure that is translation-bounded with constant C, and let γ be any autocorrelation measure for μ. Then:*

((1)) *γ is a positive measure that is translation-bounded with constant C.*
((2)) *γ is a positive-definite measure (in the sense of tempered distributions). That is, the Fourier transform $\hat{\gamma}$ is a distribution of positive type.*
((3)) *The Fourier transform $\hat{\gamma}$ is a translation-bounded positive measure.*

PROOF. Properties (1) and (2) hold for all measures $\nu_{T,\boldsymbol{x}}$ and are inherited by γ. Part (3) follows from Hof [**H92**, Proposition 3.3], and is a result of Argabright and de Lamadrid [**AL**, Thms. 2.5 and 4.1]. The translation-boundedness constant C' for $\hat{\gamma}$ generally differs from that of γ. See Appendix A for a discussion of positive-definite measures. □

DEFINITION 2.4. A *diffraction measure* for a Delone set Λ is the Fourier transform $\hat{\gamma}$ of an autocorrelation measure γ of μ_Λ regarded as a tempered distribution.

The tempered distribution $\hat{\gamma}$ is identified with a translation-bounded positive measure by Lemma 2.3. We mainly consider cases in which the set Λ has a unique autocorrelation measure γ_Λ; in this case we call γ_Λ *the* autocorrelation measure of Λ and $\hat{\gamma}_\Lambda$ *the* diffraction measure of Λ.

A diffraction measure $\hat{\gamma}$ is a mathematical analogue of X-ray diffraction in the sense that values of the measure $\hat{\gamma}$ evaluated on "bump functions" ("pixels") are analogues of physical X-ray diffraction pictures, see Gähler and Klitzing [**GK**].

DEFINITION 2.5. A *Patterson set* or *perfectly diffractive Delone set* is a Delone set Λ that has a unique autocorrelation measure γ_Λ whose associated diffraction measure $\hat{\gamma}_\Lambda$ is a pure discrete measure. That is, there is a countable set $\sigma_P(X)$

such that

$$\hat{\gamma}_\Lambda := \sum_{\boldsymbol{y} \in \sigma_P(\Lambda)} p(\boldsymbol{y}) \delta_{\boldsymbol{y}} \ , \tag{2.6}$$

with all $p(\boldsymbol{y}) > 0$ for $\boldsymbol{y} \in \sigma_P(\Lambda)$. We call $\sigma_P(\Lambda)$ the *Patterson spectrum* of Λ.

The name 'Patterson set' reflects the fact that the autocorrelation is termed the *Patterson series* in X-ray crystallography, see Azároff [**Az**, p. 307], or [**Cow**, Ch. 5.3] for general background.

We note some elementary facts about Patterson sets. The positive-definiteness of the autocorrelation measure γ_Λ guarantees that $\sigma_P(\Lambda) = -\sigma_P(\Lambda)$ and

$$p(\boldsymbol{y}) = p(-\boldsymbol{y}) \geq 0 \ . \tag{2.7}$$

Furthermore $p(\boldsymbol{y}) \leq C'$ follows from the translation-boundedness of μ_Λ with constant C'. In interesting examples the Patterson spectrum $Y = \sigma_P(\Lambda)$ is a dense set. However, for each $\epsilon > 0$ the set

$$Y_\epsilon := \{ \boldsymbol{y} \in Y : p(\boldsymbol{y}) \geq \epsilon \} \ , \tag{2.8}$$

is a closed discrete set, as a consequence of the translation-boundedness of δ_Λ. In an actual X-ray diffraction spectrum only sufficiently large intensities will be detected above background levels, and the discreteness of Y_ϵ in (2.8) justifies how a Patterson set produces a pattern of discrete "bright spots."

The property of being a Patterson set is not affected by "small" changes in the set Λ. If Λ is a Delone set with a unique autocorrelation and Λ' is any Delone set, such that

$$\Lambda \ \Delta \ \Lambda' := (\Lambda \setminus \Lambda') \cup (\Lambda' \setminus \Lambda) \tag{2.9}$$

has density zero, in the sense that

$$\lim_{T \to \infty} \frac{1}{(2T)^n} \#(\Lambda \ \Delta \ \Lambda') \cap [-T, T]^n = 0 \ , \tag{2.10}$$

then Λ' has the same autocorrelation measure as Λ. (See Hof [**H95a**].)

Many constructions of Patterson sets are based on the Poisson summation formula, which we state in the following form.

THEOREM 2.6. (*Poisson summation formula*). *For a full rank lattice L in $\mathbb{R}^n$ the tempered distribution*

$$\mu_L = \sum_{\boldsymbol{x} \in L} \delta_{\boldsymbol{x}} \ , \tag{2.11}$$

has Fourier transform

$$\hat{\mu}_L = \frac{1}{|\det(L)|} \mu_{L^*} = \frac{1}{|\det(L)|} \sum_{\boldsymbol{y} \in L^*} \delta_{\boldsymbol{y}} \ , \tag{2.12}$$

in which L^* is the dual lattice

$$L^* = \{ \boldsymbol{y} \in \mathbb{R}^n : \langle \boldsymbol{y}, \boldsymbol{x} \rangle \in \mathbb{Z} \quad \textit{for all} \quad \boldsymbol{x} \in \Lambda \} \ . \tag{2.13}$$

The formula is equivalent to the assertion that for a Schwartz function $g \in \mathcal{S}(\mathbb{R}^n)$ one has

$$\sum_{\boldsymbol{x} \in L} g(\boldsymbol{x}) = \frac{1}{|\det(L)|} \sum_{\boldsymbol{y} \in L^*} \hat{g}(\boldsymbol{y}) \ . \tag{2.14}$$

The Poisson summation formula is often stated in a more general form explicitly exhibiting the action of a translation $\boldsymbol{t} \in \mathbb{R}^n$,

$$\sum_{\boldsymbol{x} \in L} g(\boldsymbol{x} - \boldsymbol{t}) = \frac{1}{|\det(L)|} \sum_{\boldsymbol{y} \in L^*} \hat{g}(\boldsymbol{y}) e^{2\pi i \langle \boldsymbol{y}, \boldsymbol{t} \rangle} . \tag{2.15}$$

For a proof of the validity of (2.14), which applied to a wider class of test functions than the Schwartz class, see Katznelson [**K68**, p. 129] and Gröchenig [**Gr**]. A generalization of the Poisson summation formula to a class of unbounded measures on a general locally compact Abelian group appears in Argabright and de Lamadrid [**AL**, Thm. 3.3].

Using this formula it is easy to verify that all ideal crystals are Patterson sets.

THEOREM 2.7. *An ideal crystal $\Lambda = L + F$, in which L is a full rank lattice in $\mathbb{R}^n$ and F is a finite set, has a unique autocorrelation measure*

$$\gamma_\Lambda = \frac{1}{|\det(L)|} \sum_{\boldsymbol{f}_1 \in F} \sum_{\boldsymbol{f}_2 \in F} \left(\sum_{\boldsymbol{x} \in L} \delta_{\boldsymbol{x} + \boldsymbol{f}_1 - \boldsymbol{f}_2} \right) . \tag{2.16}$$

Its Fourier transform $\hat{\gamma}_\Lambda$ is given by

$$\hat{\gamma}_\Lambda = \frac{1}{|\det(L)|^2} \sum_{\boldsymbol{y} \in L^*} \left(\sum_{\boldsymbol{f}_1 \in F} \sum_{\boldsymbol{f}_2 \in F} e^{2\pi i \langle \boldsymbol{f}_1 - \boldsymbol{f}_2, \boldsymbol{\xi} \rangle} \right) \delta_{\boldsymbol{y}} . \tag{2.17}$$

Thus Λ is a Patterson set with spectrum $\sigma_P(\Lambda)$ contained in the dual lattice L^*.

PROOF. To obtain (2.16) we use (2.5) and count elements of $(L+F) - (L+F)$ on a box $[-T, T]^n$ and let $T \to \infty$. These points fall in $L + (F - F)$ and the density yields a weight $\frac{1}{|\det(L)|}$; we omit the estimates. The Poisson summation formula yields (2.17). □

In the special case that Λ is a lattice L, its autocorrelation measure γ_L is equal to the measure μ_L up to a scale factor, namely

$$\gamma_L = \frac{1}{|\det(L)|} \mu_L = \frac{1}{|\det(L)|} \sum_{\boldsymbol{x} \in L} \delta_{\boldsymbol{x}} . \tag{2.18}$$

In this case the Patterson spectrum $\sigma_P(L) = L^*$. For a general ideal crystal $\Lambda = L + F$ one can have $\sigma_p(L) \neq L^*$. For the one-dimensional example

$$\Lambda := \mathbb{Z} \cup (\mathbb{Z} + a) \cup (\mathbb{Z} + b) \cup (\mathbb{Z} + c)$$

one can find irrational a, b, c such that

$$1 + e^{2\pi i n a} + e^{2\pi i n b} + e^{2\pi i n c} = 0$$

holds only for $n = \pm 1$, in which case $\sigma_P(\Lambda) = \mathbb{Z} \setminus \{\pm 1\}$.

There is a strong connection between Patterson sets and summation formulas. Recall that a Delone set of finite type is a Delone set Λ such that $\Lambda - \Lambda$ is a closed discrete set.

LEMMA 2.8. *If Λ is a Delone set of finite type then any autocorrelation measure γ of μ_Λ is a pure discrete measure of the form*

$$\gamma = \sum_{\boldsymbol{y} \in \Lambda - \Lambda} n(\boldsymbol{y}) \delta_{\boldsymbol{y}} , \tag{2.19}$$

in which $n(\boldsymbol{y}) = n(-\boldsymbol{y}) \geq 0$.

PROOF. Each measure $\mu_{T,\boldsymbol{w}}$ in (2.5) is pure discrete, and has the form (2.19) with $n(\boldsymbol{y}) = n(-\boldsymbol{y}) \geq 0$. Since $\Lambda - \Lambda$ is a closed discrete set, any limit point in the vague topology of $\mu_{T,\boldsymbol{w}}$ inherits these properties. □

Thus we deduce:

THEOREM 2.9. (*Quasicrystal Summation Formula*). *Suppose that Λ is a Delone set of finite type in $\mathbb{R}^n$. If Λ is a Patterson set then its autocorrelation measure γ_Λ and Fourier transform $\hat{\gamma}_\Lambda$ have the form*

$$\gamma_\Lambda = \sum_{\boldsymbol{y} \in \Lambda - \Lambda} n(\boldsymbol{y}) \delta_{\boldsymbol{y}} \quad \text{and} \quad \hat{\gamma}_\Lambda = \sum_{\boldsymbol{z} \in \sigma_P(\Lambda)} p(\boldsymbol{z}) \delta_{\boldsymbol{z}} \ . \tag{2.20}$$

Both γ_Λ and $\hat{\gamma}_\Lambda$ are translation-bounded measures on $\mathbb{R}^n$. For each function g in the Schwartz space $\mathcal{S}(\mathbb{R}^n)$,

$$\sum_{\boldsymbol{y} \in \Lambda - \Lambda} n(\boldsymbol{y}) \hat{g}(\boldsymbol{y}) = \sum_{\boldsymbol{z} \in \sigma_P(\Lambda)} p(\boldsymbol{z}) g(\boldsymbol{z}) \ . \tag{2.21}$$

PROOF. This follows from Lemma 2.3 and the definition of Patterson set. For a test function $g \in \mathcal{S}(\mathbb{R}^n)$, the left side of (2.21) is $\langle \gamma_\Lambda, \hat{g} \rangle$ while the right side is $\langle \hat{\gamma}_\Lambda, g \rangle$. □

The quasicrystal summation formula (2.21) may be valid for wider classes of functions $g(\boldsymbol{y})$ than just those functions in the Schwartz space $\mathcal{S}(\mathbb{R}^n)$. This is the case for the Poisson summation formula, see for example Gröchenig [**Gr**] and Kahane and Lemarié-Rieusset [**KLR**]. There are nontrivial limits to the range of validity of the Poisson summation formula, however. Katznelson ([**K67**], [**K68**, p. 155]) gives an example of a function $g \in L^1(\mathbb{R})$ such that $\hat{g} \in L^1(\hat{\mathbb{R}})$ and both sides of (2.21) converge absolutely but do not agree.

Theorem 2.9 applies more generally to sets Λ that are not Delone sets but retain the "finite local complexity" property that $\Lambda - \Lambda$ is a discrete closed set [2]. An interesting example of such a set having a pure point diffraction spectrum is the set of visible lattice points in $\mathbb{Z}^2$, as was recently shown by Baake, Moody and Pleasants [**BMP**].

There exist many interesting summation formulas known which are formally of the general type

$$\gamma_\Lambda = \sum_{\boldsymbol{y} \in Y} n(\boldsymbol{y}) \delta_{\boldsymbol{y}} \quad \text{and} \quad \hat{\gamma}_\Lambda = \sum_{\boldsymbol{z} \in Z(\Lambda)} p(\boldsymbol{z}) \delta_{\boldsymbol{z}} \ ,$$

where Y and Z are countable sets, $n(\boldsymbol{y})$ and $p(\boldsymbol{z})$ are weights, which the formula applies to specific spaces of test functions (usually different from the Schwartz space), see Guinand [**Gu**, Sec. 10].

We now consider examples of Patterson sets. The most general method found so far for proving that certain Delone sets Λ in $\mathbb{R}^n$ are Patterson sets uses properties of an associated dynamical system$([[\Lambda]], \mathbb{R}^n)$.

DEFINITION 2.10. Given any Delone set Λ of finite type, the set $[[\Lambda]]$ is the collection of all Delone sets Λ' which are pointwise limits of some sequence of translates $\{\Lambda + \boldsymbol{x}_i : i = 1, 2, 3, \ldots\}$ of Λ.

---

[2] Such sets must be uniformly discrete, but need not be relatively dense.

The *natural topology* on $[[\Lambda]]$ defines two sets Λ and Λ' as being within distance ϵ if there is a translation $\boldsymbol{t}$ with $\|\boldsymbol{t}\| < \epsilon$ such that $\Lambda + \boldsymbol{t}$ agrees with Λ' on a ball of radius $1/\epsilon$ around $\mathbf{0}$; the set $[[\Lambda]]$ is compact in this topology. More generally, for any Delone set one can define $[[\Lambda]]$ as the closure of the set of translates of $\Lambda + \boldsymbol{x}$ in an appropriate topology, and $[[\Lambda]]$ is a compact set in this topology, see Solomyak [**So98b**]. The set $[[\Lambda]]$ is closed under translations, and we let $([[\Lambda]], \mathbb{R}^n)$ denote the (topological) dynamical system with this $\mathbb{R}^n$-action.

DEFINITION 2.11. (i) A topological dynamical system $\mathcal{X}$ with $\mathbb{R}^n$-action is *minimal* if every orbit of a point under translation by $\mathbb{R}^n$ is dense in $\mathcal{X}$.

(ii) A topological dynamical system is *uniquely ergodic* if it has a unique invariant measure μ; in this case we can regard it as the metrical dynamical system with measure μ.

(iii) A topological dynamical system is *strictly ergodic* if it is minimal and uniquely ergodic.

In the case of a topological dynamical system $\mathcal{X} = ([[\Lambda]], \mathbb{R}^n)$ these concepts have the following characterizations. $\mathcal{X}$ is minimal if and only if Λ is *repetitive*, which means that for each T-patch $\Lambda \cap B(\boldsymbol{x}, T)$ of Λ there is a radius T' (depending only on T) such that Λ contains a translate of this patch inside any ball of radius T'. Such an $\mathcal{X}$ is uniquely ergodic if and only if any T-patch has a uniform limiting frequency of occurrence inside T'-patches, as $T' \to \infty$. Such an $\mathcal{X}$ is strictly ergodic if and only if it is uniquely ergodic and every T-patch has a uniform limiting frequency that is positive.

To any metrical dynamical system $([[\Lambda]], \mathbb{R}^n, \mu)$ we associate a family of commuting unitary operators $U(\boldsymbol{t}) : L^2([[\Lambda]], \mu) \to L^2([[\Lambda]], \mu)$ indexed by $\boldsymbol{t} \in \mathbb{R}^n$, given by

$$U(\boldsymbol{t})f(\Lambda') = f(\Lambda' - \boldsymbol{t}) \text{ for } \Lambda' \in [[\Lambda]].$$

DEFINITION 2.12. (i) A *measurable eigenfunction* $f \in L^2([[\Lambda]], \mathbb{R}^n, \mu)$ with eigenvalue $\boldsymbol{\lambda} \in \mathbb{R}^n$ is one that satisfies

$$U(\boldsymbol{t})f(\Lambda) = e^{2\pi i \langle \boldsymbol{\lambda}, \boldsymbol{t} \rangle} f(\Lambda), \quad \text{for all} \quad \boldsymbol{t} \in \mathbb{R}^n \ .$$

(ii) A *continuous eigenfunction* $f \in C(([[\Lambda]], \mathbb{R}^n)$ is an eigenfunction which is continuous in the natural topology on $[[\Lambda]]$.

DEFINITION 2.13. (i) The *spectrum* of $([[\Lambda]], \mathbb{R}^n, \mu)$ is the joint spectrum of the family of commuting operators $\{U(\boldsymbol{t}) : \boldsymbol{t} \in \mathbb{R}^n\}$.

(ii) A dynamical system $([[\Lambda]], \mathbb{R}^n, \mu)$ has *pure discrete spectrum* or *pure point spectrum* if the set of measurable eigenfunctions spans $L^2([[\Lambda]], \mu)$.

THEOREM 2.14. *If Λ is a Delone set of finite type such that the dynamical system $([[\Lambda]], \mathbb{R}^n)$ is strictly ergodic and has pure discrete spectrum, then every set Λ' in $[[\Lambda]]$ is a Patterson set.*

PROOF. The essential idea of this result appears in Dworkin [**Dw**]. A proof is sketched in Hof [**H97**, pp. 253–257]. □

It is known that if the dynamical system $([[\Lambda]], \mathbb{R}^n)$ is strictly ergodic and has purely continuous spectrum, then no set Λ' in $[[\Lambda]]$ is a Patterson set. If it has mixed spectrum — some discrete and some continuous — it is not known whether some Λ' in $[[\Lambda]]$ can be a Patterson set.

Essentially all model sets with a reasonable window set B have been proved to be Patterson sets by this method. The following result is due to Schlottmann [**S98**] [**S99**, Thm. 4.5].

THEOREM 2.15. *(Schlottmann) If Λ is a model set in $\mathbb{R}^n$ whose window set B is compact, with non-empty interior and with a boundary of Haar measure zero, then Λ is a Patterson set, whose spectrum $\sigma_p(\Lambda)$ has*

$$\sigma_P(\Lambda) \subseteq \pi_{||}(L^*) \tag{2.22}$$

where L^* is the dual lattice of L.

Schlottmann proves that the associated dynamical system has a pure point spectrum, and Theorem 2.15 then follows from Theorem 2.14. That a result like this should hold was suggested by Meyer [**Me95**], and this result improves on an earlier result of Hof [**H97**, Sec. 4.4], whose proof did not use dynamical systems.

A number of self-replicating Delone sets have been proved to be Patterson sets using the associated dynamical system. For self-replicating Delone sets, Solomyak [**So97**] gives an algorithmic method for testing whether the dynamical system associated to a primitive self-replicating Delone set Λ of finite type in $\mathbb{R}^2$ has pure point spectrum. He applies this to several examples in §7 of his paper. His example 7.2 implies that the set Λ of vertices of the "sphinx tiling" of Godrèche [**Go**] gives a dynamical system with purely discrete spectrum. Thus all elements Λ' of $[[\Lambda]]$ are Patterson sets. In this example the spectrum of the associated dynamical system $([[\Lambda]], \mathbb{R}^2)$ is not contained in any finite-dimensional $\mathbb{Z}$-module. This spectrum is contained in $\mathbb{Z}[\frac{1}{2}] \times \mathbb{Z}[\frac{1}{2}]$, and involves rationals with arbitrarily high powers of 2 in the denominator. This indicates that there is some set Λ' in $[[\Lambda]]$ which has a Patterson spectrum $\sigma_P(\Lambda')$ which is not contained in any finite-dimensional $\mathbb{Z}$-module. This would happen if Λ' had the same spectrum as that of the dynamical system, i.e. no coefficients were "extinguished." Note that this sort of spectrum differs from that of any cut-and-project set, because such sets have spectra $\sigma_P(\Lambda)$ contained in a finite-dimensional $\mathbb{Z}$-module by (2.22). However the sets constructed by this type of dynamical system may be model sets. The chair tiling in in $\mathbb{R}^2$ yields model sets based on a p-adic "internal space", as is shown in Baake, Moody and Schlottmann [**BMS**]. A similar result was established for the n-dimensional chair tiling by Lee and Moody [**LM**], who also showed that the sphinx tiling is a union of 36 model sets using such an "internal space." The dynamical systems associated to self-similar structures can be viewed as a generalization of substitution dynamical systems, the spectral properties of which have been extensively studied, see Queffélec [**Q**].

We say that a strictly ergodic dynamical system acting with an $\mathbb{R}^n$-action on a compact space Ω with invariant measure μ is *homogeneous* if $L^2(\Omega, \mu)$ has a basis of continuous eigenfunctions, see [**Ro94**, p. 494]. Such a dynamical system necessarily has pure discrete spectrum. Many of the constructions above yield Λ such that $([[\Lambda]], \mathbb{R}^n)$ is a homogeneous dynamical system. The potential relevance of such dynamical systems to the problem of defining "Fourier coefficients" for certain Delone sets Λ is discussed at the end of §3.

3. Fourier Quasicrystals

For an ideal crystal Λ it is well-known that the Fourier transform $\hat{\mu}_\Lambda$ is the density function of a measure which contains "phase information" that is lost in the X-ray diffraction measure. Indeed, if

$$\Lambda = \bigcup_{j=1}^{k} (L + \boldsymbol{f}_j) \ , \tag{3.1}$$

where L is a full rank lattice on $\mathbb{R}^n$ having dual lattice L^*, then the Poisson summation formula gives

$$\hat{\mu}_\Lambda = \sum_{\boldsymbol{y} \in L^*} c(\boldsymbol{y}) \delta_{\boldsymbol{y}} \tag{3.2}$$

in which

$$c(\boldsymbol{y}) = \frac{1}{|\det(L)|} \sum_{j=1}^{k} \exp(2\pi i \langle \boldsymbol{f}_j, \boldsymbol{y} \rangle) \ . \tag{3.3}$$

By Theorem 2.7 the autocorrelation measure γ_Λ of Λ has Fourier transform given by

$$\hat{\gamma}_\Lambda = \sum_{\boldsymbol{y} \in L^*} |c(\boldsymbol{y})|^2 \delta_{\boldsymbol{y}} \ , \tag{3.4}$$

because

$$|c(\boldsymbol{y})|^2 = \frac{1}{|\det(L)|^2} \sum_{i=1}^{k} \sum_{j=1}^{k} \exp(2\pi i \langle \boldsymbol{f}_i - \boldsymbol{f}_j, \boldsymbol{y} \rangle) \ . \tag{3.5}$$

Knowledge of the Fourier coefficients $\{c(\boldsymbol{y}) : \boldsymbol{y} \in L^*\}$ suffices to uniquely reconstruct Λ, but it is well-known that knowledge of the intensities $\{|c(\boldsymbol{y})|^2 : \boldsymbol{y} \in L^*\}$ does not always uniquely determine the translation-equivalence class of Λ. This ambiguity is an important obstacle to the reconstruction of crystal structure from X-ray diffraction data.

This raises the problem:

Phase Problem. For which Patterson sets Λ can one define "phase information" $\{c(\boldsymbol{y}) : \boldsymbol{y} \in \sigma_P(\Lambda)\}$ such that the distribution $\hat{\mu}_\Lambda$ has a "formal δ-function expansion"

$$\hat{\mu}_\Lambda \sim \sum_{\boldsymbol{y} \in Y} c(\boldsymbol{y}) \delta_{\boldsymbol{y}} \ , \tag{3.6}$$

in which $Y = \sigma_P(\Lambda)$ and for which

$$\hat{\gamma}_\Lambda = \sum_{\boldsymbol{y} \in \sigma_P(\Lambda)} |c(\boldsymbol{y})|^2 \delta_{\boldsymbol{y}} \ , \tag{3.7}$$

both hold?

The phase problem can be divided into two subproblems. The first problem is that of defining a "formal δ-function expansion" (3.6) for the distribution $\hat{\mu}_\Lambda$, for some countable spectrum Y. The second problem is obtaining conditions on a Patterson set Λ such that the coefficients $p(\boldsymbol{y})$ of the diffraction measure $\hat{\gamma}_\Lambda$ given by

$$\hat{\gamma}_\Lambda = \sum_{\boldsymbol{y} \in \sigma_P(\Lambda)} p(\boldsymbol{y}) \delta_{\boldsymbol{y}} \ . \tag{3.8}$$

are related to the coefficients $c(\boldsymbol{y})$ of the formal δ-function expansion by

$$p(\boldsymbol{y}) = |c(\boldsymbol{y})|^2 \ , \tag{3.9}$$

We call (3.9) the *consistent phase property.*

We first deal with the problem of defining a "formal δ-function expansion" (3.6). Here we do not assume that Λ is a Patterson set. The narrowest such definition is the following.

DEFINITION 3.1. A Delone set Λ is a *strongly almost periodic set* if the tempered distribution $\hat{\mu}_\Lambda$ is a translation-bounded measure that is a pure point measure.

In this case the Fourier transform of μ_Λ can be written

$$\hat{\mu}_\Lambda := \sum_{\boldsymbol{y} \in Y} c(\boldsymbol{y}) \delta_{\boldsymbol{y}} \ , \tag{3.10}$$

in which Y is a countable set. All such sets can be classified using the following result of Cordoba [**Co89**].

THEOREM 3.2. (*Cordoba*) *Suppose that* $\Lambda = \cup_{i=1}^k \Lambda_i$ *is a uniformly discrete set in* $\mathbb{R}^n$*, and let* g_Λ *denote the tempered distribution*

$$g_\Lambda = \sum_{i=1}^{k} w_i \left(\sum_{\boldsymbol{x} \in \Lambda_i} \delta_{\boldsymbol{x}} \right) \tag{3.11}$$

in which $\{w_1, \ldots, w_k\}$ *are complex numbers. If the Fourier transform* $\hat{g}_\Lambda$ *is a translation-bounded measure which is pure point, i.e.*

$$\hat{g}_\Lambda = \sum_{\boldsymbol{y} \in Y} m(\boldsymbol{y}) \delta_{\boldsymbol{y}} \ , \tag{3.12}$$

with

$$\sum_{\boldsymbol{y} \in \boldsymbol{z} + [0,1]^n} |m(\boldsymbol{y})| \le C, \quad \text{for all} \quad \boldsymbol{z} \in \mathbb{R}^n \ ,$$

then Λ *and each set* Λ_i *are a finite union of translates of some full rank lattice* L *in* $\mathbb{R}^n$.

Cordoba's theorem as stated in [**Co89**] only concludes that each Λ_i is a finite disjoint union of translates of n-dimensional lattices. However the union of two such translates $(L_1 + \boldsymbol{a}_1) \cup (L_2 + \boldsymbol{a}_2)$ cannot be uniformly discrete unless the lattices L_1 and L_2 are commensurable, i.e. unless both can be written as a finite union of cosets of a common full-rank lattice L. This follows from Kronecker's theorem in Diophantine approximation. Since Λ is uniformly discrete, there must be a common refining lattice L for all these lattices simultaneously, which gives Theorem 3.2.

We immediately obtain:

COROLLARY 3.3. *A strongly almost periodic set is an ideal crystal and conversely.*

PROOF. Apply Theorem 3.2 with $\Lambda = \Lambda_1$ and $w_1 = 1$. □

The hypotheses of Theorem 3.2 cannot be relaxed to merely requiring that both g_Λ and $\hat{g}_\Lambda$ be translation-bounded pure discrete measures. Indeed, de Bruijn ([**dB86**], Theorem 11.1) gives examples of measures

$$\mu = \sum_{\boldsymbol{y} \in \Lambda} n(\boldsymbol{y}) \delta_{\boldsymbol{y}}$$

in which Λ is a Delone set, and μ and its Fourier transform $\hat{\mu}$ are both translation-bounded pure discrete measures, but Λ is not contained in a finite union of translates of a lattice. These examples are obtained from cut-and-project sets by a smoothing operation. In these examples the coefficients $m(\boldsymbol{y})$ necessarily assume infinitely many values.

For general Delone sets Λ the distribution $\hat{\mu}_\Lambda$ need not be a measure, so we cannot assign a direct meaning of "pure discrete measure" to $\hat{\mu}_\Lambda$. As an example, Hof [**H97**, p. 246] observes that any Delone set $\Lambda \subset \mathbb{Z}^n$ that is not fully periodic has $\hat{\mu}_\Lambda$ not a measure. To proceed, we observe that the existence of a Fourier transform $\hat{\mu}_\Lambda$ satisfying (3.2) can be rephrased as saying that μ_Λ has a "Fourier series"

$$\mu_\Lambda \sim \sum_{\boldsymbol{y} \in L^*} c(\boldsymbol{y}) \exp(-2\pi i \langle \boldsymbol{y}, \cdot \rangle) \ , \tag{3.13}$$

because the distributional Fourier transform of the function $\exp(-2\pi i \langle \boldsymbol{y}, \cdot \rangle)$ is $\delta_{\boldsymbol{y}}$. We therefore seek to directly define such a "Fourier series" associated to μ_Λ. To accomplish this, we consider various classes of almost periodic functions.

H. Bohr [**Bo1**] developed a theory of uniformly almost periodic functions on the real line, which was extended to $\mathbb{R}^n$ by S. Bochner. Uniformly almost periodic functions are those bounded continuous functions $h(\boldsymbol{x})$ that can be uniformly approximated on all of $\mathbb{R}^n$ by trigonometric polynomials. They have a well-defined "Fourier series"

$$h(\boldsymbol{x}) \sim \sum_{\boldsymbol{y} \in Y} m(\boldsymbol{y}) \exp(-2\pi i \langle \boldsymbol{y}, \boldsymbol{x} \rangle) \tag{3.14}$$

in which Y is a countable set, and the coefficients are square-summable,

$$\|h\|^2 := \sum_{\boldsymbol{y} \in Y} |m(\boldsymbol{y})|^2 < \infty \ . \tag{3.15}$$

The Fourier series data $\{m(\boldsymbol{y}) : \boldsymbol{y} \in Y\}$ permits unique reconstruction of the function $h(\boldsymbol{x})$. However not all countable sets Y and data $\{m(\boldsymbol{y}) : \boldsymbol{y} \in Y\}$ satisfying (3.15) give "Fourier series" of uniformly almost periodic functions. The condition

$$\sum_{\boldsymbol{y} \in Y} |m(\boldsymbol{y})| < \infty \ , \tag{3.16}$$

is known to be a sufficient condition for (3.14) to be the Fourier series of a uniformly almost periodic function.

L. Schwartz [**Sch**, Sec. V1.9] introduced the following notion of uniformly almost periodic distribution based on uniformly almost periodic function.

DEFINITION 3.4. A tempered distribution f is a *uniformly almost periodic distribution* if for each compactly supported C^∞-function $g \in C_c^\infty(\mathbb{R}^n)$ the convolution $g * f$ is a uniformly almost periodic function on $\mathbb{R}^n$. (Here $g * f(\boldsymbol{y}) = \langle f, g_{-\boldsymbol{y}} \rangle$ where $g_{\boldsymbol{y}}(\boldsymbol{x}) = g(\boldsymbol{x} + \boldsymbol{y})$.) More generally, if $\mathcal{B}$ is a class of almost periodic functions, a *$\mathcal{B}$-almost periodic distribution* f is a tempered distribution f such that for each $g \in C_c^\infty(\mathbb{R}^n)$ the convolution $g * f \in \mathcal{B}$.

A uniformly almost periodic distribution f has a well-defined "Fourier series"

$$f \sim \sum_{\boldsymbol{y} \in Y} m(\boldsymbol{y}) \exp(-2\pi i \langle \boldsymbol{y}, \cdot \rangle) \tag{3.17}$$

in which Y is a countable set. To construct it, given $\boldsymbol{y} \in \mathbb{R}^n$ take $g \in C_c^\infty(\mathbb{R}^n)$ to be a test function which has $\hat{g}(\boldsymbol{y}) \neq 0$, and if the uniformly almost periodic function $g * f$ has "Fourier series"

$$g * f(x) \sim \sum_{\boldsymbol{z} \in \mathbb{R}^n} m_g(\boldsymbol{z}) \exp(-2\pi i \langle \boldsymbol{z}, \cdot \rangle) \tag{3.18}$$

where only countably many $m_g(\boldsymbol{z}) \neq 0$, then we set

$$m(\boldsymbol{y}) := \frac{m_g(\boldsymbol{y})}{\hat{g}(\boldsymbol{y})} \ . \tag{3.19}$$

It can be checked that this definition is independent of the choice of test function g having $g(\boldsymbol{y}) \neq 0$. One can prove that the coefficients $m(\boldsymbol{y})$ are (uniformly) locally square-summable: there is a constant C such that for all $\boldsymbol{x} \in \mathbb{R}^n$,

$$\sum_{\boldsymbol{y} \in \boldsymbol{x} + [0,1]^n} |m(\boldsymbol{y})|^2 < C \ . \tag{3.20}$$

However a drawback is that not all data $\{m(\boldsymbol{y}) : \boldsymbol{y} \in Y\}$ satisfying (3.20) are the "Fourier series" of a (uniformly) almost periodic distribution f. Burkhill and Rennie [**BR**] develop a theory of almost periodic distributions extending that of Schwartz.

DEFINITION 3.5. A Delone set Λ is a *Bohr almost periodic set* Λ if its associated measure μ_Λ is a uniformly almost periodic distribution.

We view the Fourier transform $\hat{\mu}_\Lambda$ of a Bohr almost periodic set Λ as having a "formal δ-function expansion"

$$\hat{\mu}_\Lambda \sim \sum_{\boldsymbol{y} \in Y} m(\boldsymbol{y}) \delta_{\boldsymbol{y}} \tag{3.21}$$

which is its "Fourier series" (3.18).

The unique reconstructability of uniformly almost periodic functions from their "Fourier series" has the following consequence for Bohr almost periodic sets:

(1) The "Fourier series" of a Bohr almost periodic set μ_Λ permits unique reconstruction of Λ.
(2) If Λ is a Bohr almost periodic set and G is a nonempty finite set disjoint from Λ, then $\Lambda \cup G$ is not a Bohr almost periodic set.

A simple sufficient condition for f to be a uniformly almost periodic distribution is the following.

LEMMA 3.6. *If a tempered distribution f and its Fourier transform $\hat{f}$ on $\mathbb{R}^n$ are both translation-bounded measures that are pure discrete, then f and $\hat{f}$ are both (uniformly) almost periodic distributions.*

PROOF. This is easy to verify using test functions $g \in C_c^\infty(\mathbb{R}^n)$ because (3.18) holds for $g * f$ and for $g * \hat{f}$. □

Lemma 3.6 implies that ideal crystals Λ are Bohr almost periodic sets. As mentioned earlier, de Bruijn ([**dB86, dB87**]) constructs a large number of distributions f which he calls "*Poisson combs*" that apparently satisfy the hypotheses of Lemma 3.6. (He works in the Gelfand-Shilov space $S_{1/2}^{1/2}$ of distributions, however, rather than with tempered distributions, see van Eijndhoven [**Eij**].) These sets are not Bohr almost periodic sets because points are assigned variable weights rather than having weight one at all points.

The concept of "Bohr almost periodic set" is so narrow as to exclude various Patterson sets. Hof [**H92**, p. 90] observes that the tempered distribution

$$f = \sum_{n \in \mathbb{Z}} w_n \delta_n \tag{3.22}$$

where $\{w_n : n \in \mathbb{Z}\}$ is a zero-one sequence that describes a "Fibonacci quasicrystal" is not a (uniformly) almost-periodic distribution. The same remains true even if the type of almost-periodicity used in defining the distribution is relaxed from that of Bohr to the wider classes of Stepanov or Wiener. The set

$$\Lambda_w := \{n \in \mathbb{Z} : w_n = 1\} \tag{3.23}$$

is a Meyer set and is known to be a Patterson set. Other examples are given by certain one-dimensional cut-and-project sets Λ do not have μ_Λ being an uniformly almost periodic measure, also due to Hof[**H97**, p. 257]

It seems to be unknown whether there exist any Bohr almost periodic sets that are not ideal crystals. A strong constraint on the nature of Bohr almost periodic sets arises from the restriction that

$$\mu_\Lambda = \sum_{\boldsymbol{x} \in \Lambda} n(\boldsymbol{x}) \delta_{\boldsymbol{x}} \tag{3.24}$$

has all coefficients $n(\boldsymbol{x}) = 1$. In regard to this property, we mention another result of Cordoba [**Co88**].

Theorem 3.7. (*Cordoba*). *Suppose that X and Y are discrete sets in $\mathbb{R}^n$, that $\{p(\boldsymbol{y}) : \boldsymbol{y} \in Y\}$ are positive real numbers, and that the two distributions*

$$f_1 = \sum_{\boldsymbol{x} \in X} \delta_{\boldsymbol{x}} \quad \text{and} \quad f_2 = \sum_{\boldsymbol{y} \in Y} p(\boldsymbol{y}) \delta_{\boldsymbol{y}} \tag{3.25}$$

are tempered distributions. If $f_2 = \hat{f}_1$, then X is a full rank lattice L in $\mathbb{R}^n$ and Y is the dual lattice L^*, and all $p(\boldsymbol{y}) = \frac{1}{|\det(L)|}$.

This result appears in [**Co88**, Thm. 2], except that Cordoba asserts that $|\det(L)| = 1$, which is too strong a conclusion. His method appears to establish the result above.

In Theorem 3.7 X is a discrete set, not necessarily a Delone set, while Y is required to be a discrete set, but translation-boundedness is not required, the growth on the sizes of the coefficients $|p(\boldsymbol{y})|$ being sufficient to give a tempered distribution. This result puts further restriction on any Bohr periodic set that is not an ideal crystal.

To obtain a wider class of sets Λ for which $\hat{\mu}_\Lambda$ has a well-defined δ-function expansion, we must relax the definition of "almost periodic distribution" to allow a wider class of almost periodic functions. We would like a definition that includes all cut-and-project sets which are Patterson sets. For this it seems that one needs a class $\mathcal{B} \subseteq L_2(\mathbb{R}^n)$ of almost periodic functions with the following three properties.

(1) *Translation-closure property.* If $f(\boldsymbol{x}) \in \mathcal{B}$ with "formal Fourier series"

$$f(\boldsymbol{x}) \sim \sum_{\boldsymbol{y} \in Y} c(\boldsymbol{y}) e^{2\pi i \langle \boldsymbol{y}, \boldsymbol{x} \rangle} \tag{3.26}$$

then for each translation $\boldsymbol{t} \in \mathbb{R}^n$, $f_t(\boldsymbol{x}) = f(\boldsymbol{x} - \boldsymbol{t}) \in \mathcal{B}$ and the "formal Fourier series" of f_t has the same spectrum Y as f with Fourier coefficients

$$c_t(\boldsymbol{y}) = c(\boldsymbol{y}) e^{-2\pi i \langle \boldsymbol{y}, \boldsymbol{t} \rangle} . \tag{3.27}$$

(2) *Parseval property.* The "formal Fourier series" (3.26) of $f(\boldsymbol{x}) \in \mathcal{B}$ satisfies

$$\|f\|_2^2 = \sum_{\boldsymbol{y} \in Y} |c(\boldsymbol{y})|^2 . \tag{3.28}$$

(3) *Riesz-Fischer property.* For any countable set Y and set of coefficients $\{c(\boldsymbol{y}) : \boldsymbol{y} \in Y\}$ that are square-summable,

$$\sum_{\boldsymbol{y} \in Y} |c(\boldsymbol{y})|^2 < \infty , \tag{3.29}$$

there exists a function $f(\boldsymbol{x}) \in \mathcal{B}$ which has "formal Fourier series"

$$f(\boldsymbol{x}) \sim \sum_{\boldsymbol{y} \in Y} c(\boldsymbol{y}) e^{2\pi i \langle \boldsymbol{y}, \boldsymbol{x} \rangle} . \tag{3.30}$$

In the one-dimensional case the Besicovitch class of B^2-almost periodic functions has these properties, see Appendix B. Definition 3.4 yields a notion of B^2-*almost periodic distribution* and we then also obtain an associated notion of *Besicovitch almost periodic set (of class* B^2 analogous to Definition 3.5. Hof [**H97**, p. 258] observes that certain one-dimensional cut-and-project sets are Besicovitch almost periodic sets in this sense. The Besicovitch theory does not seem to have been extended to $\mathbb{R}^n$ for $n \geq 2$, but Følner [**Fø**] has developed a theory of almost periodic functions on $\mathbb{R}^n$ which has the Parseval and Riesz-Fischer properties.

DEFINITION 3.8. A Delone set Λ is a *Bescovitch almost periodic set* of class $\mathcal{B}$ if its associated measure μ_Λ is a uniformly almost periodic distribution of class $\mathcal{B}$.

This definition depends on the class $\mathcal{B}$, and one hopes that a suitable class $\mathcal{B}$ of functions define a concept of *Besicovitch almost periodic set* on $\mathbb{R}^n$ which will include all reasonable cut-and-project sets. Such a theory has not yet been worked out in any detail.

A price one pays in allowing larger classes of almost periodic functions with the Riesz-Fischer property is that a $\mathcal{B}$-almost periodic function cannot be reconstructed from its "formal Fourier series". For example, there are two B^2-almost periodic functions f and g on $\mathbb{R}$ which disagree on a set of infinite Lebesgue measures but have the same B^2-Fourier series. Thus we cannot hope to reconstruct a set Λ uniquely from "phase information" supplied by a "formal Fourier series" of this sort.

We conclude this section by describing results from another approach for associating "discrete spectrum" to the tempered distribution $\hat{\mu}_\Lambda$, which was originally explored by Bombieri and Taylor [**BT86**], [**BT87**]. In some circumstances a tempered distribution $f(\boldsymbol{x})$ has a limit

$$m_{\boldsymbol{\xi}} := \lim_{T \to \infty} \frac{1}{(2T)^n} \int_{[-T,T]^n + \boldsymbol{a}} e^{-2\pi i \langle \boldsymbol{\xi}, \boldsymbol{x} \rangle} f(\boldsymbol{x}) d\boldsymbol{x} , \tag{3.31}$$

which is independent of the translation $\boldsymbol{a} \in \mathbb{R}^n$. We can view $m_{\boldsymbol{\xi}}$ as defining a "Fourier coefficient" of the distribution $f(\boldsymbol{x})$ at the frequency $\boldsymbol{\xi}$. Hof ([**H95a**]) obtained the following result.

THEOREM 3.9. (*Hof*). *Let μ be a translation-bounded measure on $\mathbb{R}^n$ that has a unique autocorrelation measure γ and suppose that for some $\boldsymbol{\xi} \in \mathbb{R}^n$ the limit*

$$m_{\boldsymbol{\xi}} = \lim_{T\to\infty} \frac{1}{(2T)^n} \int_{[-T,T]^n+\boldsymbol{a}} e^{-2\pi i\langle \boldsymbol{\xi}, \boldsymbol{x}\rangle} d\mu(\boldsymbol{x}) \tag{3.32}$$

exists uniformly in $\boldsymbol{a}$. Then the pure discrete component $\hat{\gamma}(\{\boldsymbol{\xi}\})$ of $\hat{\gamma}$ at $\boldsymbol{\xi}$ has

$$\hat{\gamma}(\{\boldsymbol{\xi}\}) = |m_{\boldsymbol{\xi}}|^2 \ . \tag{3.33}$$

The conclusion (3.33) asserts that the consistent phase property (3.9) holds at the point $\boldsymbol{\xi}$. The hypothesis (3.32) above is a uniformity condition which asserts that for each $\epsilon > 0$ there is a value T_ϵ such that for $T \geq T_\epsilon$,

$$\left| m_{\boldsymbol{\xi}} - \frac{1}{(2T)^n} \int_{[-T,T]^n+\boldsymbol{a}} e^{2\pi i\langle \boldsymbol{\xi}, \boldsymbol{x}\rangle} d\mu(\boldsymbol{x}) \right| \leq \epsilon \tag{3.34}$$

holds for all $\boldsymbol{a} \in \mathbb{R}^n$. The uniformity condition (3.32) is known to hold for all $\boldsymbol{\xi} \in \mathbb{R}^n$ for cut-and-project sets with polytope masks B, see Hof [**H95a**, pp. 248–251] for precise results. The uniformity condition (3.32) for all $\boldsymbol{\xi} \in \mathbb{R}^n$ has also been verified for special classes of self-repetitive Delone sets, see Gähler and Klitzing [**GK**, Thm. 3.1], Hof [**H95a**, p. 247], and Solomyak [**So97**, Thm. 5.1].

Hof [**H97**, p. 247] presents an example based on Allouche and Mendes-France [**AM-F**, p. 336]) showing that some type of uniformity hypothesis is necessary for the conclusion (3.33) in Theorem 3.9 to hold. This example takes

$$f_\mu := \sum_{m\in\mathbb{Z}} e^{2\pi i m^\alpha} \delta_m \tag{3.35}$$

with $\alpha = \frac{1}{2k+1}$ for some integer $k \geq 1$. It has a well-defined "Fourier coefficient" (3.29) at $\xi = 0$, namely $m_0 = 0$, but $\hat{\gamma}(\{0\}) = 1$. We also note that Theorem 3.9 does not provide any information regarding a possible continuous component of the measure $\hat{\gamma}$, either singular continuous or absolutely continuous.

To conclude this section, we observe that Theorem 3.2 provides a mechanism to define "Fourier coefficients" for a sizeable class of aperiodic Delone sets Λ. This is evidenced by the examples above, and it may also apply to a class of Λ whose associated dynamical system has suitably strong properties. Suppose that Λ is a Delone set of finite type whose associated dynamical system $([[\Lambda]], \mathbb{R}^n)$ is minimal and uniquely ergodic. It is then expected that the uniformity condition (3.32) holds for those $\boldsymbol{\xi}$ not in the discrete spectrum of the dynamical system, and for those $\boldsymbol{\xi}$ for which the dynamical system has a continuous eigenfunction. An analogous theorem for a general uniquely ergodic transformation T on a compact space (with a $\mathbb{Z}$-action) was proved by E. A. Robinson, Jr. [**Ro94**, Theorem 1]. Assuming that a version of Robinson's result is valid for $\mathbb{R}^n$-actions, we could conclude that whenever the dynamical system $([[\Lambda]], \mathbb{R}^n)$ is homogeneous, i.e. $L^2(\Omega, \mu)$ has a basis of continuous eigenfunctions, then property (3.32) will hold for all $\boldsymbol{\xi} \in \mathbb{R}^n$. Theorem 3.2 then assigns "Fourier coefficients" at *every* $\boldsymbol{\xi} \in \mathbb{R}^n$, which satisfy the consistent phase property. Homogeneous dynamical systems have pure discrete spectrum, so that these "Fourier coefficients" would account for the entire spectrum. It follows that this class of sets Λ , which includes ideal crystals, would have a satisfactory definition of "phase information".

4. Open Problems

The first set of problems concerns Patterson sets and summation formulas. Aside from ideal crystals, all known constructions of Patterson sets Λ produce a Patterson spectrum $\sigma_P(\Lambda)$ that is a dense set in $\mathbb{R}^n$. What constraints does the assumption that $\sigma_P(\Lambda)$ is a discrete set put on $\Lambda - \Lambda$ and $\sigma_P(\Lambda)$? We first formulate a version of this question purely in terms of summation formulas.

PROBLEM 4.1. (a) Suppose that γ is a positive definite translation-bounded measure in $\mathbb{R}^n$ that is supported on a Delone set Λ in $\mathbb{R}^n$, with

$$\gamma = \sum_{\boldsymbol{x} \in \Lambda} n(\boldsymbol{x}) \delta_{\boldsymbol{x}} \ , \tag{4.1}$$

and that its Fourier transform $\hat{\gamma}$ is also a discrete measure supported as a Delone set Y in $\mathbb{R}^n$

$$\hat{\gamma} = \sum_{\boldsymbol{y} \in Y} p(\boldsymbol{y}) \delta_{\boldsymbol{y}} \ . \tag{4.2}$$

Is it true that there always exists a lattice L and a finite set F such that

$$X \subseteq L + F \quad \text{and} \quad Y \subseteq L^* \tag{4.3}$$

holds?

(b) If (a) is true, does the weaker hypothesis that X and Y are both discrete sets in $\mathbb{R}^n$ still imply that (4.3) holds?

An affirmative answer to this problem would significantly strengthen the result of Cordoba given as Theorem 3.7.

Since Problem 4.1 may be hard, we propose the following weaker version that involves Delone sets of finite type.

PROBLEM 4.2. (a) Let Λ be a Delone set of finite type in $\mathbb{R}^n$ that is a Patterson set and suppose that Patterson spectrum $\sigma_P(\Lambda)$ is a Delone set. Does there exist a lattice L such that

$$\sigma_P(\Lambda) \subseteq L^* \ , \tag{4.4}$$

holds?

(b) If (a) is true, does the weaker hypothesis that $\sigma_P(\Lambda)$ is a discrete set still imply (4.4)?

Next we ask a question concerning which substitution Delone sets are Patterson sets.

PROBLEM 4.3. Suppose that Λ is a Delone set of finite type that is a primitive self-replicating Delone set. If the dynamical system $([[\Lambda]], \mathbb{R}^n)$ has some continuous spectrum does it follow that every element of $[[\Lambda]]$ is not a Patterson set?

We next consider problems related to Bohr almost periodic sets.

PROBLEM 4.4. Is a Bohr almost periodic set necessarily an ideal crystal?

This problem was discussed in §3. In a related direction, one can ask for a classification of uniformly almost periodic measures whose Fourier transform is a uniformly almost periodic function.

PROBLEM 4.5. Characterize all translation-bounded measures μ in $\mathbb{R}^n$ that are uniformly almost periodic measures and whose (distributional) Fourier transform $\hat{\mu}$ is also a uniformly almost periodic measure.

A theory of Besicovitch almost periodic sets in $\mathbb{R}^n$ has not been worked out in any detail. At this point it is not clear what is the best class $\mathcal{B}$ of almost periodic distributions to take in order to get a good class of *$\mathcal{B}$-almost periodic Delone sets*. We will assume that the class of $\mathcal{B}$-almost periodic functions used necessarily satisfies properties (1)–(3) given in §3.

PROBLEM 4.6. Define a suitable class of $\mathcal{B}$-quasicrystals with the properties:

(1) Those Patterson sets that are $\mathcal{B}$-quasicrystals, have the consistent phase property (3.9).
(2) All cut-and-project sets that are Patterson sets are $\mathcal{B}$-quasicrystals.
(3) All self-replicating Delone sets that are Patterson sets are $\mathcal{B}$-quasicrystals.

More generally, we we may ask:

PROBLEM 4.7. Are all $\mathcal{B}$-quasicrystals necessarily Patterson sets? If so, do they all have the consistent phase property (3.12)?

We also consider the relation of the "phase information" determined by a $\mathcal{B}$-quasicrystal "formal Fourier expansion" to that determined by Theorem 3.9.

PROBLEM 4.8. Suppose that μ is a translation-bounded measure on $\mathbb{R}^n$ that is a $\mathcal{B}$-almost periodic measure with "formal Fourier series"

$$\mu \sim \sum_{\boldsymbol{\xi} \in Y} c(\boldsymbol{\xi}) e^{2\pi i \langle \boldsymbol{\xi}, \boldsymbol{x} \rangle} . \tag{4.5}$$

If for a given $\boldsymbol{\xi} \in \mathbb{R}^n$ the limit

$$m_{\boldsymbol{\xi}} := \lim_{T \to \infty} \frac{1}{(2T)^d} \int_{[-T,T]^d + \boldsymbol{a}} e^{-2\pi i \langle \boldsymbol{\xi}, \boldsymbol{x} \rangle} d\mu(\boldsymbol{x}) \tag{4.6}$$

exists uniformly in $\boldsymbol{a} \in \mathbb{R}^n$, then does

$$c(\boldsymbol{\xi}) = m_{\boldsymbol{\xi}} \tag{4.7}$$

always hold?

We have noted that the information contained in the spectrum of a Patterson set Λ does not suffice to reconstruct the set Λ up to a translation. Could this be done if extra information about the set Λ was known? Recall that a Delone set of finite type Λ is *repetitive* if for each radius T there is a finite bound $M_\Lambda(T)$ such that inside any patch of X of diameter $M_X(T)$ one can find a translate of each type of T-patch of Λ.

PROBLEM 4.9. (i) Suppose that Λ is a Delone set of finite type which is repetitive, and suppose that Λ is a Patterson set. Is it true that all repetitive Delone sets of finite type with the same autocorrelation measure as Λ are contained in the translation-closure $[[\Lambda]]$?

(ii) As an important special case, suppose further that $([[\Lambda]], \mathbb{R}^n)$ is uniquely ergodic. Is it true that the repetitive Delone sets of finite type with the same autocorrelation measure as Λ are exactly the translation closure Λ?

Note that reconstructing crystal structure from "phase information" is only possible by using the extra information that an ideal crystal is a fully periodic set, and in particular, that it is repetitive. An affirmative answer to this problem would extend the reconstruction results for crystals to some aperiodic sets.

We next consider a problem relating Patterson sets and Meyer sets.

PROBLEM 4.10. Suppose that Λ is a Delone set of finite type which is a repetitive. If Λ is a Patterson set, must Λ be a Meyer set?

In case this problem is too hard, one can ask it for special subclasses of sets. The following one is of particular interest.

PROBLEM 4.11. Suppose that Λ is a primitive self-replicating Delone set. If Λ is a Patterson set, must Λ be a Meyer set?

Note that a primitive self-replicating Delone set is necessarily a Delone set of finite type that is repetitive.

To conclude, a very general problem is to characterize summation formulae generalizing the Poisson summation formula. These would involve "weighted discrete sets" whose Fourier transform is also a "weighted discrete set", in an appropriate framework of almost periodic functions. This question however extends far outside the framework of quasicrystals. The "explicit formula" of prime number theory which relates the primes to the zeros of the Riemann zeta function can be viewed as a kind of summation formula. Guinand [**Gu**] has introduced a very general notion of uniform almost periodicity for weighted discrete sequences, with respect to a given family of test functions. In this framework he is able to show, for particular weights, that the truth of the Riemann hypothesis would say that the discrete set $\{m \log p \;:\; m \geq 0, p \text{ a prime}\}$ with weights $\frac{\log p}{p^{m/2}}$ has Fourier transform supported on $\{\gamma \;:\; \zeta(\frac{1}{2} + i\gamma) = 0\}$ with associated weight $\frac{1}{2\pi}$, see [**Gu**, p. 263].

Acknowledgments. I am indebted to M. Baake, A. Hof, R. V. Moody, P. A. B. Pleasants, A. Robinson Jr. and B. Solomyak for helpful comments. I am grateful to the referees for many constructive suggestions.

Appendix A. Measures and Distributions.

This appendix gives basic facts on measures and distributions. See also the appendices in Hof [**H97**]. This approach uses a theory of measures viewed as linear functionals on a suitable space of test functions.

DEFINITION A.1. A (complex-valued)*measure* μ is a continuous linear functional on the space $\mathcal{K}(\mathbb{R}^n)$ of compactly supported continuous functions on $\mathbb{R}^n$. Here continuity means that for each compact K there is a constant a_K such that

$$|\mu(f)| \leq a_K ||f||_\infty$$

for all $f \in \mathcal{K}(\mathbb{R}^n)$ with support in K and $||.||_\infty$ is the supremum norm.

DEFINITION A.2. (i) A *positive measure* is a measure μ such that $f \in \mathcal{K}(\mathbb{R}^n)$ with $f \geq 0 \Rightarrow \mu(f) \geq 0$.

(ii) For every measure μ there is a smallest positive measure ρ such that $|\mu(f)| \leq \rho(|f|)$ for all $f \in \mathcal{K}(\mathbb{R}^n)$. This measure ρ is called the *absolute value* of μ, and is denoted $|\mu|$.

(iii) A measure is *bounded* if $|\mu|(\mathbb{R}^n)$ is finite, and is *unbounded* otherwise.

Every function $\phi(\boldsymbol{x})$ that is locally L^1 defines a measure μ_ϕ by

$$\mu_\phi(\boldsymbol{x}) = \int_{\mathbb{R}^n} f(\boldsymbol{x})\phi(\boldsymbol{x})d\boldsymbol{x} \text{ for } f \in \mathcal{K}(\mathbb{R}^n).$$

where $d\boldsymbol{x}$ is Lebesgue measure on $\mathbb{R}^n$. The convolution $\mu * \nu$ of two measures is given by

$$\mu * \nu(f) = \int_{\mathbb{R}^n \times \mathbb{R}^n} f(\boldsymbol{x}+\boldsymbol{y})d\mu(\boldsymbol{x})d\nu(\boldsymbol{y}),$$

and is well-defined if at least one of them has compact support.

A sequence of measures μ_n converges to a limit measure ν in the *vague topology* if for each test function $f \in \mathcal{K}(\mathbb{R}^n)$ the limit $\mu_n(f) \to \nu(f)$. (This is the weak-$*$ topology on the space of measures $\mathcal{M}(\mathbb{R}^n)$.)

This linear functional version of measure is related to concepts in classical measure theory via the Riesz-Markov representation theorem stated below.

DEFINITION A.3. (i) A *Borel measure* is a measure defined on the Borel sets $\mathcal{B}$ of $\mathbb{R}^n$ Such measures take values in $\mathbb{C}$, and may be unbounded.

(ii) A Borel measure is *positive* if it takes values in the nonnegative reals $\mathbb{R}_{\geq 0}$. Associated to a Borel measure μ is a measure $|\mu|$ which is the smallest positive measure such that

$$|\mu(X)| \leq |\mu|(X)$$

for all compact sets X.

DEFINITION A.3. A positive Borel measure μ is *regular* if it has the two properties:

(a) (Outer regular) For each set A in $\mathbb{R}^n$,

$$\mu(A) = \inf\{\mu(U) : \ A \ \subset \ U, \ U \text{ open } \}.$$

(b) (Inner regular) For each μ-measurable set $A \in \mathbb{R}^n$,

$$\mu(A) = \sup\{\mu(K) : \ K \subset \ A, \ K \text{ compact}\}.$$

A general Borel measure μ is *regular* if $|\mu|$ is.

If two regular Borel measures coincide on all open (resp. compact) sets, they are equal. If a positive Borel measure μ is not regular we can obtain a regularization by defining $\nu(A) = inf\{\mu(U) : A \subset U : U \text{ open}\}$.

THEOREM A.1. (*Lebesgue decomposition theorem*) *Any regular Borel measure μ on $\mathbb{R}^n$ has a unique decomposition as*

$$\mu = \mu_{pp} + \mu_{ac} + \mu_{sc} \tag{A.1}$$

where μ_{pp} is a pure point measure, μ_{ac} is absolutely continuous with respect to Lebesgue measure and μ_{sc} is singular continuous with respect to Lebesgue measure.

PROOF. See Reed and Simon [**RS**, Thm. I.14]. □

Here a *pure point measure* is a sum of weighted delta functions on a countable set X. There is no other restriction on the set X, which could be dense.

DEFINITION A.5. A Borel measure μ is a *Radon measure* if for each compact set $K \subset \mathbb{R}^n$, the measure $|\mu|(K)$ is finite.

The property that $|\mu|(K)$ is finite for all compact sets K in $\mathbb{R}^n$ implies that a Radon measure is a regular Borel measure, see Rudin [**Ru74**, Thm. 2.18] and Evans and Gariepy [**EG**, Thm. 1.1.4].

THEOREM A.2. (*Riesz-Markov representation theorem*) *There is a one to one correspondence between positive measures and positive Radon measures; for each positive measure ψ there is a unique Borel measure μ such that $\psi(f) = \int f d\mu$ for each $f \in \mathcal{K}(\mathbb{R}^n)$.*

PROOF. See Dieudonne [**Di**, Chapter XIII] or Rudin [**Ru74**, p. 42] or Reed and Simon [**RS**, Thm. IV.18]. □

To relate measures and distributions, note that *distributions* are continuous linear functionals on the space $\mathcal{D}(\mathbb{R}^n)$ of compactly supported smooth functions on $\mathbb{R}^n$, while *tempered distributions* are continuous linear functionals on the Schwartz space $\mathcal{S}$ of rapidly decreasing smooth functions on $\mathbb{R}^n$, with continuity with respect to an appropriate topology. Since $\mathcal{D}(\mathbb{R}^n) \subset \mathcal{K}(\mathbb{R}^n)$ we can associate to each measure μ a unique distribution, defined by

$$\mu(g) = \int_{\mathbb{R}^n} g(x) d\mu(\boldsymbol{x}) \text{ for } g \in \mathcal{D}(\mathbb{R}^n). \tag{A.2}$$

We identify the measure with this distribution, noting that any measure is uniquely reconstructible from its associated distribution μ. If the distribution associated to a measure is a tempered distribution, we call it a *tempered measure.* Not all measures are tempered.

To have a well-defined Fourier transform, some restriction on the class of measures is required. There is an elegant theory of the Fourier transform for tempered distributions, described in Schwartz [**Sch**] and Rudin [**Ru73**, Ch. 7]. This theory applies to tempered measures, and the following subclass of measures are suitable for modeling diffraction questions.

DEFINITION A.6. A Radon measure μ on $\mathbb{R}^n$ is *translation-bounded* if there is a constant α such that

$$|\mu|([0,1]^n + \boldsymbol{y}) \leq \alpha \quad \text{for all } \boldsymbol{y} \in \mathbb{R}^n \ .$$

Translation-bounded measures are tempered measures. For tempered measures the Fourier transform $\hat{\mu}$ is well-defined as a tempered distribution, but in general it is not a measure.

DEFINITION A.7. A tempered distribution T on $\mathbb{R}^n$ is of *positive type* if $T(\overline{\phi(-\boldsymbol{x})} * \phi(\boldsymbol{x})) \geq 0$ for all compactly supported C^∞-test functions $\phi \in \mathcal{D}(\mathbb{R}^n)$.

L. Schwartz showed that a distribution is of positive type if and only if it is the Fourier transform of a positive measure μ of at most polynomial growth, see Reed and Simon [**RS**, p. 331]. This generalizes Bochner's theorem characterizing positive definite functions, and we therefore call a measure μ that is a distribution of positive type a *positive definite measure.* Such measures satisfy

$$\int_{\mathbb{R}^n} f(\boldsymbol{x}) * \overline{f(-\boldsymbol{x})} d\mu(\boldsymbol{x}) \text{ for } f \in \mathcal{K}(\mathbb{R}^n),$$

which is the definition of positive definite measure used in [**AL**] below. Such measures are tempered measures.

THEOREM A.3. *If μ is a translation bounded positive definite measure then its Fourier transform $\hat{\mu}$ is a translation-bounded positive measure.*

PROOF. The first part follows from Proposition 3.3 of Hof [**H95a**]. Finally $\hat{\mu}$ is a positive measure by Reed and Simon [**RS**, Theorem IX.10]. See also Berg and Forst [**BF**, Prop. 1.4.4]. □

A more general subclass of measures whose Fourier transforms are measures was introduced and studied by Argabright and de Lamadrid [**AL**].

DEFINITION A.8. A measure μ is a *transformable measure* if there exists a measure $\hat{\mu}$ defined on the character space $\hat{\mathbb{R}}^n := \{\boldsymbol{\xi} : \chi_{\boldsymbol{\xi}}(\boldsymbol{x}) = e^{2\pi i \langle \boldsymbol{\xi}, \boldsymbol{x} \rangle}\}$ such that

$$\int_{\mathbb{R}^n} f * f^*(\boldsymbol{x}) d\mu(\boldsymbol{x}) = \int_{\hat{\mathbb{R}}^n} |\check{f}(\boldsymbol{\xi})|^2 d\hat{\mu}(\boldsymbol{\xi}),$$

where $f^*(\boldsymbol{x}) = \overline{f(-\boldsymbol{x})}$ and $\check{f}(\boldsymbol{\xi})$ is the inverse Fourier transform of f. The measure $\hat{\mu}$ is called the *Fourier transform* of μ,

They show that transformable measures are necessarily tempered, and that on $\mathbb{R}^n$ their notion of Fourier transform agrees with that of tempered distributions, see [**AL**, Thm. 7.2]. The Fourier transform $\hat{\mu}$ of a transformable measure is a translation-bounded measure [**AL**, Thm. 2.5]. All positive definite measures are transformable [**AL**, Thm. 4.1], and a transformable measure is positive definite if and only if $\hat{\mu}(\boldsymbol{x})$ is a positive measure. This class of measures is not symmetric under Fourier transform, i.e. if μ is transformable it need not be the case that $\hat{\mu}$ is transformable. There exist transformable measures that are not translation-bounded [**AL**, Ch. 7].

Appendix B. Almost Periodic Functions and Almost Periodic Measures. This appendix describes various notions of almost periodic functions on $\mathbb{R}^n$ and uses them to define various notions of almost periodic measure μ. To such a measure μ one can associate a "formal Fourier series"

$$\mu \sim \sum_{\boldsymbol{\xi} \in \sigma(\mu)} c(\boldsymbol{\xi}) e^{2\pi i \langle \boldsymbol{\xi}, \boldsymbol{x} \rangle} ,$$

in which $\sigma(\mu)$ is a countable set of frequencies is a spectrum of μ. In such a case the tempered distribution $\hat{\mu}$ will have a "formal δ-function expansion"

$$\hat{\mu} \sim \sum_{\boldsymbol{\xi} \in \sigma(\mu)} c(\boldsymbol{\xi}) \delta_{\boldsymbol{\xi}} .$$

We first describe the theory of uniformly almost periodic functions as given in Bohr [**Bo1**].

DEFINITION B.1. A continuous function $f \in L^{\infty}(\mathbb{R}^n)$ is *uniformly almost periodic* (in the sense of Bohr) if for each $\epsilon > 0$ there exists a relatively dense set $\Lambda_{\epsilon}(f)$ of ϵ-almost periods of f. Here an *ϵ-almost period* is a value τ such that

$$\sup_{x \in \mathbb{R}^n} |f(\boldsymbol{x} + \boldsymbol{\tau}) - f(\boldsymbol{x})| \le \epsilon . \tag{B.1}$$

Let $AP(\mathbb{R}^n)$ denote the set of uniformly almost periodic functions on $\mathbb{R}^n$. It is closed under uniform limits: If $\{f_j\} \subseteq AP(\mathbb{R}^n)$ have $||f - f_j||_{\infty} \to 0$, then $f \in AP(\mathbb{R}^n)$. It is well-known that a function $f \in AP(\mathbb{R}^n)$ if and only if for each $\epsilon > 0$ there exists a finite trigonometric sum

$$P_{\epsilon}(\boldsymbol{x}) = \sum_{\boldsymbol{\lambda} \in F_{\epsilon}} c(\lambda, \epsilon) e^{2\pi i \langle \boldsymbol{\lambda}, \boldsymbol{x} \rangle}$$

such that $||f - P_{\epsilon}||_{\infty} \le \epsilon$.

There is a notion of *Fourier series* and a *Parseval relation* valid for uniformly almost periodic functions. For any almost periodic function f, for $\boldsymbol{x} \in \mathbb{R}^n$ the limit

$$\mathcal{M}(f) := \lim_{R\to\infty} \frac{1}{R^n} \int_{C(\boldsymbol{x},R)} f(\boldsymbol{y}) d\boldsymbol{y} \tag{B.2}$$

exists, where $C(\boldsymbol{x}, R) = R[0,1]^n + \boldsymbol{x}$. This limit is independent of $\boldsymbol{x}$, and is attained uniformly in $\boldsymbol{x}$ as $R \to \infty$. The function $e^{-2\pi i\langle \boldsymbol{\xi}, \boldsymbol{x}\rangle} f(\boldsymbol{x})$ is also uniformly almost periodic, and for $\boldsymbol{\xi} \in \mathbb{R}^n$ we define the Fourier coefficient $\gamma(\boldsymbol{\xi})$ of $f(\boldsymbol{x})$ by

$$\gamma(\boldsymbol{\xi}) := \mathcal{M}(e^{-2\pi i\langle \boldsymbol{\xi}, \boldsymbol{x}\rangle} f(\boldsymbol{x})) \ . \tag{B.3}$$

DEFINITION B.2. For a uniformly almost periodic function the set

$$\sigma_U(f) := \{\boldsymbol{\xi} : \gamma(\boldsymbol{\xi}) \neq 0\} \tag{B.4}$$

is called the *uap spectrum of f* or Bohr spectrum of f. (Note that Bohr's [**Bo1**] definition of the spectrum differs slightly, being $2\pi\sigma_U(f)$.)

THEOREM B.1. *If f is uniformly almost periodic on $\mathbb{R}^n$, then so is $|f|^2$ and*

$$\mathcal{M}(|f|^2) = \sum_{\boldsymbol{\xi} \in \sigma_U(f)} |\gamma(\xi)|^2 \ . \tag{B.5}$$

This theorem implies that $\sigma_U(f)$ is at most a countable set. Thus f has a formal "Fourier expansion."

$$f(\boldsymbol{x}) \approx \sum_{\xi \in \sigma_U(f)} \gamma(\boldsymbol{\xi}) e^{2\pi i\langle \boldsymbol{\xi}, \boldsymbol{x}\rangle} \ , \tag{B.6}$$

in the sense of mean values (Bohr [**Bo1**, p. 47]) and (B.5) can be viewed as a Parseval-type relation. Any Fourier expansion of an almost-periodic function satisfies

$$\sum_{\boldsymbol{\xi} \in S} |\gamma(\boldsymbol{\xi})|^2 < \infty \tag{B.7}$$

where $S = \sigma_U(f)$. However not all countable sets S and sequences (B.7) are "Fourier expansions" of some uniformly almost periodic functions. For any countable set S and any coefficient set $\{\gamma(\boldsymbol{\xi}) : \boldsymbol{\xi} \in S\}$ the condition

$$\sum_{\boldsymbol{\xi} \in S} |\gamma(\boldsymbol{\xi})| < \infty$$

is sufficient for there to exist a (unique) almost-periodic function f with "Fourier expansion" (B.6).

The Fourier expansion of a uniformly almost periodic function f uniquely determines f.

THEOREM B.2. *If f_1 and f_2 are uniformly almost periodic functions on $\mathbb{R}^n$ and if*

$$\mathcal{M}(e^{-2\pi i\langle \boldsymbol{\xi}, \boldsymbol{x}\rangle} f_1(\boldsymbol{x})) = \mathcal{M}(e^{-2\pi i\langle \boldsymbol{\xi}, \boldsymbol{x}\rangle} f_2(\boldsymbol{x}))$$

for all $\boldsymbol{\xi} \in \mathbb{R}^n$, then $f_1 \equiv f_2$.

The "Fourier expansion" (B.6) of a uniformly almost periodic function f can be used to reconstruct f using a Cesaro-like summation procedure.

THEOREM B.3. *Given any countable set S, there exists a family of* weight functions $\{\beta_{S,\epsilon}(\boldsymbol{\xi})\}$ *depending on: the parameter $\epsilon > 0$, such that:*

(1) $0 \le \beta_{S,\epsilon}(\xi) \le 1$,
(2) $\lim_{\epsilon \downarrow 0} \beta_{S,\epsilon}(\xi) = 1$ *if* $\boldsymbol{\xi} \in S$,
(3) *For each ϵ there is a finite set $F_S(\epsilon)$ such that $\beta_{S,\epsilon}(\boldsymbol{\xi}) = 0$ if $\boldsymbol{\xi} \notin F_S(\epsilon)$.*
(4) *For every uniformly almost periodic function with spectrum contained in S, if*

$$P_{f,\epsilon}(x) := \sum_{\boldsymbol{\xi} \in S} \beta_{S,\epsilon}(\boldsymbol{\xi}) \gamma(\boldsymbol{\xi}) e^{2\pi i \langle \boldsymbol{\xi}, \boldsymbol{x} \rangle}$$

then $||f - P_{f,\epsilon}||_\infty \to 0$ *as* $\epsilon \to 0$.

The notion of almost periodic function was extended to measures by Schwartz [**Sch**, Sect. VI.9].

DEFINITION B.3. An (unbounded) Radon measure μ is a *uniformly almost periodic measure* if for each compactly supported C^∞-function g on $\mathbb{R}^n$ ($g \in \mathcal{D}(\mathbb{R}^n)$) the convolution

$$g * \mu(\boldsymbol{x}) = \int_{\mathbb{R}^n} g(\boldsymbol{x} - \boldsymbol{y}) d\mu(\boldsymbol{y}) \tag{B.8}$$

is a uniformly almost-periodic function.

We assign to a uniformly almost periodic measure μ the "formal Fourier expansion"

$$\mu \sim \sum_{\boldsymbol{\xi} \in \sigma_U(\mu)} c(\boldsymbol{\xi}) e^{2\pi i \langle \boldsymbol{\xi}, \boldsymbol{x} \rangle} , \tag{B.9}$$

in which the "Fourier coefficient" $c(\boldsymbol{\xi})$ is defined by observing that for each $g \in C_c^\infty(\mathbb{R}^n)$ the uniformly almost periodic function $\mu * g$ has the Fourier expansion

$$\mu * g \approx \sum_{\boldsymbol{\xi} \in \sigma_U(\mu * g)} c(\boldsymbol{\xi}) \hat{g}(-\boldsymbol{\xi}) e^{2\pi i \langle \boldsymbol{\xi}, \boldsymbol{x} \rangle} , \tag{B.10}$$

and $c(\boldsymbol{\xi})$ is determined using any $g(x)$ such that $\hat{g}(-\boldsymbol{\xi}) \neq 0$, and is well-defined. Here we set

$$\sigma_U(\mu) := \bigcup_{g \in C_c^\infty} \sigma_U(\mu * g) , \tag{B.11}$$

and $\sigma_U(\mu)$ can be proved to be a countable set.

Thus one may think of an uniformly almost periodic measure μ as having a fixed countable spectrum $\sigma_U(\mu)$, which contains the spectra of all $\mu * g$, and the formula (B.10) giving the "Fourier coefficients" of $\mu * g$ as a "weak summation formula."

The closed graph theorem implies that any uniformly almost periodic measure has

$$\sup_{\boldsymbol{x} \in \mathbb{R}^n} \int_{C(\boldsymbol{x}, R)} |d\mu| = C(R) < \infty , \tag{B.12}$$

where $C(\boldsymbol{x}, R) = \boldsymbol{x} + R[0,1]^n$ is a scaled unit cube. Thus any almost periodic measure is necessarily *translation-bounded.* This in turn implies that the convolution

$\mu * g$ makes sense for any function $g \in \mathcal{S}(\mathbb{R}^n)$, the Schwartz space of rapidly-decreasing C^∞-functions. The tempered distribution $\hat{\mu}$ can be viewed as having a "formal δ-function expansion"

$$\hat{\mu} \sim \sum_{\boldsymbol{\xi} \in \sigma_U(\mu)} c(\boldsymbol{\xi}) \delta_{\boldsymbol{\xi}} \tag{B.13}$$

given the term-by-term Fourier transform of the right side of (B.12).

For any full-rank lattice $L \in \mathbb{R}^n$, the measure

$$\mu_L(\boldsymbol{x}) := \sum_{\boldsymbol{\lambda} \in L} \delta_{\boldsymbol{\lambda}} \ . \tag{B.14}$$

is an almost-periodic measure. For any compactly supported continuous function $f(\boldsymbol{x})$, the function

$$\mu_L * f(\boldsymbol{y}) = \sum_{\boldsymbol{\lambda} \in L} f(\boldsymbol{y} - \boldsymbol{\lambda}) \ , \tag{B.15}$$

is periodic with period lattice L, hence is uniformly almost-periodic.

The "Fourier expansion" of the almost periodic measure μ_L for a lattice L is related to the Poisson summation formula. This states (Theorem 2.6) that the (distributional) Fourier transform of μ_L is

$$\hat{\mu}_L = \frac{1}{|det(L)|} \sum_{\boldsymbol{\xi} \in L^*} \delta(\boldsymbol{\xi}) \ , \tag{B.16}$$

where L^* is the dual lattice

$$L^* = \{\boldsymbol{\xi} \in \mathbb{R}^n : \langle \boldsymbol{\lambda}, \boldsymbol{\xi} \rangle \in \mathbb{Z} \text{ for all } \boldsymbol{\lambda} \in L\} \ . \tag{B.17}$$

However, taking the Fourier transform of (B.16) formally, term-by-term, gives

$$\mu_L(\boldsymbol{x}) \sim \frac{1}{|det(L)|} \sum_{\boldsymbol{\xi} \in L^*} \exp(2\pi i \langle \boldsymbol{\xi}, \boldsymbol{x} \rangle) \ . \tag{B.18}$$

This indicates that the spectrum $\sigma_U(\mu_L * f)$ of the periodic function $\mu_L * f$ is contained in L^*.

The space of uniformly almost periodic measures is not large enough to include measures μ_Λ associated to all regular cut-and-project sets. We can obtain a sufficiently large class of measures by relaxing the notion of almost periodic function used to define almost periodic measures. It was observed by Besicovitch and Bohr [**BeBo**] that various notions of almost periodicity are obtained by changing the topology of convergence used for approximation by finite trigonometric polynomials. In this way one can define the almost periodic functions of Stepanov, Wiener and others, see Besicovitch [**Be**]. We would like a class of almost periodic functions wide enough to permit as valid Fourier series expansions all expressions

$$\sum_{\boldsymbol{\xi} \in S} c(\boldsymbol{\xi}) e^{2\pi i \langle \boldsymbol{\xi}, \boldsymbol{x} \rangle} \tag{B.19}$$

for any countable set S and any square-summable sequence

$$\sum_{\boldsymbol{\xi} \in S} |c(\boldsymbol{\xi})|^2 < \infty \ , \tag{B.20}$$

and which satisfy a Parseval identity. The class $B^2(\mathbb{R})$ of Besicovitch almost periodic functions on $\mathbb{R}$ satisfy these conditions.

DEFINITION B.4. The *Besicovitch B^2-distance* between two functions $f, g \in L^2(\mathbb{R})$ is

$$D_{B^2}[f,g] = \left(\limsup_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} |f(x) - g(x)|^2 dx \right)^{1/2} . \tag{B.21}$$

The class $B^2(\mathbb{R})$ of *Besicovitch almost periodic functions* consists of all functions $f \in L^2(\mathbb{R})$ such that there is a sequence of trigonometric polynomials $\{f_n\}$ with

$$D_{B^2}[f, f_n] \to 0 \quad \text{as} \quad n \to \infty . \tag{B.22}$$

Besicovitch's original definition of B^2-almost periodic functions incorporated a notion of ϵ-almost period which is parallel to definition (B.1) of uniformly almost periodic functions. Call a set P of real numbers *satisfactorily uniform* if there exists a number l such that the ratio of the maximum number of terms of P to the minimum number of terms in P in an interval of length l is less than 2. A function in $L^2(\mathbb{R})$ is B^2-almost periodic if for each $\epsilon > 0$ there exists a satisfactorily uniform set

$$P_\epsilon = \{\tau_i : \cdots < \tau_{-1} < \tau_0 < \tau_1 < \tau_2 < \cdots\}$$

such that for each $i \in \mathbb{Z}$,

$$D_{B_2}[f, f_{\tau_i}] < \epsilon ,$$

where f_{τ_i} is the translated function $f(\cdot - \tau_i)$, and for every positive $c > 0$,

$$\limsup_{x\to\infty} \left(\limsup_{i\to\infty} \frac{1}{c} \int_{x}^{x+c} |f(x+\tau_i) - f(x)|^2 dx \right) < \epsilon^2 .$$

This equivalence of this definition to the earlier one is given in Besicovitch [**Be**, p. 78 and p. 100].

We can associate to B^2-almost periodic function on the line a B^2-Fourier series

$$f \sim_{B^2} \sum_{\xi \in \sigma_B(f)} c(\xi) e^{2\pi i \xi x} \tag{B.23}$$

which is supported on a countable set $\sigma_B(f)$ which we call the *Besicovitch spectrum* of f, cf. [**Be**, p. 104]. To do this we a mean value $\mathcal{M}(f)$ of a B^2-polynomial. Take a series of trigonometric polynomials

$$s_n(x) = \sum_{\xi \in F_n} c(\xi) e^{2\pi i \xi x} \tag{B.24}$$

where F_n is a finite set, with $D_{B_2}[s_n(x) - f(x)] \to 0$. Each $s_n(x)$ has a mean value, and these have a limiting mean value, so we can define

$$\mathcal{M}(f) := \lim_{n\to\infty} \mathcal{M}(s_n(x)) . \tag{B.25}$$

Now $\{e^{2\pi i \xi x} s_n(x)\}_{n\to\infty}$ converges to $e^{2\pi i \xi x} f(x)$ in the B^2-sense, and we define

$$c(\xi) \sim_{B^2} \mathcal{M}(f e^{-2\pi i \xi x}) . \tag{B.26}$$

THEOREM B.4. *If* $f \in B^2(\mathbb{R})$ *then* f *has a* B^2*-Fourier series supported on a countable set* $\sigma_B(f)$*,*

$$f \sim_{B^2} \sum_{\xi \in \sigma_B(f)} c(\xi) e^{2\pi i \xi x} \ . \tag{B.27}$$

Also f *satisfies the Parseval identity*

$$\|f\|^2 = D_{B_2}[f, 0] = \sum_{\xi \in \sigma_B(f)} |c(\xi)|^2 \ . \tag{B.28}$$

PROOF. See Besicovitch [**Be**, p. 109]. □

THEOREM B.5. *If* S *is any countable set and* $\{c(\xi) : \xi \in S\}$ *is a square-summable sequence in* $\mathbb{R}$*, so that*

$$\sum_{\xi \in S} |c(\xi)|^2 < \infty \ ,$$

then there exists $f \in B^2(\mathbb{R})$ *which has* B^2*-Fourier series*

$$f \sim \sum_{\xi \in S} c(\xi) e^{2\pi i \xi x} \ . \tag{B.29}$$

PROOF. See Besicovitch [**Be**, p. 110]. □

Finally, the uniqueness theorem for B^2-Fourier series is as follows.

THEOREM B.6. *The functions* $f, g \in B^2(\mathbb{R})$ *have the same* B_2*- Fourier series, if and only if*

$$D_{B^2}[f, g] = 0 \ . \tag{B.30}$$

PROOF. See Besicovitch [**Be**, p. 109]. □

One can find two functions f, $g \in B^2(\mathbb{R})$ which differ on a set of infinite Lebesgue measure and which have $D_{B^2}(f, g) = 0$, so that they have the same B^2-Fourier series. This ambiguity is similar to the ambiguity one encounters in the definition of the diffraction measure presented in §2, where the diffraction measure remains unaffected by "small" changes, cf. (2.9). However the Fourier coefficients of a B^2-almost periodic function f do contain "phase information" in the sense that the translated function $f_t(\boldsymbol{x}) = f(\boldsymbol{x} - t)$ has the same spectrum $\sigma_B(f_t) = \sigma_B(f)$ and its Fourier coefficients are

$$c_t(\boldsymbol{\xi}) = c(\boldsymbol{\xi}) e^{2\pi i t \xi} \ . \tag{B.31}$$

We define B^2-almost periodic measures in exactly the same way as was done for uniformly almost periodic measures.

DEFINITION B.5. An unbounded Radon measure μ is a *Besicovitch almost periodic measure* or *B^2-almost periodic measure* if for each compactly supported C^∞-function g on $\mathbb{R}$ the convolution $\mu * g(\boldsymbol{y})$ is a B^2-almost periodic function.

One can now define a B^2-Fourier series and a B^2-almost periodic spectrum $\sigma_B(\mu)$ for a B^2-almost periodic measure, or distribution. Hof [**H97**, p. 257] indicates that certain one-dimensional cut-and-project sets Λ give B^2-almost periodic measures μ_Λ in this sense.

Besicovitch developed the theory of B^2-almost periodic functions on the real line $\mathbb{R}$, and apparently did not extend it to $\mathbb{R}^n$. In the 1950's Følner [**Fø**] developed an analogue of the Besicovitch theory which is valid on arbitrary infinite groups G, and in particular $\mathbb{R}^n$. He proves analogues of the Theorems B.4.–B.6. for his almost periodic functions. However, he notes that his function space does not agree with Besicovitch's class $B^2(\mathbb{R})$ on $\mathbb{R}$. Later Davis [**Da68**] gave an extension of B^p-almost periodic functions valid on an arbitrary locally compact Abelian group. His definition does extend Besicovitch's to $\mathbb{R}^n$ (choosing a suitable "complete homogeneous Bohr net" on $\mathbb{R}^n$). His functions have well-defined Fourier series with a countable spectrum, and he gives a sense in which the Fourier series recovers the function, cf. [**Da68**, Thm. 3.1]. However he does not work out the case of B^2-almost periodic functions in any detail.

The most interesting special case for this paper is that where the Besicovitch almost-periodic distribution f has a Fourier transform $\hat{f}$ that is itself a Besicovitch almost-periodic distribution. In this case both f and $\hat{f}$ have spectra — in the B^2-almost-periodic sense — that is supported in a countable set. Can one characterize such pairs of distributions? Is there some analogue of a "summation formula" associated to such a pair of distributions?

References

[AM-F] J. P. Allouche and M. Mendes-France, *Automata and automatic sequences*, in: *Beyond Quasicrystals*, eds. F. Axel and D. Gratias, Springer, Berlin (1995), pp. 293–367.

[AL] L. Argabright and J. G. de Lamadrid, *Fourier Analysis of Unbounded Measures on Locally Compact Abelian Groups*, Memoirs of the AMS, vol. 145, Amer. Math. Soc., Providence, RI (1974).

[AuM] L. Auslander and Y. Meyer, *A generalized Poisson summation formula*, Appl. Comp. Harmonic Anal. **3** (1996), 372–376.

[Az] L. D. Azároff, *Elements of X-ray Crystallography*, McGraw-Hill, New York (1968).

[Ba] M. Baake, *A guide to mathematical quasicrystals*, in: *Quasicrystals*, eds. J.-B. Suck, M. Schreiber and P. Häussler, Springer, Berlin (2000), in press; math-ph/9904014.

[BH] M. Baake and M. Höffe, *Diffraction of random tilings: some rigorous results*, J. Stat. Phys. **99** (2000), 216–261; math-ph/9904005.

[BMP] M. Baake, R. V. Moody and P. A. B. Pleasants, *Diffraction from visible lattice points and k-th power free integers*, Discr. Math., **221** (2000), 3–42; math.MG/9906132.

[BMS] M. Baake, R. V. Moody and M. Schlottmann, *Limit-(quasi)periodic point sets as quasicrystals with p-adic internal spaces*, J. Phys. **A 31** (1998), 5755–5765.

[BF] C. Berg and G. Forst, *Potential Theory in Locally Compact Abelian Groups*, Springer-Verlag, New York 1975.

[Be] A. S. Besicovitch, *Almost Periodic Functions*, Cambridge Univ. Press., Cambridge (1932); reprint: Dover, New York (1954).

[BeBo] A. S. Besicovitch and H. Bohr, *Almost periodicity and general trigonometric series*, Acta Math. **57** (1931), 203–292; reprinted in [**Bo2**].

[Boc] S. Bochner, *A generalization of Poisson's summation formula*, Duke Math. J. **6** (1940), 229–234.

[BocNe] S. Bochner and J. von Neumann, *Almost periodic functions in groups II*, Trans. Amer. Math. Soc. **37** (1935), 21–50.

[Bo1] H. Bohr, *Fastperiodische Funktionen*, Springer, Berlin (1932); reprinted in [**Bo2**]; English edition: *Almost Periodic Functions*, Chelsea, New York (1947).

[Bo2] H. Bohr, *Collected Mathematical Works, Vol. II: Almost Periodic Functions*, eds. E. Følner and B. Jessen, Dansk Matematisk Forening, Copenhagen (1952).

[BT86] E. Bombieri and J. Taylor, *Which distributions of matter diffract? An initial investigation*, J. Phys. Colloq. C3 **47** (1986), 19–28.

[BT87] E. Bombieri and J. E. Taylor, *Quasicrystals, tilings and algebraic number theory: some preliminary connections*, in: *The Legacy of Sonya Kovalevskaya*, ed. L. Keen, Contemporary Math., vol. 64, Amer. Math. Soc., Providence, RI (1987), pp. 241–264.

[dB81] N. G. de Bruijn, *Algebraic theory of Penrose's nonperiodic tiling of the plane I & II*, Nederl. Akad. Wetensch. Proc. Ser. **A 84** (1981), 39–52 and 53–66.

[dB86] N. G. de Bruijn, *Quasicrystals and their Fourier transform*, Nederl. Akad. Wetensch. Proc. Ser. **A 89** (1986), 123–152.

[dB87] N. G. de Bruijn, *Modulated quasicrystals*, Nederl. Akad. Wetensch. Proc. Ser. **A 90** (1987), 121–132.

[BR] H. Burkhill and B. C. Rennie, *Almost periodic generalized functions*, Math. Proc. Camb. Phil. Soc. **94** (1983), 149–166.

[CT] J. W. Cahn and J. E. Taylor, *An introduction to quasicrystals*, in: *The Legacy of Sonya Kovalevskaya*, ed. L. Keen, Contemp. Math., Vol. 64, Amer. Math. Soc., Providence, RI (1987), pp. 287–297.

[Co88] A. Cordoba, *La formule sommatoire de Poisson*, C. R. Acad. Sci. Paris **306**, Serie I (1988), 373–376.

[Co89] A. Cordoba, *Dirac combs*, Lett. Math. Phys. **17** (1989), 191–196.

[Cow] J. M. Cowley, *Diffraction Physics*, 3rd ed., North-Holland, Amsterdam (1995).

[Da68] H. W. Davis, *On completing the von Neumann almost periodic functions*, Duke Math. J. **35** (1968), 199–215.

[Da74] H. W. Davis, *Generalized almost periodicity in groups*, Trans. Amer. Math. Soc. **191** (1974), 329–352.

[D] B. N. Delone, *Neue Darstellung der geometrischen Kristallographie*, Z. Kristallographie **84** (1932), 109–149.

[DDSG] B. N. Delone, N. P. Dolbilin, M. I. Štogrin and R. V. Galiulin, *A local criterion for regularity in a system of points*, Sov. Math. Dokl. **17** (1976), 319–322.

[Di] J. Dieudonné, *Treatise of Analysis,* Volume II, Academic Press, New York (1970).

[DuKa] M. Duneau and A. Katz, *Quasiperiodic structures*, Phys. Rev. Lett. **54** (1985), 2688–2691.

[DEK] A. L. Duran, R. Estrada and R. P. Kanwal, *Extensions of the Poisson summation formula*, J. Math. Anal. Appl. **218** (1998), 581–606.

[Dw] S. Dworkin, *Spectral theory and X-ray diffraction*, J. Math. Phys. **34** (1993), 2965–2967.

[Eij] S. J. L. van Eijndhoven, *Functional analytic characterizations of the Gelfand-Shilov spaces* S_α^β, Indag. Math. **49** (1987), 133–144.

[Els] V. Elser, *The diffraction pattern of projected structures*, Acta. Cryst. **A 42** (1986), 36–43.

[EG] L. C. Evans and R. F. Gariepy, *Measure Theory and Fine Properties of Functions*, CRC Press, Boca Raton, FL (1992).

[Fø] E. Følner, *Besicovitch almost periodic functions in arbitrary groups*, Math. Scand. **5** (1957), 47–53.

[GK] F. Gähler and R. Klitzing, *The diffraction pattern of self-similar tilings*, in: *The Mathematics of Long-Range Aperiodic Order*, ed. R. V. Moody, NATO ASI Series C 489, Kluwer, Dordrecht (1997), pp. 141–174.

[Go] C. Godrèche, *The sphinx: a limit periodic tiling of the plane*, J. Phys. **A 22** (1989), L1163–L1168.

[Gr] K. H. Gröchenig, *An uncertainty principle related to the Poisson summation formula*, Studia Math. **121** (1996), 97–104.

[GHR] K. Gröchenig, A. Haas and A. Raugi, *Self-affine tilings with several tiles I*, Appl. Comp. Harm. Anal. 7 (1999), 211–238.

[Gu] A. P. Guinand, *Concordance and the Harmonic Analysis of Sequences*, Acta Math. **101** (1959), 235–271.

[H92] A. Hof, *Quasicrystals, Aperiodicity and Lattice Systems*, PhD-thesis, Univ. Groningen (1992).

[H95a] A. Hof, *On diffraction by aperiodic structures*, Commun. Math. Phys. **169** (1995), 25–43.

[H95b] A. Hof, *Diffraction by aperiodic structures at high temperatures*, J. Phys. **A 28** (1995), 57–62.

[H97] A. Hof, *Diffraction by aperiodic structures*, in: *The Mathematics of Long-Range Aperiodic Order*, ed. R. V. Moody, NATO ASI Series C 489, Kluwer, Dordrecht (1997), pp. 239–268.

[Jan] C. Janot, *Quasicrystals: A Primer*, 2nd ed., Clarendon Press, Oxford (1994).

[KLR] J.-P. Kahane and P.-G. Lemarié-Rieusset, *Remarques sur la formule sommatoire de Poisson*, Studia Math. **109** (1994), 303–316.

[K67] Y. Katznelson, *Une remarque concernant la formule de Poisson*, Studia Math. **29** (1967), 107–108.

[K68] Y. Katznelson, *An Introduction to Harmonic Analysis*, 2nd ed., Wiley, New York (1968); reprint: Dover, New York (1974).

[Ke90] R. Kenyon, *Self-Similar Tilings*, PhD-thesis, Princeton (1990).

[Ke92] R. Kenyon, *Self-replicating tilings*, in: *Symbolic Dynamics and Its Applications*, ed. P. Walters, Contemp. Math., Vol. 135, Amer. Math. Soc, Providence, RI (1992), pp. 239–264.

[Ke94] R. Kenyon, *Inflationary tilings with self-similar structure*, Comm. Math. Helv. **69** (1994), 169–198.

[Ke96] R. Kenyon, *The construction of self-similar tilings*, Geom. Funct. Anal. **6** (1996), 471–488.

[La95] J. C. Lagarias, *Meyer's concept of quasicrystal and quasiregular sets*, Commun. Math. Phys. **179** (1996), 365–376.

[La99a] J. C. Lagarias, *Geometric models for quasicrystals I. Delone sets of finite type*, Discr. Comput. Geom. **21** (1999), 161–191.

[La99b] J. C. Lagarias, *Geometric models for quasicrystals II. Local rules under isometries*, Discr. Comput. Geom. **21** (1999), 345–372.

[LaWa1] J. C. Lagarias and Y. Wang, *Self-affine tiles in* $\mathbb{R}^n$, Adv. Math. **121** (1996), 21–49.

[LaWa2] J. C. Lagarias and Y. Wang, *Integral self-affine tiles in* $\mathbb{R}^n$ *I. Standard and nonstandard digit sets*, J. London Math. Soc. **54** (1996), 161–179.

[LaWa3] J. C. Lagarias and Y. Wang, *Substitution Delone sets*, Discr. Comput. Geom., to appear; math.MG/0110222.

[LPS] T. Q. T. Le, S. A. Piunikhin and V. A. Sadov, *The geometry of quasicrystals*, Russian Math. Surveys **48** (1993), 37–100.

[LM] J.-Y. Lee and R. V. Moody, *Lattice substitution systems and model sets*, Discr. Comput. Geom. **25** (2001), 173–201; math.MG/0002019.

[LSt] D. Levine and P. J. Steinhardt, *Quasicrystals: a new class of ordered structures*, Phys. Rev. Lett. **53** (1984), 2477–2480.

[LuP] W. F. Lunnon and P. A. B. Pleasants, *Quasicrystallographic tilings*, J. Math. Pures Appl. **66** (1987), 217–263.

[Me72] Y. Meyer, *Algebraic Numbers and Harmonic Analysis*, North-Holland, Amsterdam (1972).

[Me95] Y. Meyer, *Quasicrystals, Diophantine approximation and algebraic numbers*, in: *Beyond Quasicrystals*, eds. F. Axel and D. Gratias, Springer, Berlin (1995), pp. 3–16.

[Mo95] R. V. Moody, *Meyer Sets and the Finite Generation of Quasicrystals*, in: *Symmetries in Science VIII*, ed. B. Gruber, Plenum, New York (1995), pp. 379–394.

[Mo97] R. V. Moody, *Meyer sets and their duals*, in: *The Mathematics of Long Range Aperiodic Order* ed. R. V. Moody, NATO ASI Series C 489, Kluwer, Dordrecht (1997), pp. 403–442.

[Mo99] R. V. Moody, *Model sets: a survey*, in: *Order, Chance, and Risk*, eds. F. Axel and J.-P. Gazeau, Springer, New York (2000); math.MG/0002020.

[Q] M. Queffélec, *Substitution Dynamical Systems — Spectral Analysis*, Lecture Notes in Mathematics, vol. 1294, Springer, Berlin (1987).

[RS] M. Reed and B. Simon, *Functional Analysis*, 2nd ed., Academic Press, New York (1980).
[Ren] B. C. Rennie, *On generalized functions*, J. Appl. Prob. **19 A** (1982), 139–156.
[Ro94] E. A. Robinson, Jr., On uniform convergence in the Wiener-Wintner theorem, J. London Math. Soc. **49** (1994), 493–501.
[Ro96a] E. A. Robinson, Jr., *The dynamical properties of Penrose tilings*, Trans. Amer. Math. Soc. **348** (1996), 4447–4464.
[Ro96b] E. A. Robinson, Jr., *The dynamical theory of tilings and quasicrystallography*, in: *Ergodic Theory of $\mathbb{Z}^d$-actions*, eds. M. Pollicott and K. Schmidt, London Math. Soc. Lecture Notes, vol. 228, Cambridge University Press, Cambridge (1996), pp. 451–473.
[Ru73] W. Rudin, *Functional Analysis*, 2nd ed., McGraw-Hill, New York (1991).
[Ru74] W. Rudin, *Real and Complex Analysis*, 3rd ed., McGraw-Hill, New York (1987).
[S98] M. Schlottmann, *Cut-and-project sets in locally compact Abelian groups*, in: *Quasicrystals and Discrete Geometry*, ed. J. Patera, Fields Institute Monographs, vol. 10, Amer. Math. Soc., Providence, RI (1998), pp. 247–264.
[S99] M. Schlottmann, *Generalized model sets and dynamical systems*, in: *Directions in Mathematical Quasicrystals*, eds. M. Baake and R. V. Moody, CRM Monograph Series, Amer. Math. Soc., Providence, RI (2000), this volume.
[Sch] L. Schwartz, *Theorie des Distributions*, 3rd ed., Hermann, Paris (1998).
[Sen] M. Senechal, *Quasicrystals and Geometry*, Cambridge University Press, Cambridge (1995); corr. reprint (1996).
[SBGC] D. Shechtman, I. Blech, D. Gratias and J. W. Cahn, *Metallic phase with long-range orientational order and no translational symmetry*, Phys. Rev. Lett. **53** (1984), 1951–1953.
[So97] B. Solomyak, *Dynamics of self-similar tilings*, Ergod. Th. & Dyn. Syst. **17** (1997), 695–738.
[So98a] B. Solomyak, *Non-periodicity implies unique composition for self-similar translationally finite tilings*, Discr. Comput. Geom. **20** (1998), 265–279.
[So98b] B. Solomyak, *Spectrum of dynamical systems arising from Delone sets*, in: *Quasicrystals and Discrete Geometry*, ed. J. Patera, Fields Institute Monographs, vol. 10, Amer. Math. Soc., Providence, RI (1998), pp. 265–275.
[Vin1] A. Vince, *Replicating tesselations*, SIAM J. Discr. Math. **6** (1993), 501–521.
[Vin2] A. Vince, *Digit tiling of Euclidean space*, in: *Directions in Mathematical Quasicrystals*, eds. M. Baake and R. V. Moody, CRM Monograph Series, Amer. Math. Soc. Providence, RI (2000), 329–369.

AT&T Labs–Research, Florham Park, NJ 07932-0971, USA
E-mail address: jcl@research.att.com