



Positive Definite Measures with Discrete Fourier Transform and Pure Point Diffraction

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Abstract. In this paper we characterize the positive definite measures with discrete Fourier transform. As an application we provide a characterization of pure point diffraction in locally compact Abelian groups.

1 Introduction

Physical quasicrystals were discovered in 1984 by Shechtman, Blech, Gratias, and Cahn and independently in 1985 by Ishimasa, Nissen, and Fukano. They are aperiodic solids having an essentially discrete diffraction diagram.

The mathematical framework for diffraction was set in the 1990's by Hof [9]. Given a point set Λ , which represents the positions of the atoms in a solid, its autocorrelation measure γ (see below for a precise definition) is a positive and positive definite measure. The Fourier transform $\widehat{\gamma}$ of γ is called the diffraction pattern of Λ . If $\widehat{\gamma}$ is a discrete measure, we say that Λ is pure point diffractive. The key to understanding the structure of quasicrystals is the understanding of pure point diffraction.

Gil de Lamadrid and Argabright [10] showed that discreteness of $\widehat{\gamma}$ is equivalent to the strong almost periodicity of γ , and this holds in the setting of arbitrary locally compact Abelian groups. As a consequence we get that pure point diffraction is equivalent to the strong almost periodicity of the corresponding autocorrelation measure. However, this type of almost periodicity is generally hard to check, and one would like to relax this condition. For weighted Dirac combs with Meyer support, and in particular for point sets verifying the Meyer condition, Baake and Moody [3] proved that pure point diffraction is equivalent to norm-almost periodicity of the autocorrelation measure. For Meyer sets the almost periodicity of the autocorrelation has been replaced by the almost periodicity of the underlying set in a suitable topology by Moody and Strungaru [13], and this has been generalized to arbitrary point sets in \mathbb{R}^d by Gouéré [7]. Gouéré also proved that for a Delone set $\Lambda \subset \mathbb{R}^d$, with autocorrelation measure γ , pure point diffraction is equivalent with the condition:

- (i) For all $R > 0$ and all $\epsilon > 0$ the set $\{t \in \mathbb{R}^d \mid \gamma(t + B_R(0)) \geq \gamma(\{0\}) - \epsilon\}$ is relatively dense.

Received by the editors May 9, 2008; revised November 28, 2010.

Published electronically April 6, 2011.

This work was done while the author was a Postdoctoral Fellow at the University of Victoria and was supported by the Natural Sciences and Engineering Research Council of Canada.

AMS subject classification: 43A25.

Keywords: pure point diffraction, positive definite measure, Fourier transform of measures.

While this condition is easy to understand, Gouéré’s proof is based on the Schwartz class of functions and thus on the geometry of \mathbb{R}^d .

The goal of this paper is to generalize this equivalence from the case of \mathbb{R}^d to an arbitrary locally compact Abelian group G (and in some sense, beyond point sets). In Theorem 5.4 we prove that for Delone sets in arbitrary locally compact Abelian groups, pure point diffraction is equivalent to the following condition:

- (i) For all sets V in a basis of precompact open neighborhoods of 0 and all $\epsilon > 0$ the set $\{t \in G \mid \gamma(T_t V) > \gamma(\{0\}) - \epsilon\}$ is relatively dense.

Along the way we get a more general result about the discreteness of the Fourier transform of a positive definite measure, which might be of independent interest.

The main tools used in this paper are the equivalence of strong almost periodicity of the autocorrelation and pure point diffraction [10], as well as Krein’s inequality for positive definite functions [4].

The paper is organized as follows. In Section 2 we introduce the concept of almost periodicity and its connection to the discreteness of the Fourier transform. We also introduce Krein’s inequality. In Theorem 3.3 we provide a new characterization for the discreteness of the Fourier transform of a positive definite measure, while in Section 4 we show that if the measure is also positive and has 0 as an isolated point for its support, then the conditions in Theorem 3.3 can be simplified. In Section 5 we introduce the reader to the diffraction theory and see how Theorems 3.3 and 4.2 can be used to characterize pure point diffraction.

2 Preliminaries

Throughout the paper, G denotes a locally compact Abelian group. We will denote by $C_U(G)$ the space of bounded and uniformly continuous functions on G , and by $C_c(G)$ the space of compactly supported continuous functions on G .

Definition 2.1 For a function f on G , f^\dagger and \tilde{f} denote the functions defined by ¹

$$f^\dagger(x) = f(-x) \quad \text{and} \quad \tilde{f}(x) = \overline{f^\dagger(x)} = \overline{f(-x)} \quad \forall x \in G.$$

Definition 2.2 For $f, g \in C_c(G)$ their *convolution* is defined by

$$f * g(x) = \int_G f(x - t)g(t)dt.$$

The *convolution* of a function $f \in C_c(G)$ and a measure μ is the function $f * \mu$ defined by

$$f * \mu(x) = \int_G f(x - t)d\mu(t).$$

Almost periodic functions were first introduced by Bohr on the real line, and later generalized to arbitrary locally compact groups. We recall the standard definition of an almost periodic function.

¹The author is not familiar with any standard notation for f^\dagger . Argabright and de Lamadrid [10] denote this function by f' , Berg and Forest [4] use the \check{f} notation, while Hewitt and Ross [8] use f^* .

Definition 2.3 A function $f \in C_U(G)$ is called *almost periodic* if the set

$$\{t \in G \mid \|f - T_t f\|_\infty < \epsilon\},$$

is relatively dense for each $\epsilon > 0$, where $T_t f(x) := f(x - t)$.

The importance of almost periodicity in the study of discreteness of the Fourier transform was observed by Eberlein, who proved that a finite measure is discrete if and only if its Fourier transform is an almost periodic function [6]. This result was later generalized to unbounded measures by Argabright and de Lamadrid in the following way.

Theorem 2.4 ([10]) *For a Fourier transformable translation bounded measure μ the following are equivalent:*

- (i) μ is a discrete measure;
- (ii) for all $f \in C_c(\widehat{G})$ the function $f * \widehat{\mu}$ is an almost periodic function.

Crystallographers are interested in the Fourier dual of this result. Thus we have to make an extra assumption, namely that the measure μ is double Fourier transformable (i.e., μ is Fourier transformable, and its Fourier transform $\widehat{\mu}$ is also Fourier transformable). This is usually the case, since the autocorrelation measure is usually positive and positive definite (see Section 5), thus double Fourier transformable by [4]. Hence, by applying Theorem 2.4 to the inverse Fourier transform of μ we get the following.

Proposition 2.5 *For a double Fourier transformable measure μ the following are equivalent:*

- (i) $\widehat{\mu}$ is a discrete measure;
- (ii) for all $f \in C_c(G)$ the function $f * \mu$ is an almost periodic function.

An immediate consequence of this is the following.

Proposition 2.6 *Let μ be a double Fourier transformable measure with discrete Fourier transform. Then, for all $f \in C_c(G)$ and all $\epsilon > 0$, the set*

$$\{t \in G \mid \operatorname{Re}(\mu(T_t f)) > \operatorname{Re}(\mu(f)) - \epsilon\}$$

is relatively dense.

In general the reverse is not true, but in the case of positive definite functions, Krein's inequality provides the link to proving that equivalence holds in Proposition 2.6.

Proposition 2.7 (Krein's inequality) *Let f be a positive definite function on G . Then, for all $x, t \in G$ we have*

$$|f(t + x) - f(x)|^2 \leq 2f(0)[f(0) - \operatorname{Re} f(t)].$$

In particular,

$$\|f - T_t f\|_\infty^2 \leq 2f(0)[f(0) - \operatorname{Re} f(t)].$$

3 Positive Definite Measures

As we mentioned in the introduction, we will try to simplify the condition in Theorem 2.4 by using Krein’s inequality for positive definite functions. Given a positive definite measure μ , we will convolve it with a function of the type $f * \tilde{f}$ and get a positive definite function. Proposition 2.7 will give a simpler characterization for the ϵ -almost periods of $\mu * f * \tilde{f}$. In order to use Theorem 2.4 we only need $f * \tilde{f} \in C_c(G)$, thus we only need to assume that f is compactly supported and an L^2 function on G [8].

We will denote by $BCL(G)$ the set of bounded compactly supported L^2 functions on G . That is,

$$BCL(G) := \{f: G \rightarrow \mathbb{C} \mid \|f\|_\infty < \infty, \|f\|_2 < \infty \text{ and } \text{supp}(f) \text{ is compact}\}.$$

Let $\Delta: BCL(G) \rightarrow C_c(G)$ be defined by $\Delta(f) := f * \tilde{f}$. For a precompact open set U , we will denote by $\Delta(U)$ the function $\Delta(U) := \Delta(1_U)$. It is clear that $\Delta(f)$ is always positive definite, and if $f \geq 0$, then $\Delta(f) \geq 0$.

Definition 3.1 A subset $\mathcal{U} \subset BCL(G)$ is called *Fourier separable* if for any open precompact set $V \subset G$ there exists $f \in \mathcal{U}$ so that \tilde{f} does not vanish on V .

Lemma 3.2 Let μ be a double Fourier transformable positive definite measure, and let $\mathcal{U} \subset BCL(G)$ be a Fourier separable set. Then the following are equivalent:

- (i) $\hat{\mu}$ is a discrete measure;
- (ii) for all $f \in \mathcal{U}$ and all $\epsilon > 0$, the set

$$\{t \in G \mid \text{Re}[\mu(T_t \Delta(f))] > \mu(\Delta(f)) - \epsilon\}$$

is relatively dense.

Proof The implication (i) \Rightarrow (ii) follows from Proposition 2.6.

For (ii) \Rightarrow (i), fix an $f \in \mathcal{U}$. Since both μ and $\Delta(f^\dagger)$ are positive definite, $\Delta(f^\dagger) * \mu$ is a positive definite function, thus we can use Krein’s inequality

$$(3.1) \quad \begin{aligned} |\Delta(f^\dagger) * \mu(t+s) - \Delta(f^\dagger) * \mu(s)|^2 \leq \\ 2\Delta(f^\dagger) * \mu(0)[\Delta(f^\dagger) * \mu(0) - \text{Re}(\Delta(f^\dagger) * \mu(t))] \end{aligned}$$

for all $s, t \in G$, since

$$\Delta(f^\dagger) * \mu(t) = \int_G \Delta(f^\dagger)(t-s) d\mu(s) = \int_G \Delta(f)(s-t) d\mu(s) = \mu(T_t \Delta(f)).$$

Let $\epsilon > 0$. Then, by (ii), the set

$$R := \left\{ t \in G \mid \mu(\Delta(f)) - \text{Re}(\mu(T_t \Delta(f))) < \frac{\epsilon^2}{2\mu * \Delta(f)(0) + 1} \right\}$$

is relatively dense. Combining with (3.1), we get that the set

$$\{t \in G \mid \|\Delta(f^\dagger) * \mu - T_t(\Delta(f^\dagger) * \mu)\|_\infty < \epsilon\},$$

is relatively dense.

Thus, since $\epsilon > 0$ was arbitrary, $\Delta(f^\dagger) * \mu$ is an almost periodic function.

Then, for all $g \in C_c(G)$, the function $\Delta(f^\dagger) * \mu * g$ is almost periodic (see [10], for example). Thus, the measure $\Delta(f^\dagger) * \mu$ is Fourier transformable (since positive definite) and verifies Proposition 2.5(ii). Therefore, its Fourier transform $|\widehat{f^\dagger}|^2 \widehat{\mu} = (|\widehat{f}|^2)^\dagger \widehat{\mu}$ is a discrete measure.

Since $(|\widehat{f}|^2)^\dagger \widehat{\mu}$ is a discrete measure for all $f \in \mathcal{U}$, by the Fourier separability assumption, $\widehat{\mu}$ is a discrete measure. ■

Using the fact that the set $\{1_U \mid U \subset G \text{ precompact open set}\}$ is Fourier separable, by combining Proposition 2.6 and Lemma 3.2 we get the following

Theorem 3.3 *Let μ be a double Fourier transformable, positive definite measure, let \mathcal{V} be a fixed basis of precompact open sets on G , and let $\mathcal{U} \subset BCL(G)$ be a Fourier separable set. The following are equivalent:*

- (i) $\widehat{\mu}$ is a discrete measure;
- (ii) for all precompact open sets U and all $\epsilon > 0$, the set

$$\{t \in G \mid \operatorname{Re}[\mu(t + \Delta(U))] > \mu(\Delta(U)) - \epsilon\}$$

is relatively dense;

- (iii) for all open sets $U \in \mathcal{V}$ and all $\epsilon > 0$, the set

$$\{t \in G \mid \operatorname{Re}[\mu(t + \Delta(U))] > \mu(\Delta(U)) - \epsilon\}$$

is relatively dense;

- (iv) for all $f \in C_c(G)$ and all $\epsilon > 0$, the set

$$\{t \in G \mid \operatorname{Re}[\mu(T_t \Delta(f))] > \mu(\Delta(f)) - \epsilon\}$$

is relatively dense;

- (v) for all $f \in BCL(G)$ and all $\epsilon > 0$, the set

$$\{t \in G \mid \operatorname{Re}[\mu(T_t \Delta(f))] > \mu(\Delta(f)) - \epsilon\}$$

is relatively dense;

- (vi) for all $f \in \mathcal{U}$ and all $\epsilon > 0$, the set

$$\{t \in G \mid \operatorname{Re}[\mu(T_t \Delta(f))] > \mu(\Delta(f)) - \epsilon\}$$

is relatively dense.

An immediate consequence of this result is the following.

Corollary 3.4 *If the group G has a function $f \in BCL(G)$ with nowhere vanishing Fourier transform, then for all the double Fourier transformable, positive definite measures μ on G the following are equivalent:*

- (i) $\widehat{\mu}$ is a discrete measure;
- (ii) for all $\epsilon > 0$ the set

$$\{t \in G \mid \operatorname{Re}[\mu(T_t \Delta(f))] > \mu(\Delta(f)) - \epsilon\}$$

is relatively dense.

4 Positive and Positive Definite Measures

For this section μ is a positive and positive definite measure for which 0 is an isolated point of its support. That is, there exists an open neighborhood U of 0 so that

$$\mu|_U = \mu(\{0\})\delta_0.$$

The following is a weaker version of Proposition 2.6.

Lemma 4.1 *Let V be an open neighborhood of 0. If $\widehat{\mu}$ is a discrete measure, then, for all $\epsilon > 0$, the set*

$$\{t \in G \mid \mu(T_t V) > \mu(\{0\}) - \epsilon\}$$

is relatively dense.

Proof Let $f \in C_c(G)$ be such that $f \leq 1_V$ and $f(0) = 1$. Since $\widehat{\mu}$ is a discrete measure, $\widetilde{f} * \mu$ is an almost periodic function, hence the set

$$P := \{t \in G \mid \|\widetilde{f} * \mu - T_t(\widetilde{f}) * \mu\|_\infty < \epsilon\}$$

is relatively dense.

Let us observe that for all $t \in P$ we have $|\mu(f) - \mu(T_t f)| < \epsilon$.

In particular,

$$\mu(T_t V) \geq \mu(T_t f) > \mu(f) - \epsilon \geq \mu(\{0\})f(0) - \epsilon = \mu(\{0\}) - \epsilon. \quad \blacksquare$$

In the remainder of this section we will prove that, under the settings from the beginning of the section, the converse of Lemma 4.1 is also true. The main idea is that for all $f \in BCL(G)$ such that $\operatorname{supp}(f) - \operatorname{supp}(f) \subset U$ we have $\mu(\Delta(f)) = \mu(\{0\})(\Delta(f)(0))$. Thus, in Theorem 3.3(iv) we can replace $\mu(\Delta(f))$ with $\mu(\{0\})(\Delta(f)(0))$. Also, since μ is positive, it preserves inequalities, and this allows us to switch between functions and small open sets in Theorem 3.3(vi).

Theorem 4.2 *Let μ be a positive and positive definite measure such that 0 is an isolated point of its support, and \mathcal{V} a fixed basis of precompact open neighborhoods of 0. Then the following are equivalent:*

- (i) $\widehat{\mu}$ is a discrete measure;
- (ii) for all W precompact open neighborhoods of 0 and all $\epsilon > 0$, the set

$$\{t \in G \mid \mu(T_t W) > \mu(\{0\}) - \epsilon\}$$

is relatively dense;

- (iii) for all $V \in \mathcal{V}$ and all $\epsilon > 0$, the set

$$\{t \in G \mid \mu(T_t V) > \mu(\{0\}) - \epsilon\}$$

is relatively dense.

Proof The implication (i) \Rightarrow (ii) follows from Lemma 4.1, while (ii) \Rightarrow (iii) is clear. We now prove (iii) \Rightarrow (i).

Let $\mathcal{U} := \{f \in C_c(G) \mid f \geq 0, f \not\equiv 0, \text{supp}(f * \widetilde{f}) \subset U\}$. Let $f \in \mathcal{U}$ and $0 < \epsilon < \Delta(f)(0)$. Since $\Delta(f)$ is continuous at 0, there exists a $V \in \mathcal{V}$ so that

$$|\Delta(f)(x) - \Delta(f)(0)| < \epsilon \quad \forall x \in V.$$

Hence,

$$\Delta(f) \geq (\Delta(f)(0) - \epsilon)1_V.$$

We know by (iii) that the set $R := \{t \in G \mid \mu(T_t V) > \mu(\{0\}) - \frac{\epsilon}{|\Delta(f)(0) - \epsilon| + 1}\}$ is relatively dense. Now let $t \in R$.

Then

$$\begin{aligned} \text{Re}[\mu(T_t \Delta(f))] &= \mu(T_t \Delta(f)) \geq (\Delta(f)(0) - \epsilon) \mu(T_t 1_V) \\ &> (\Delta(f)(0) - \epsilon) \mu(\{0\}) - \epsilon = \mu(\Delta(f)) - \epsilon(1 + \mu(\{0\})) \\ &= \text{Re}[\mu(\Delta(f))] - \epsilon(1 + \mu(\{0\})). \end{aligned}$$

So, if we show that \mathcal{U} is a Fourier separable set, the equivalence (vi) \Leftrightarrow (i) in Theorem 3.3 completes the proof.

Let $V \subset \widehat{G}$ be an open precompact set, and let K be its closure. Since G is the dual group of \widehat{G} and \mathcal{V} is a basis of open sets at 0, there exists a $W \in \mathcal{V}$ so that $W - W \subset U$ and

$$W \subset N(K, 1/4) := \{x \in G \mid |\langle x, \chi \rangle - 1| < 1/4 \forall \chi \in K\}.$$

Since the Haar measure $\theta_{\widehat{G}}$ is regular, there exists a compact set $K_1 \subset W$ so that

$$\theta_{\widehat{G}}(K_1) > 4/5 \theta_{\widehat{G}}(W).$$

We know that there exists a continuous function f with $1_W \geq f \geq 1_{K_1}$. Then $f \in \mathcal{U}$, and for all $\chi \in K$ we have

$$\begin{aligned} \operatorname{Re}[\widehat{f}(\chi)] &= \operatorname{Re}\left[\int_G f(x)\chi(x)dx\right] = \int_W f(x) \operatorname{Re}[\chi(x)]dx \\ &= \int_{K_1} f(x) \operatorname{Re}[\chi(x)]dx + \int_{W \setminus K_1} f(x) \operatorname{Re}[\chi(x)]dx \\ &\geq \int_{K_1} \operatorname{Re}[\chi(x)]dx + \int_{W \setminus K_1} f(x) \operatorname{Re}[\chi(x)]dx \\ &\geq \int_{K_1} 3/4dx - \int_{W \setminus K_1} 1dx = 3/4\theta_{\widehat{G}}(K_1) - \theta_{\widehat{G}}(W \setminus K_1) \\ &= 7/4\theta_{\widehat{G}}(K_1) - \theta_{\widehat{G}}(W) > 0. \end{aligned}$$

Thus, $\operatorname{Re}[\widehat{f}(\chi)] \neq 0 \forall \chi \in K$. ■

5 Diffraction Theory

5.1 A Short Review

Recall that a measure ν is called *translation bounded* (or *shift bounded*) if for all compact sets $K \subset G$, there exists a constant $C_K < \infty$ so that

$$(5.1) \quad \|\nu\|_K := \sup_{t \in G} \{|\nu|(t + K)\} \leq C_K.$$

It is easy to see that ν is translation bounded if and only if (5.1) holds for one compact set K with non-empty interior.

For some $C > 0$ and some compact set K with non-empty interior, we denote by

$$\mathcal{M}_{C,K}(G) := \{\nu \mid \|\nu\|_K \leq C\}.$$

By [2] $\mathcal{M}_{C,K}(G)$ is vaguely compact.

A *van Hove sequence* is a sequence of compact sets $B_n \subset G$ with the property that for all compact sets $K \subset G$

$$\lim_{n \rightarrow \infty} \frac{\theta_G(\partial^K(B_n))}{\theta_G(B_n)} = 0,$$

where the K -boundary is defined by

$$\partial^K(B_n) = \overline{(B_n + K) \setminus B_n} \cup ((\overline{G \setminus B_n} - K) \cap B_n).$$

For a point set M we define the measure δ_M by $\delta_M := \sum_{x \in M} \delta_x$. Given a Delone set Λ , the sequence

$$(5.2) \quad \frac{\delta_{\Lambda \cap B_n} * \widetilde{\delta_{\Lambda \cap B_n}}}{\theta_G(B_n)}$$

lives in some $\mathcal{M}_{C,K}(G)$ and thus has a vague cluster point $\gamma(\Lambda)$. We will call any such cluster point $\gamma(\Lambda)$ an *autocorrelation measure* of Λ . $\gamma(\Lambda)$ is a positive and positive definite measure, and thus double Fourier transformable. Its Fourier transform is called a *diffraction measure* for Λ .

More generally we can define an autocorrelation of a translation bounded measure ν as a vague cluster point of

$$(5.3) \quad \frac{\nu|_{B_n} * \widetilde{\nu|_{B_n}}}{\theta_G(B_n)}.$$

Again, such a cluster point exist because all these measures belong to some $\mathcal{M}_{C,K}(G)$. Moreover, any cluster point is positive definite, and thus Fourier transformable.

Note that in both cases, by going to a van Hove subsequence of $\{B_n\}$, we can assume that γ is the limit of (5.2) or (5.3).

5.2 Pure Point Diffraction

Definition 5.1 A measure ν , with an autocorrelation $\gamma(\nu)$, is called *pure point diffractive* if the diffraction measure $\widehat{\gamma(\nu)}$ is a discrete (pure point) measure. A Delone set Λ is called pure point diffractive if the corresponding measure δ_Λ is pure point diffractive.

Remark 5.2 The definition of pure point diffractiveness depends on the choice of the cluster point in the definition of the autocorrelation. So, whenever we say that Λ or ν is pure point diffractive, we understand that Definition 5.1 holds for Λ or ν and our choice of the autocorrelation. For an example, see Example 5.9.

Given a translation bounded measure ν with an autocorrelation γ that verifies the assumptions from Section 4, Theorem 4.2 gives us the following.

Proposition 5.3 *Let ν be a translation bounded measure with an autocorrelation γ . Let \mathcal{V} be a fixed basis of precompact open neighborhoods of 0. If γ is positive and has 0 as an isolated point for its support, then the following are equivalent:*

- (i) Λ is pure point diffractive;
- (ii) for all $V \in \mathcal{V}$ precompact open neighborhoods of 0 and all $\epsilon > 0$, the set

$$\{t \in G \mid \gamma(T_t V) > \gamma(\{0\}) - \epsilon\}$$

is relatively dense;

- (iii) for all $V \in \mathcal{V}$ and all $\epsilon > 0$, the set

$$\{t \in G \mid \gamma(T_t V) > \gamma(\{0\}) - \epsilon\}$$

is relatively dense.

In particular, since the autocorrelation of a Delone set always verifies these assumptions, we get the following.

Theorem 5.4 Let Λ be a Delone set with an autocorrelation γ . Let \mathcal{V} be a fixed basis of precompact open neighborhoods of 0. Then the following are equivalent:

- (i) Λ is pure point diffractive;
- (ii) for all V precompact open neighborhoods of 0 and all $\epsilon > 0$, the set

$$\{t \in G \mid \gamma(T_t V) > \gamma(\{0\}) - \epsilon\}$$

is relatively dense;

- (iii) for all $V \in \mathcal{V}$ and all $\epsilon > 0$, the set

$$\{t \in G \mid \gamma(T_t V) > \gamma(\{0\}) - \epsilon\},$$

is relatively dense.

Remark 5.5 Theorem 5.4 also holds for positive weighted Dirac combs with uniformly discrete support.

For the diffraction of a general translation bounded measure, by Theorem 3.3 we also get the following.

Theorem 5.6 Let ν be a translation bounded measure with double Fourier transformable autocorrelation γ , and let \mathcal{U} be a fixed basis of precompact open sets. The following are equivalent:

- (i) ν is pure point diffractive;
- (ii) for all precompact open sets U and all $\epsilon > 0$, the set

$$\{t \in G \mid \operatorname{Re}[\gamma(t + \Delta(U))] > \gamma(\Delta(U)) - \epsilon\}$$

is relatively dense;

- (iii) For all open sets $U \in \mathcal{U}$ and all $\epsilon > 0$, the set

$$\{t \in G \mid \operatorname{Re}[\gamma(t + \Delta(U))] > \gamma(\Delta(U)) - \epsilon\}$$

is relatively dense;

- (iv) for all $f \in C_c(G)$ and all $\epsilon > 0$, the set

$$\{t \in G \mid \operatorname{Re}[\gamma(T_t \Delta(f))] > \gamma(\Delta(f)) - \epsilon\}$$

is relatively dense;

- (v) for all $f \in BCL(G)$ and all $\epsilon > 0$, the set

$$\{t \in G \mid \operatorname{Re}[\gamma(T_t \Delta(f))] > \gamma(\Delta(f)) - \epsilon\}$$

is relatively dense.

Example 5.7 Let $\Lambda := \mathbb{Z}$. A simple computation shows that the autocorrelation of Λ is $\gamma := \delta_{\mathbb{Z}}$. Then for each $0 \in U \subset \mathbb{R}$ open and each $\epsilon > 0$, we have

$$\gamma(t + U) \geq \gamma(\{t\}) = 1 > 1 - \epsilon = \gamma(\{0\}) - \epsilon \quad \forall t \in \mathbb{Z}.$$

Hence $\Lambda = \mathbb{Z}$ is pure point diffractive, which is not surprising since it is known that the diffraction of \mathbb{Z} is $\widehat{\gamma} = \delta_{\mathbb{Z}}$.

Example 5.8 Let $\Lambda \subset \mathbb{Z}$ be constructed the following way. For each $t \in \mathbb{Z}$ we keep t with probability $1/2$. Such an Λ is called a *Bernoulli set*.

Let $\{B_n\}_n$ be a van Hove sequence.

Then

$$\begin{aligned} \frac{\delta_{\Lambda|_{B_n}} * \widetilde{\delta_{\Lambda|_{B_n}}}}{\text{vol}(B_n)} &= \sum_{t \in \mathbb{Z}} \frac{\#\{(x, y) | x, y \in \Lambda \cap B_n, x - y = t\}}{\text{vol}(B_n)} \delta_t \\ &= \sum_{t \in \mathbb{Z}} \frac{\#\{y \in \mathbb{Z} | y, y + t \in \Lambda \cap B_n\}}{\text{vol}(B_n)} \delta_t. \end{aligned}$$

Note that we count how many times on average y and $t + y$ belong to Λ . If $t \in \mathbb{Z} \setminus \{0\}$, the two events are independent, so the probability that $y, t + y$ are simultaneously in Λ is $1/4$. If $t = 0$, then we only have one condition, namely $y \in \Lambda$, which happens with probability $1/2$.

Thus, for almost surely all Bernoulli sets Λ , the autocorrelation is

$$\gamma = \frac{1}{2} \delta_0 + \frac{1}{4} \sum_{t \in \mathbb{Z}^*} \delta_t = \frac{1}{4} \delta_0 + \frac{1}{4} \delta_{\mathbb{Z}}.$$

It is easy to see that for all open sets U with diameter less than $1/4$ and all $t \in \mathbb{R}$ we have

$$\gamma(t + U) \leq \frac{1}{4} = \gamma(\{0\}) - \frac{1}{4}.$$

Hence, almost surely all Bernoulli sets are not pure point diffractive.

The reason we only get an almost surely statement is because, with probability zero, we could still get a point set like $\Lambda = 2\mathbb{Z}$ (which is pure point diffractive).

Example 5.9 Let $\Lambda := [\mathbb{Z} \cap (0, \infty)] \cup [\Lambda' \cap (-\infty, 0]]$, where Λ' is a Bernoulli set. Let

$$B_{2n} := [-n^2, n], \quad B_{2n+1} := [-n, n^2].$$

Then, almost surely, Λ has two autocorrelations with respect to the van Hove sequence B_n : $\gamma_1 = \delta_{\mathbb{Z}}$ given by $\{B_{2n+1}\}$ and $\gamma_2 = \frac{1}{4}(\delta_0 + \delta_{\mathbb{Z}})$ given by $\{B_{2n}\}$.

Note that Λ is pure point diffractive when we chose the first autocorrelation but not when we chose the second. Also note that when we chose the first autocorrelation we get the diffraction of \mathbb{Z} , while when we chose the second we get the diffraction of a generic Bernoulli set.

Also note that every real solid that is modeled by this set has arbitrary large subsets with different statistical properties. Thus, if one chooses a sample to diffract, the diffraction depends on whether the sample is chosen from the left or right side of 0. Different large samples will have different diffraction patterns.

Acknowledgments I am grateful to Michael Baake, Robert Moody, Ian Putnam, and Robert Engel for various remarks and suggestions that improved this paper. I would also like to thank the anonymous referees for careful reading of the manuscript and making some suggestions.

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