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Diffraction of Weighted Lattice Subsets

Dedicated to Robert V. Moody on the occasion of his 60th birthday

Michael Baake

Abstract. A Dirac comb of point measures in Euclidean space with bounded complex weights that is supported on a lattice Γ inherits certain general properties from the lattice structure. In particular, its autocorrelation admits a factorization into a continuous function and the uniform lattice Dirac comb, and its diffraction measure is periodic, with the dual lattice Γ^* as lattice of periods. This statement remains true in the setting of a locally compact Abelian group whose topology has a countable base.

1 Introduction

Mathematical diffraction theory is concerned with the Fourier analysis of the autocorrelation measures of unbounded, but translation bounded, complex measures in Euclidean space, compare [10, 27, 14, 2, 17] and references listed there. More generally, the same question is also analyzed in the setting of σ-compact locally compact Abelian groups [1, 7, 26]. There are many interesting and relevant open questions connected with it, in particular how to assess the spectral type of the (positive) diffraction measure, which is the Fourier transform of the autocorrelation.

One important subclass of translation bounded measures consists of the set of discrete Dirac combs which are supported on a lattice or a subset thereof. This paper provides a characterization of the autocorrelation and diffraction measures associated to measures of this class. As an application, we derive a relation between the diffraction measures of complementary lattice subsets. Other recent (sometimes implicit) applications of this characterization include deterministic cases such as the visible lattice points or the k-th power free integers [5, 4] and the class of substitution lattice systems [19, 20], but also a wide class of lattice gas models [2, 12]. The latter are presently gaining practical importance in crystallography due to the need for a better understanding of diffuse scattering, compare [2, 13, 27] and references given there.

The article is organized as follows. First, we describe the problem in the Euclidean setting and state the corresponding result in Theorem 1. The next section then covers the step by step proof of this result. All details, or at least precise references, are given in order to make the presentation relatively self-contained and accessible also to readers with a more applied background. As general references for topological concepts and results, we use [8, 22]. As one application, we then compare lattice subsets with their complements, with special emphasis on the homometry problem (see

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Theorem 2). This is followed by an extension of Theorem 1 to the more general situation that Euclidean space $\mathbb{R}^n$ is replaced by a locally compact Abelian group (LCA group) G whose topology has a countable base. An analogous result is true here, and is summarized in Theorem 3.

2 Euclidean Lattices

Let $\varGamma$ be a lattice in $\mathbb{R}^n$, *i.e.* the integer span of n vectors that are linearly independent over $\mathbb{R}$. We are interested in the *weighted* Dirac comb [9]

$$\omega = \sum_{t\in\varGamma} w(t)\,\delta_t \tag{1}$$

where $w\colon \varGamma \to \mathbb{C}$ is a bounded function and δ_t denotes the normalized point (or Dirac) measure located at t, so that $\delta_t(\varphi) = \varphi(t)$ for continuous functions φ. Since $\varGamma$ is uniformly discrete and w is bounded, ω is a translation bounded (or shift bounded) complex measure, *cf.* [7, Chapter I.1]. By a measure, we always mean a regular (complex) Borel measure, identified with the corresponding linear functional on $\mathcal{K}(\mathbb{R}^n)$, the space of continuous functions of compact support. This is justified by the Riesz-Markov theorem, compare [23, 7, 14, 2] for details. The space of measures is then equipped with the vague topology which we will use throughout.

Let us first assume that the *natural autocorrelation measure* of ω exists. It is defined with respect to an increasing sequence of balls around the origin, and denoted by γ_ω. So, we assume for the moment that

$$\gamma_\omega = \lim_{r\to\infty} \frac{\omega_r * \tilde{\omega}_r}{\mathrm{vol}\big(B_r(0)\big)} \tag{2}$$

exists as a vague limit, where ω_r means the restriction of ω to the (open) ball $B_r(0)$ of radius r around 0, $\tilde{\omega}_r := (\omega_r)^{\sim}$, and $\tilde{\omega}$ is the measure defined by $\tilde{\omega}(\varphi) = \overline{\omega(\tilde{\varphi})}$ for any continuous function φ of compact support, with $\tilde{\varphi}(x) := \overline{\varphi(-x)}$. In particular, for ω of (1), we have $\tilde{\omega} = \sum_{t\in\varGamma} \overline{w(t)}\,\delta_{-t}$.

Since $\varGamma$ is a lattice, the natural autocorrelation is a pure point measure of the form $\gamma_\omega = \sum_{z\in\varGamma} \nu(z)\,\delta_z$ with the coefficients being given by

$$\begin{aligned} \nu(z) &= \lim_{r\to\infty} \frac{1}{\mathrm{vol}\big(B_r(0)\big)} \sum_{\substack{t,t'\in\varGamma_r \\ t-t'=z}} w(t)\overline{w(t')} \\ &= \lim_{r\to\infty} \frac{1}{\mathrm{vol}\big(B_r(0)\big)} \sum_{t\in\varGamma_r} w(t)\overline{w(t-z)}. \end{aligned} \tag{3}$$

Here, $\varGamma_r = \varGamma \cap B_r(0)$, and there are several variants to write $\nu(z)$ as a limit. For fixed z and $r \gg |z|$, the two approximations for finite radius used in (3), prior to dividing by $\mathrm{vol}\big(B_r(0)\big)$, differ by surface contributions which are uniformly small in comparison to the bulk. To make this precise, one needs an estimate for the number

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of lattice points in spherical shells of thickness s and radius $r \gg s$ which is $O(r^{n-1})$ in n dimensions, see [16]. Hence, the above limit does not depend on such details, and we will make use of this freedom in the Euclidean setting without further mentioning.

Since Γ is a lattice in $\mathbb{R}^n$, its density is well-defined as a limit, namely

$$\operatorname{dens}(\Gamma) = \lim_{r\to\infty} \frac{|\Gamma \cap B_r(a)|}{\operatorname{vol}\big(B_r(0)\big)} \tag{4}$$

with $a \in \mathbb{R}^n$ and $|A|$ denoting the cardinality of a (finite) set A. This limit exists *uniformly* in a, see [14, 26]. As a lattice, Γ is uniformly discrete (*i.e.* the minimal distance between any two distinct points is strictly positive), and the natural autocorrelation thus exists if and only if the coefficients $\nu(z)$ of (3) exist for all $z \in \Gamma$.

So far, we explicitly assumed the existence of the natural autocorrelation as a limit, and hence its uniqueness. This is the standard situation investigated *e.g.* in crystallography, and it seems very adequate in view of the usual homogeneity of the systems analyzed. Mathematically, however, this assumption is not necessary, and we will thus formulate our results in a slightly more general setting.

Our key assumption is that the complex weight function w is bounded, so that the measure ω is translation bounded. This is already sufficient to ensure that all finite approximations to the autocorrelation are uniformly translation bounded, see [14, Proposition 2.2]. Consequently, there is always at least one vague limit point, but, in general, we might have several. To make this precise, let us define

$$\gamma_\omega^{(r)} = \frac{\omega_r * \tilde{\omega}_r}{\operatorname{vol}\big(B_r(0)\big)}$$

and consider the family of autocorrelation approximants $\{\gamma_\omega^{(r)} \mid r > 0\}$, all of which are positive definite measures by construction. When restricted to a compact set K, the corresponding family of finite measures is precompact in the vague topology.

Let us now consider *any* vague limit point γ of the family $\{\gamma_\omega^{(r)} \mid r > 0\}$. It is then possible to select a diverging sequence of radii $(r_i)_{i\in\mathbb{N}}$ such that $\gamma_\omega^{(r_i)} \to \gamma$ vaguely as $i \to \infty$. As we will see, the proof of our main result (Theorem 1) will only depend on the existence of such a sequence, so we can formulate it as a result for each limit point.

The standard tools from Fourier analysis are also needed. The Fourier transform of a rapidly decreasing (or Schwartz) function φ is

$$\hat{\varphi}(x) = \int_{\mathbb{R}^n} e^{-2\pi i x y} \varphi(y)\, dy$$

where xy is the standard Euclidean scalar product in $\mathbb{R}^n$. From here, we take the usual route to the Fourier transform of measures that are, at the same time, tempered distributions, see [23, Chapter IX.1] or [25, Chapter 7] for general background and [2] for our conventions. An alternative approach, without any reference to Schwartz functions, could follow [7, Chapter I.4] and employ the positive definiteness of γ_ω which guarantees the existence of $\hat{\gamma}_\omega$.

We call a Borel set A *regular*, if $A^\circ \neq \varnothing$ and if ∂A has Lebesgue measure 0, and say that a measure μ is *supported* on a regular Borel set A, if μ and $\mu|_A$, the restriction of μ to A, are identical as measures on $\mathbb{R}^n$. The central result can now be phrased as follows.

Theorem 1 *Let Γ be a lattice in $\mathbb{R}^n$ and ω a weighted Dirac comb on Γ with bounded complex weights. Let γ_ω be any of its autocorrelations, i.e. any of the limit points of the family $\{\gamma_\omega^{(r)} \mid r > 0\}$. Then the following holds.*

(1) *The autocorrelation γ_ω can be represented as*

$$\gamma_\omega = \Phi \cdot \delta_\Gamma = \sum_{x\in\Gamma} \Phi(x)\, \delta_x$$

where $\Phi\colon \mathbb{R}^n \to \mathbb{C}$ is a bounded continuous positive definite function that interpolates the autocorrelation coefficients $\nu(x)$ as defined at $x \in \Gamma$. Moreover, there exists such a Φ which extends to an entire function $\Phi\colon \mathbb{C}^n \to \mathbb{C}$ with the additional growth restriction that there are constants $C, R \geq 0$ and $N \in \mathbb{Z}$ such that $|\Phi(z)| \leq C(1+|z|)^N \exp\big(R\,|\operatorname{Im}(z)|\big)$ for all $z \in \mathbb{C}^n$.

(2) *The Fourier transform $\hat{\gamma}_\omega$, also called a diffraction measure of ω, is a translation bounded positive measure that is periodic with the dual lattice $\Gamma^* = \{u \mid uv \in \mathbb{Z}$ for all $v \in \Gamma\}$ as lattice of periods. Furthermore, $\hat{\gamma}_\omega$ has a representation as a convolution,*

$$\hat{\gamma}_\omega = \varrho * \delta_{\Gamma^*},$$

in which ϱ is a finite positive measure supported on a fundamental domain of Γ^* that is contained in the ball of radius R around the origin.

Remarks The interpolating function Φ is not unique. It can be changed by adding any positive definite continuous (entire) function which vanishes on Γ. Also, the positive measure ϱ depends on the choice of the fundamental domain of Γ^*. As soon as the latter is fixed (as a regular Borel set, say, to avoid pathologies with singular versus continuous parts), ϱ is unique. This is so because $\hat{\gamma}_\omega$ is Γ^*-periodic and thus defines a unique measure on the factor group $\mathbb{R}^n/\Gamma^*$, which, in turn, gives rise to a unique measure ϱ on the fundamental domain chosen.

A rather natural fundamental domain of Γ^* can be constructed from the Voronoi cell of Γ^*, which is a polytope, namely the set of all points of $\mathbb{R}^n$ which are not farther apart from the origin than from any other point of Γ^*. It is the intersection of finitely many closed half-spaces and hence a zonotope. A fundamental domain emerges from it by removal of certain boundaries, starting with the $(n-1)$-boundaries, then the $(n-2)$-boundaries, and so on down to the 0-boundaries. Due to the lattice structure of Γ^*, these boundaries always come in translation pairs, one member of which is removed. What remains, is a regular Borel set E which is a true fundamental domain of Γ^*, *i.e.* the Γ^*-translates of E form a partition of $\mathbb{R}^n$. Its existence is vital for the above statement because ϱ may contain point measures. The radius R in the above growth estimate can be taken as the radius of the circumsphere of the fundamental domain of Γ^* chosen. This follows from the Paley-Wiener theorem for distributions with compact support [25, Theorem 7.23]. If a fundamental domain is constructed on the basis of the Voronoi cell of Γ^*, then its circumradius R, the covering radius of Γ^*, is minimal among all fundamental domains of Γ^*.

If there is only one limit point to the family $\{\gamma_\omega^{(r)} \mid r > 0\}$, we are in the standard situation of crystallography, where the homogeneity of the systems makes this a very natural assumption. In this case, Theorem 1 simply refers to *the* autocorrelation.

The above mentioned question of the spectral type of $\hat{\gamma}_\omega$ is now obviously reduced to that of the spectral type of ϱ. The latter is a finite positive measure and admits the unique decomposition

$$\varrho = (\varrho)_{pp} + (\varrho)_{sc} + (\varrho)_{ac}$$

with respect to Lebesgue measure, which is the natural reference measure in this context. As usual, *pp*, *sc* and *ac* stand for pure point, singular continuous and absolutely continuous, see [23, Section I.4] for details.

The result of Theorem 1 is not really restricted to Dirac combs. If h is a (continuous) L^1-function, say, and ω a Dirac comb of the above type, then $h * \omega$ is a well-defined translation bounded measure, with autocorrelation $\gamma = (h * \tilde{h}) * \gamma_\omega$ and diffraction measure $\hat{\gamma} = |\hat{h}|^2 \hat{\gamma}_\omega$ by the convolution theorem. This can be considered as a situation where h describes a more realistic profile of the scatterers (*e.g.* atoms), and Theorem 1 can then be applied to γ_ω and $\hat{\gamma}_\omega$. Convolution is also a key ingredient to tackle the problem of diffraction at high temperature, compare [15].

Various applications were already mentioned in the Introduction. Also, the case that $\varrho = (\varrho)_{pp}$ can now be analyzed in more detail, and a set of necessary and sufficient conditions is given in [4]. Arrangements of scatterers where $\hat{\gamma}_\omega$ is a pure point measure are often called pure point diffractive. These cases are of particular interest because they include perfect crystals, but also several aperiodic lattice substitution systems, see [6, 19] for details.

3 Proof of Theorem 1

The key idea is to use an appropriate regularization of the point measure ω of (1) for the construction of the function Φ and the measure ϱ. It relies on the existence of a properly converging sequence of approximating measures. We will employ Ascoli's Theorem to construct a (Lipschitz) continuous interpolation of the autocorrelation coefficients of (3), and a combination of Bochner's Theorem with the convolution property of the Fourier transform to conclude on the existence of the measure ϱ.

Let $c \in C_c^\infty$ be a non-negative bump function with compact support contained in $B_\varepsilon(0)$ where $\varepsilon > 0$ is at most half the packing radius of Γ (the technical reason for this restriction will become clear below). Let $c(0) = c_0$ be the maximal value of c, so that $0 \le c(x) \le c_0$ for all $x \in \mathbb{R}^n$. Such a function, which is also called an approximate identity, can be constructed as follows, compare [18, p. 168]. Start from $\phi(x) = \exp\big(|x|^2/(|x|^2 - 1)\big)$ for $|x| < 1$ and $\phi(x) = 0$ otherwise. This is a C^∞-function with support in the closed unit ball, with $\phi(0) = 1$. Now, set $c(x) = c_0\phi(x/\varepsilon)$. Clearly, $0 \le c(x) \le c_0$, the support is in the closed ball of radius ε, and c is integrable, *i.e.* $\|c\|_1 < \infty$. Also, $(c * \tilde{c})(0) = \int_{\mathbb{R}^n} c(x)\tilde{c}(-x)\,dx = \|c\|_2^2 < \infty$, and,

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for fixed $\varepsilon > 0$, we can always adjust c_0 so that $\|c\|_2^2 = 1$. We henceforth assume that such a function c is given.

Recall that a function c is (globally) Lipschitz, with Lipschitz constant $L_c < \infty$, if $|c(x) - c(y)| \le L_c|x - y|$ for all $x, y \in \mathbb{R}^n$, and L_c is the smallest number with this property. In particular, c is then uniformly continuous.

Lemma 1 *A non-negative bump function $c \in C_c^\infty$ is Lipschitz. Furthermore, also $\tilde{c}$ and $c * \tilde{c}$ are Lipschitz, with $L_{\tilde{c}} = L_c$ and $L_{c*\tilde{c}} \le \|c\|_1 L_c$.*

Proof It is clear that c is Lipschitz because it is smooth and has compact support, so $L_c \le \sup_{x\in\mathbb{R}^n} \bigl|\operatorname{grad}\bigl(c(x)\bigr)\bigr| < \infty$. Since c is a real function, we have $\tilde{c}(x) = \overline{c(-x)} = c(-x)$, so that $L_c = L_{\tilde{c}}$ is obvious. Finally, consider

$$\begin{aligned}
|(c * \tilde{c})(x) - (c * \tilde{c})(y)| &= \Bigl| \int_{\mathbb{R}^n} c(z)\bigl(\tilde{c}(x - z) - \tilde{c}(y - z)\bigr)\, dz \Bigr| \\
&\le \int_{\mathbb{R}^n} c(z) |\tilde{c}(x - z) - \tilde{c}(y - z)|\, dz \\
&\le L_c|x - y| \int_{\mathbb{R}^n} c(z)\, dz = \|c\|_1 L_c |x - y|
\end{aligned}$$

which establishes the assertion. ■

Fix a radius $r > 0$ and set $\Gamma_r = \Gamma \cap B_r(0)$. Let $\omega_r = \sum_{t\in\Gamma_r} w(t)\delta_t$ be the weighted Dirac comb of Γ_r. Define $f_r = c * \omega_r$, so that

$$f_r(z) = \sum_{t\in\Gamma_r} w(t) c(z - t). \tag{5}$$

This is a continuous function, as is $\tilde{f}_r$. A simple calculation then shows that $f_r * \tilde{f}_r = (c * \tilde{c}) * (\omega_r * \tilde{\omega}_r)$ which is the continuous positive definite function

$$(f_r * \tilde{f}_r)(z) = \sum_{u,v\in\Gamma_r} w(u)\overline{w(v)}(c * \tilde{c})(z - u - v). \tag{6}$$

Due to the small support of c (recall that ε is at most half the packing radius of Γ), and hence that of $c * \tilde{c}$, most terms of the double sum vanish, and it effectively collapses to a single sum. In particular, if $z = t$ is in the lattice, $(c * \tilde{c})(t - u - v)$ is either 0 or 1 by construction. In fact, for $u \in \Gamma$, the value 1 is taken precisely for $v = t - u$. This is a consequence of the above choice of ε, and also motivates it, a posteriori.

Let us now define $g_r = \frac{1}{\operatorname{vol}(B_r(0))} f_r * \tilde{f}_r$. Then it is clear from the above that $g_r(t) \to \nu(t)$ as $r \to \infty$ for all $t \in \Gamma$. We have thus constructed a family of continuous positive definite functions $\{g_r \mid r > 0\}$ that pointwise converges to the autocorrelation coefficients for all $t \in \Gamma$. We now have to check whether it will result in a continuous interpolation.

Lemma 2 *The family $\{g_r \mid r > 0\}$ is uniformly Lipschitz, hence in particular equicontinuous, and uniformly bounded.*

Proof The function f_r of (5), for any $r > 0$, is a finite linear combination of Lipschitz functions and hence Lipschitz, by Lemma 1. With $W := \sup_{t\in\Gamma} |w(t)|$, we can estimate the Lipschitz constant of f_r as $L_{f_r} \le |\Gamma_r| W L_c$ since the support of c is so small that no two bumps in f_r overlap. Lemma 1 then gives $L_{f_r * \tilde{f}_r} \le \|f_r\|_1 L_{f_r}$, and with $\|f_r\|_1 \le W\|c\|_1$ we obtain

$$L_{f_r * \tilde{f}_r} \le |\Gamma_r| W^2 \|c\|_1 L_c < \infty.$$

Consequently, also g_r is Lipschitz, and we have

$$L_{g_r} \le \frac{|\Gamma_r|}{\mathrm{vol}\,\big(B_r(0)\big)} W^2 \|c\|_1 L_c.$$

The first factor on the right hand side is the number of lattice points in a ball of radius r, divided by its volume. This is known [16] to be

$$\frac{|\Gamma_r|}{\mathrm{vol}\,\big(B_r(0)\big)} = \mathrm{dens}(\Gamma) + \mathcal{O}(r^{-1}) \quad \text{as } r \to \infty \tag{7}$$

from which the uniform Lipschitz condition follows, and hence also the equi-continuity of the family $\{g_r \mid r > 0\}$.

Similarly, consider $g_r = (c * \tilde{c}) * \frac{\omega_r * \tilde{\omega}_r}{\mathrm{vol}\,(B_r(0))}$ which is a continuous function composed of non-overlapping little bumps. Consequently, using (2) and (3) and observing that $\|c * \tilde{c}\|_\infty = \|c\|_2^2 = 1$ (due to our choice of c_0), we see that

$$|g_r(z)| \le \|g_r\|_\infty \le \frac{|\Gamma_r|}{\mathrm{vol}\,\big(B_r(0)\big)} W^2$$

from which, again with (7), one obtains equi-boundedness. ∎

Lemma 2 allows us to use Ascoli's Theorem, see [18, Corollary III.3.3] for a version that covers our situation (note that $\mathbb{R}^n$ is only locally compact, but a metric space with a countable dense subset, *e.g.* $\mathbb{Q}^n$. Consequently, the corresponding topology has a countable base [8, Proposition IX.12]). In particular, no matter whether we start from the entire family $\{g_r \mid r > 0\}$ or from a sequence $(g_{r_i})_{i\in\mathbb{N}}$ (as needed for the case that we have several autocorrelations), there is a diverging (sub)sequence of radii, $(r_j)_{j\in\mathbb{N}}$, such that, as $j \to \infty$, the g_{r_j} converge compactly to some function g which is then bounded and continuous. Since the family is actually equi-uniformly continuous, convergence is globally uniform. As a limit of positive definite functions, g is still positive definite. Moreover, it is also (globally) Lipschitz, and $g(t) = \nu(t)$ for all $t \in \Gamma$ by construction. So far, we have established:

Proposition 1 *Let Γ be a lattice in $\mathbb{R}^n$ and ω the Dirac comb of (1), with bounded complex weights. Let γ_ω be any of its (natural) autocorrelation measures, the latter defined as the limit of a suitable sequence $(\gamma_\omega^{(r_i)})_{i\in\mathbb{N}}$ of approximants, with $(r_i)_{i\in\mathbb{N}}$ an increasing, unbounded sequence of radii. Then, γ_ω admits a representation of the form*

$$\gamma_\omega = g \cdot \delta_\Gamma$$

where $\delta_\Gamma = \sum_{t\in\Gamma} \delta_t$ is the Dirac comb of Γ and g is a bounded, positive definite Lipschitz function on all of $\mathbb{R}^n$. ■

Now, we can invoke Bochner's Theorem [23, Theorem IX.9] which tells us that $\hat{g}$, the Fourier transform of g, is a *finite* positive measure (our above construction was crucial to ensure this). On the other hand, $\hat{\delta}_\Gamma$ is translation bounded, wherefore $\hat{g} * \hat{\delta}_\Gamma$ is well defined [7, Proposition 1.13], and it is a tempered measure. This allows us to (backwards) employ the convolution theorem, compare [7, Proposition 4.10]:

$$\hat{\gamma}_\omega = \hat{g} * \hat{\delta}_\Gamma = \mathrm{dens}(\Gamma)\, \hat{g} * \delta_{\Gamma^*} \tag{8}$$

where the second step uses the identity $\hat{\delta}_\Gamma = \mathrm{dens}(\Gamma)\delta_{\Gamma^*}$, known as Poisson's summation formula for lattice Dirac combs, see [7, Example 6.22] or [9].

Proposition 2 *The diffraction measure $\hat{\gamma}_\omega$ of (8) is Γ^*-periodic. It can thus alternatively be represented as*

$$\hat{\gamma}_\omega = \varrho * \delta_{\Gamma^*}$$

where ϱ is a bounded positive measure that is supported on a fundamental domain of Γ^* which we may choose to be bounded.

Proof The Γ^*-periodicity of $\hat{\gamma}_\omega$ is obvious from the convolution formula in (8). Also, it is a standard result that each lattice in $\mathbb{R}^n$ has a fundamental domain inside the Voronoi cell of Γ^* that is a regular Borel set, E say (the construction of such a set was described in the Remark following Theorem 1). The translates $t + E$ for $t \in \Gamma^*$ then form a disjoint partition of $\mathbb{R}^n$, and we have

$$\hat{\gamma}_\omega = \sum_{t\in\Gamma^*} \hat{\gamma}_\omega|_{t+E}$$

where $\hat{\gamma}_\omega\big|_{t+E}$ is the restriction of $\hat{\gamma}_\omega$ to the set $t + E$. But periodicity tells us that $\hat{\gamma}_\omega|_{t+E} = \hat{\gamma}_\omega|_E * \delta_t$, and the assertion follows with $\varrho := \hat{\gamma}_\omega|_E$. ■

To complete the proof of Theorem 1, it remains to go back to the autocorrelation, *i.e.*,

$$\gamma_\omega = \check{\varrho} \cdot \check{\delta}_{\Gamma^*} = \Phi \cdot \delta_\Gamma$$

where we have

$$\varrho = \mathrm{dens}(\Gamma)\, \hat{\Phi},$$

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again by Poisson's summation formula. The nice properties of the function Φ claimed in Theorem 1 are now a direct consequence of the Paley-Wiener Theorem, see [23, Theorem IX.12] or [25, Theorem 7.23], because ϱ is by construction a positive measure with compact support. This also concludes the proof of Theorem 1. ■

Remark The above proof employed the Lipschitz property of the bump function c. Alternatively, using (6) and the smallness of the support of c (and hence also of that of $c * \tilde{c}$), one can derive that

$$|g_r(z) - g_r(z')| \leq \frac{|\Gamma_r|}{\operatorname{vol}\big(B_r(0)\big)} W^2 \sup_x |(c * \tilde{c})(z - x) - (c * \tilde{c})(z' - x)|$$

for all z, z' sufficiently close. This inequality implies equi-continuity of the family $\{g_r \mid r > 0\}$ without reference to any Lipschitz property. This results in a slightly weaker version of Proposition 1, with g being a bounded, positive definite continuous function on all of $\mathbb{R}^n$ which need not be Lipschitz.

4 Complementary Lattice Subsets

A particularly interesting situation emerges in the comparison of a lattice subset $S \subset \Gamma$ with its complement $S' = \Gamma \setminus S$. Here, the Dirac combs to be compared are $\omega = \delta_S = \sum_{x \in S} \delta_x$ and $\omega' = \delta_{S'}$. Note that the Dirac comb of (1), when specialized to $w \equiv 1$, results in an autocorrelation with coefficients

$$\nu_S(z) = \lim_{r \to \infty} \frac{|S \cap (z + S) \cap B_r(0)|}{\operatorname{vol}\big(B_r(0)\big)} = \operatorname{dens}\big(S \cap (z + S)\big)$$

for all $z \in \mathbb{R}^n$, provided the limits exist. This can easily be derived from (3) and the comments following it.

Next, recall that two point sets are called *homometric* if they share the same (natural) autocorrelation. This is an important concept in crystallography, both in theory and practice, because homometric sets cannot be distinguished by diffraction [21, 24].

Theorem 2 *Let Γ be a lattice in $\mathbb{R}^n$, and let $S \subset \Gamma$ be a subset with existing (natural) autocorrelation coefficients $\nu_S(z) = \operatorname{dens}\big(S \cap (z + S)\big)$. Then the following holds.*

(1) *The autocorrelation coefficients $\nu_{S'}(z)$ of the complement set $S' = \Gamma \setminus S$ also exist. They are $\nu_{S'}(z) = 0$ for all $z \notin \Gamma$ and otherwise, for $z = t \in \Gamma$, satisfy the relation*

$$\nu_{S'}(t) - \operatorname{dens}(S') = \nu_S(t) - \operatorname{dens}(S).$$

(2) *If, in addition,* $\operatorname{dens}(S) = \operatorname{dens}(\Gamma)/2$, *then the sets S and $S' = \Gamma \setminus S$ are homometric.*

(3) *The diffraction spectra of the sets S and S' are related by*

$$\hat{\gamma}_{S'} = \hat{\gamma}_S + \big(\operatorname{dens}(S') - \operatorname{dens}(S)\big) \operatorname{dens}(\Gamma)\, \delta_{\Gamma^*}.$$

In particular, $\hat{\gamma}_{S'} = \hat{\gamma}_S$ if $\operatorname{dens}(S') = \operatorname{dens}(S)$.

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(4) *The diffraction measure $\hat{\gamma}_{S'}$ is pure point if and only if $\hat{\gamma}_S$ is pure point.*

Proof In what follows, each term involving a density is to be viewed as the limit along a fixed increasing and unbounded sequence of radii. Since Γ is the disjoint union of S and S', $\Gamma = S\dot{\cup}S'$, we get $\mathrm{dens}(S') = \mathrm{dens}(\Gamma) - \mathrm{dens}(S)$ and the natural density of S' exists because $\mathrm{dens}(S) = \nu_S(0)$. Since $S' \subset \Gamma$, we also have $\nu_{S'}(z) = 0$ whenever $z \notin \Gamma$.

So, let $z = t \in \Gamma$ from now on. Now observe that $\Gamma \cap (t + \Gamma) = \Gamma$ and thus, using $\Gamma = S\dot{\cup}S'$, we obtain

$$\begin{aligned}\mathrm{dens}(\Gamma) &= \mathrm{dens}\big(\Gamma \cap (t+\Gamma)\big)\\ &= \nu_{S'}(t) + \nu_S(t) + \mathrm{dens}\big(S \cap (t+S')\big) + \mathrm{dens}\big(S' \cap (t+S)\big).\end{aligned}$$

Since $S' = \Gamma \setminus S$, it is easy to verify that

$$\begin{aligned}\mathrm{dens}\big(S' \cap (t+S)\big) &= \mathrm{dens}\big(\Gamma \cap (t+S)\big) - \mathrm{dens}\big(S \cap (t+S)\big)\\ &= \mathrm{dens}(S) - \nu_S(t)\end{aligned}$$

because $(t+S) \subset \Gamma$ and $\mathrm{dens}(t+S) = \mathrm{dens}(S)$. Similarly,

$$\mathrm{dens}\big(S \cap (t+S')\big) = \mathrm{dens}(S) - \nu_S(-t)$$

by first shifting and then using the previous formula. Since $\nu_S(t)$ is a real positive definite function, we have $\nu_S(-t) = \nu_S(t)$, and obtain

$$\mathrm{dens}(\Gamma) = 2\,\mathrm{dens}(S) + \nu_{S'}(t) - \nu_S(t)$$

from which the first assertion follows with $\mathrm{dens}(\Gamma) = \mathrm{dens}(S) + \mathrm{dens}(S')$.

If $\mathrm{dens}(S) = \mathrm{dens}(\Gamma)/2$, then $\mathrm{dens}(S') = \mathrm{dens}(S)$ and we obtain $\nu_{S'}(z) = \nu_S(z)$, for all z, by the first assertion. This settles assertion (2).

Since $S \subset \Gamma$, its autocorrelation is $\gamma_S = \sum_{t\in\Gamma} \nu_S(t)\delta_t$, and analogously for S', the complement set in Γ. From the first assertion, we then infer

$$\gamma_{S'} = \gamma_S + c\delta_\Gamma$$

with $c = \mathrm{dens}(S') - \mathrm{dens}(S)$. Assertion (3) now follows from taking the Fourier transform and applying Poisson's summation formula to the lattice Dirac comb δ_Γ.

Finally, the difference between $\hat{\gamma}_{S'}$ and $\hat{\gamma}_S$ in the third assertion is a multiple of δ_{Γ^*} which is a uniform lattice Dirac comb and hence a pure point measure, whence the last claim is obvious. ■

In [5], it was shown that the set of visible lattice points is pure point diffractive. The last assertion of Theorem 2 then tells us that their complement, the set of *invisible* points, also is pure point diffractive. Similarly, the set of k-th power free integers, a subset of $\mathbb{Z}$, has pure point diffraction [5], so does then its complement, the set of integers divisible by the k-th power of some integer ≥ 2. This indicates that many more pure point diffractive point sets of independent interest exist, and a general criterion based on the almost periodicity of the autocorrelation is derived in [4].

5 Generalizations

Our above derivation, with little modification, can also be carried through in the case that $\mathbb{R}^n$ is replaced by an arbitrary locally compact Abelian group G whose topology has a countable base. As such, G is certainly Hausdorff, but also σ-compact and metrizable [22, Corollary 10.16]. Consequently, G is Polish, see [22, Theorem 13.16] or the Corollary in [8, Chapter IX.6.1]. In particular, we may assume G to be equipped with a metric d which induces the topology of G and with respect to which G is complete. Since this topology has a countable base by assumption, Ascoli's Theorem is again at our disposal. This class contains all groups of the form $\mathbb{R}^n \times \mathbb{Z}^m \times H$ with $n, m \geq 0$ and H compact and metrizable, which are (up to isomorphism) the so-called metrizable compactly generated LCA groups. We assume G to be equipped with an appropriately normalized Haar measure θ_G, compare [11, Chapter 2.5]. In particular, we assume $\theta_G(G) = 1$ if G is a compact group.

A *lattice* $\varGamma$ is now a discrete (hence closed) subgroup of G such that $G/\varGamma$ is compact (this is the appropriate generalization of our previous definition in the Euclidean setting). The Dirac comb ω of (1) is well defined, and it is translation bounded (or shift bounded) if and only if the function w is bounded. Note that ω is then a *finite* complex measure if G is compact. The (open) ball of radius r around a is

$$B_r(a) = \{x \in G \mid d(x,a) < r\},$$

but the autocorrelation γ_ω of the Dirac comb ω can, in general, no longer be defined as in equation (2), because balls in general groups G can have rather weird properties. So, even with $\mathrm{vol}\big(B_r(0)\big) := \theta_G\big(B_r(0)\big)$, the limit in (2) might be meaningless. There is no problem for compact G, though: one can simply write $\gamma_\omega = \omega * \tilde{\omega}$ because $\theta_G(G) = 1$ in this case, so that existence and uniqueness of the autocorrelation are automatic. This is clear since all sums involved are actually finite.

We overcome the general difficulty by employing the concept of an *averaging sequence* which, at the same time, also constitutes a restricted (monotone increasing) van Hove sequence, see [26] for details. To explain this, recall that an LCA group G is σ-compact if and only if a countable family

$$\mathcal{U} = \{U_i \mid i \in \mathbb{N}\} \tag{9}$$

of relatively compact open sets exists with $U_1 \neq \varnothing$, $\overline{U_i} \subset U_{i+1}$ for all $i \in \mathbb{N}$, and $\bigcup_{i\in\mathbb{N}} U_i = G$, see [22, Theorem 8.22]. In particular, $0 < \theta_G(U_i) < \infty$ for all $i \in \mathbb{N}$. We call such a family $\mathcal{U}$ an averaging sequence. It also constitutes a *van Hove sequence*, if one extra property is satisfied which guarantees that the surface/bulk ratio becomes sufficiently negligible in the limit $i \to \infty$. To formalize the latter, we introduce

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

for an open set U and any compact set K in G. Here, we use the convention $A \pm B := \{x \pm y \mid x \in A, y \in B\}$, with $\varnothing \pm B = \varnothing$. The set $\partial^K U$ can, cum grano salis, be seen as a 'thickened' version of the boundary of U. Then, the final condition is that

$$\lim_{i\to\infty} \frac{\theta_G(\partial^K U_i)}{\theta_G(U_i)} = 0 \tag{10}$$

for all compact $K \subset G$. The existence of such averaging sequences of van Hove type in σ-compact LCA groups is shown in [26].

Let us assume that a family $\mathcal{U} = \{U_i \mid i \in \mathbb{N}\}$ has been given which also constitutes a van Hove sequence. Since $\varGamma$, as a lattice, is a special case of a regular model set, we can then conclude from [26, p. 145] that the *density* of $\varGamma$ exists,

$$\operatorname{dens}(\varGamma) = \lim_{i\to\infty} \frac{|\varGamma \cap U_i|}{\theta_G(U_i)}, \tag{11}$$

and that the limit is independent of the van Hove sequence chosen. This is the correct analogue of the statement (4) for lattices in $\mathbb{R}^n$. If we now define $\omega_i = \omega|_{U_i}$ and, similarly, $\tilde{\omega}_i = (\omega|_{U_i})^{\sim}$, the analogue of equation (2) would read

$$\gamma_\omega = \lim_{i\to\infty} \frac{\omega_i * \tilde{\omega}_i}{\theta_G(U_i)} \tag{12}$$

provided the limit exists.

In this case, the autocorrelation is always a pure point measure of the form $\gamma_\omega = \sum_{z\in\varGamma} \nu(z)\delta_z$ with the coefficients $\nu(z)$ now being given by

$$\nu(z) = \lim_{i\to\infty} \frac{1}{\theta_G(U_i)} \sum_{\substack{t,t'\in\varGamma\cap U_i\\ t-t'=z}} w(t)\overline{w(t')}, \tag{13}$$

again with the simplification that $\nu(z) = \sum_{t\in\varGamma} w(t)\overline{w(t-z)}$ for G compact. Usually, the more interesting cases of Dirac combs will occur for groups G that are locally compact, but *not* compact, such as $\mathbb{R}^n$.

At this point, let us state the analogue of Theorem 1 in this more general setting.

Theorem 3 *Let $\varGamma$ be a lattice in an* LCA *group G whose topology has a countable base, and let $\omega = \sum_{t\in\varGamma} w(t)\delta_t$ be a Dirac comb on $\varGamma$ with bounded complex weights. Let an averaging sequence $\mathcal{U} = \{U_i \mid i \in \mathbb{N}\}$ be given which constitutes a monotone increasing van Hove sequence, and assume that the corresponding autocorrelation measure γ_ω of (12) exists. Then we have:*

(1) *The autocorrelation measure γ_ω admits the representation*

$$\gamma_\omega = g \cdot \delta_\varGamma$$

where g is a bounded, positive definite Lipschitz function on G which interpolates the autocorrelation coefficients $\nu(t)$, $t \in \varGamma$.

(2) *The Fourier transform $\hat{\gamma}_\omega$ is a translation bounded positive measure on the dual group $\hat{G}$ which is periodic with lattice of periods $\varGamma^*$, the dual lattice of $\varGamma$. It can be represented as*

$$\hat{\gamma}_\omega = \varrho * \delta_{\varGamma^*}$$

with a finite positive measure ϱ that is supported on a totally bounded and measurable fundamental domain of $\varGamma^*$.

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Proof The argument is very similar to the proof in Section 3, wherefore we only describe the changes needed.

Lemma 1 needs a replacement because the concept of a smooth bump function makes no sense in general. Instead, we can employ a different kind of Lipschitz function as follows. Choose $\varepsilon > 0$ so that $B_\varepsilon(0) \cap B_\varepsilon(t) = \varnothing$ for all $t \in \Gamma \setminus \{0\}$. Such an ε clearly exists because G is Hausdorff and our metric induces the topology of G. If we set $A = G \setminus B_\varepsilon(0)$, which is a closed set, then $0 \notin A$ and thus $d(0, A) \geq \varepsilon > 0$, where $d(x, A) = \inf_{y \in A} d(x, y)$ is the distance of x from A. We can now define

$$c(x) = \frac{c_0 d(x, A)}{d(0, A)}. \tag{14}$$

One has $c(x) \geq 0$, $c(0) = c_0$ and $c(x) = 0$ for all $x \in A$, so c is nontrivial (if $c_0 \neq 0$) and supported on the closure of $B_\varepsilon(0)$.

Lemma 3 *The function c of (14) is Lipschitz, with Lipschitz constant $L_c = c_0/d(0, A)$. The functions $\tilde{c}$ and $c * \tilde{c}$ are also Lipschitz, with $L_{\tilde{c}} = L_c$ and $L_{c*\tilde{c}} \leq \|c\|_1 L_c$.*

Proof The Lipschitz property of $d(x, A)$, with Lipschitz constant 1, is stated in [8, Proposition IX.2.3], see [3] for an explicit proof. The remainder of the proof is that of Lemma 2, with $\mathbb{R}^n$ and Lebesgue measure replaced by g and Haar measure, respectively. ■

Since both c and $c * \tilde{c}$ are integrable w.r.t. the Haar measure θ_G, the construction of a family of approximating functions $\{g_i \mid i \in \mathbb{N}\}$, relative to the sequence $\mathcal{U}$, is now possible, in complete analogy to above.

With this modification, Lemma 2 still holds. For its proof, we only need that the density of lattice points of Γ in G exists and that, if G is not compact, then $|\Gamma \cap U_i|/\theta_G(U_i)$ converges to it as $i \to \infty$. This follows from (11). We can then proceed as before: since we assume G to be locally compact and to have a countable base, we have Ascoli's Theorem at our disposal [18]. Consequently, we obtain the following modification of Proposition 1.

Proposition 3 *Let Γ be a lattice in an* LCA *group G with countable base and let ω be the Dirac comb of (1), with bounded complex weights. Let γ_ω be an autocorrelation measure which is assumed to exist as the limit of a sequence $\{\gamma_\omega^{(i)} \mid i \in \mathbb{N}\}$ of approximants with respect to a given averaging sequence $\mathcal{U} = \{U_i \mid i \in \mathbb{N}\}$. Then, γ_ω admits a representation of the form*

$$\gamma_\omega = g \cdot \delta_\Gamma$$

where g is a bounded, positive definite Lipschitz function on all of G. ■

Next, we need some results from harmonic analysis in the setting of LCA groups, see [7, Chapter I.4] or [11, Chapter 2.8] for a suitable summary. We denote the dual group by $\hat{G}$ and assume it is equipped with a matching Haar measure, $\theta_{\hat{G}}$ (a suitable normalization of it is suggested by the Fourier inversion formula, see [11, Chapter 2.8.7]). We can now, once more, invoke Bochner's Theorem [7, Theorem 4.5]:

since γ_ω is a *positive definite* measure by construction, its Fourier transform is a uniquely determined translation bounded *positive* measure on $\hat{G}$, denoted by $\hat{\gamma}_\omega$.

To make complete sense out of equation (8), we have to say what the dual lattice is and how Poisson's summation formula works. Each $k \in \hat{G}$ defines a (continuous) character on the group G, $\langle k, x\rangle$, which replaces $\exp(2\pi i k x)$ from above. Then,

$$\Gamma^* = \{k \in \hat{G} \mid \langle k, x\rangle = 1 \text{ for all } x \in \Gamma\}$$

and Γ^* (which is called $\Gamma^\perp$ in [11]) is the *annihilator* of the closed subgroup $\Gamma \subset G$ in the dual group $\hat{G}$, compare [11, Chapter 2.9.1]. We have $\Gamma^* = (G/\Gamma)^\wedge$ and $\hat{\Gamma} = \hat{G}/\Gamma^*$, see [11, Theorem 2.9.1], so that with Γ also Γ^* is a lattice because the dual of a compact group is discrete and vice versa [11, Theorem 2.8.3]. Moreover, we can interpret G/Γ and $\hat{G}/\Gamma^*$ as (measurable) fundamental domains of the lattices Γ and Γ^*. We now get, in complete analogy to before, the general Poisson summation formula

$$\hat{\delta}_\Gamma = a\, \delta_{\Gamma^*} \tag{15}$$

where a is a constant which depends on the density of Γ and on the relative normalization of θ_G and $\theta_{\hat{G}}$, see [11, Chapter 9.9] for details. So, the following modification of Proposition 2 holds in our more general setting.

Proposition 4 *Under the assumptions of Proposition 3, the corresponding diffraction measure $\hat{\gamma}_\omega$ exists and is Γ^*-periodic. It can be represented as*

$$\hat{\gamma}_\omega = \varrho * \delta_{\Gamma^*}$$

where ϱ is a bounded positive measure, supported on a fundamental domain of Γ^* which we may choose to be totally bounded. ∎

Finally, we have to combine Propositions 3 and 4 which completes the proof of Theorem 3. ∎

Remarks Similar to the situation in Theorem 1, the assumption on the existence of the autocorrelation as a limit is not essential. If $\gamma_\omega^{(i)} := \omega_i * \tilde{\omega}_i / \theta_G(U_i)$, the uniform translation boundedness of the $\gamma_\omega^{(i)}$ implies the existence of at least one limit point, γ say. We can then choose a subfamily $\{U_{i_j} \mid j \in \mathbb{N}\}$ such that $\gamma_\omega^{(i_j)} \to \gamma$ vaguely, as $j \to \infty$, and we thus obtain the corresponding results for each vague limit point γ of $\{\gamma_\omega^{(i)} \mid i \in \mathbb{N}\}$ separately, by applying Theorem 3 to ω together with this averaging subsequence.

Finally, the Remark at the end of Section 3 remains valid in this more abstract setting if elements of $\mathcal{U}$ are used instead of balls, and if one starts with a suitable continuous function c of sufficiently small support. However, as outlined above, G is automatically Polish with our assumptions, wherefore we can directly employ Lipschitz functions. So, no further generalization is gained this way.

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