Weighted Dirac combs with pure point diffraction

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Abstract

A class of translation bounded complex measures, which have the form of weighted Dirac combs, on locally compact Abelian groups is investigated. Given such a Dirac comb, we are interested in its diffraction spectrum which emerges as the Fourier transform of the autocorrelation measure. We present a sufficient set of conditions to ensure that the diffraction measure is a pure point measure. Simultaneously, we establish a natural link to the theory of the cut and project formalism and to the theory of almost periodic measures. Our conditions are general enough to cover the known theory of model sets, but also to include examples such as the visible lattice points.

Key Words: diffraction, model sets, harmonic analysis,
almost periodic and pure point measures

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1 Introduction

The diffraction properties of quasicrystals, both physical and mathematical, are among their most striking features. The customary ways of explaining diffractivity are principally of two kinds. The first is to view the quasicrystal as orginating from a cut through a higher dimensional lattice, in which case diffraction is explained as the vestiges of the diffractive properties of the lattice that survive after projection, see [22, 10] and references therein. The second is to look at the dynamical system constructed from the hull of the quasicrystal under translation and to connect the diffraction with the corresponding dynamical spectrum [37, 36, 26]. In the latter case, an important rôle is played by the repetitivity and unique ergodicity of the basic point set (or tiling) that makes up the quasicrystal in question. Despite serious efforts [38, 25, 27], no complete answer is known on how these two approaches fit together.

In this paper, we follow a different approach that accounts for the diffractivity through three basic properties of the underlying point set (or distribution of density). It is mathematically quite direct, has the advantage of clarifying where internal spaces and the higher dimensional lattices come from, and is intrinsically insensitive to density 0 changes. Furthermore, the result will be considerably more general than previous ones while the conditions can actually be verified explicitly in many relevant examples.

Before we start our analysis, let us briefly comment on the notion of diffraction used in this paper. Mathematically, as will become clear in a moment, we are dealing with certain spectral properties of measures, and the paper is rather self-contained in this respect. Physically, our question is related to the X-ray diffraction image of a solid, see [13] for background information. However, we are completely ignoring the question whether the measure under investigation is, in any sense, a realistic physical structure, such as the ground state of some given atomic interaction, compare [16, 5] and references cited there. We simply assume that it is given, and start from there. In particular, we do *not* assume that the measures we will be considering are typical in any sense. This would require us to couple our approach to ergodic theory and to Gibbs measures, something which we defer for future work.

Also, striktly speaking, our results would only apply to a static situation such as that of a solid at zero temperature (or to any situation which is sufficiently well approximated by this point of view). This poses no problem because, in a second step, one can always extend the results rigorously to cover the dynamic situation of diffraction at high temperatures, see [23] for details. In view of this, it is perfectly adequate to withdraw from the physical reality and to study the spectral properties of certain measures in their own right, without losing the possible applications to physics and crystallography.

The basic object of our study is then a translation bounded (complex) measure ω on a locally compact Abelian group G. In the standard case of a mathematical quasicrystal, represented by a point set $\varLambda$, G would be the physical space $\mathbb{R}^n$ and ω would be the point measure $\sum_{x\in\varLambda}\delta_x$ which is the Dirac comb supported on $\varLambda$. The basic assumptions are three:

1. that the averaged autocorrelation γ_ω of ω should exist,
2. that the support of γ_ω should be a uniformly discrete set $\varDelta$, and
3. that the ε-almost periods of γ_ω should be relatively dense.

Under these assumptions, we prove that the Fourier transform $\hat{\gamma}_\omega$ of the autocorrelation measure γ_ω is a pure point measure on $\hat{G}$, the dual group of G. This is precisely the mathematical meaning of saying that ω is pure point diffractive. We also show that all model sets (no matter what internal spaces are involved) based on windows with boundaries of (Haar) measure 0 satisfy these hypotheses, thus reproving the various results of this type (cf. [36] and references given there) in a new and simpler way. Here, the crucial link is made through Weyl's theorem on uniform distribution. Moreover, there are interesting situations which are not model sets, notably the visible points of a lattice (which do not form a Delone set because they fail to be relatively dense), that are also covered by our theorem. This is a simplification of the previous approach in [7].

The constructions that are used in the proof of the main theorem are as interesting to us as the result itself. We introduce first a new group, namely the subgroup L of G generated by the support of the autocorrelation measure γ_ω, and second a topology (in fact, a uniformity) on L that is derived from the autocorrelation itself. The latter is, in general, totally different from the one that L gets induced on it from G. The completion of L with respect to this autocorrelation topology is a new locally compact Abelian group H. It is this group H that is the 'internal group' of the system. Although L is, in general, neither discrete nor closed in G, it can be mapped into $G \times H$ by essentially embedding it diagonally, whereupon it appears as a *lattice*, denoted by $\tilde{L}$. Thus the internal space and the lattice, which seem normally to be without physical meaning, appear naturally as a reflection of the ε-almost periodicity of the basic measure ω, as defined through its autocorrelation.

Furthermore, G itself can be given a new topology which combines its usual topology with the autocorrelation topology of L which lies inside it. The completion of G with respect to this new topology is a *compact* group and is, in fact, nothing more than $(G \times H)/\tilde{L}$. This gives a simple explanation of the appearance of this compact group in the cut and project formalism which, though it has been used a number of times in the so-called 'torus parameterization' [4, 21, 36], did not seem to have any *intrinsic* meaning before.

The appearance of ε-almost periodicity is strongly reminiscent of the theory of almost periodic functions of Harold Bohr, though now it appears in the generalized form of measures. The concept of almost periodicity of measures in the theory of quasicrystals has appeared before [37]. In fact, during the work for this article, we became aware that the Bohr theory has already been completely generalized to measures in a fundamental but rather neglected paper of Gil de Lamadrid and Argabright [19]. In some sense, this work already partly contains the main result of this paper as will become clear in Section 9. However, our method to arrive there, for a restricted but relevant class of measures, is constructive and far more direct. Furthermore, it has the virtue, as we have mentioned, of making many of the common features in quasicrystal theory appear by themselves in a totally natural way.

The setting of this paper is that of locally compact Abelian (LCA) groups which are also σ-compact, and that of possibly unbounded, but translation bounded, complex measures. The importance of LCA groups for internal spaces of model sets has already been demonstrated, see [8] for concrete examples. The need for σ-compact LCA groups for the setting of quasicrystals themselves is not so obvious, but has been used before in [35]. We have adopted it here because it does not pose any extra complications and it is a natural setting for the theorem and its proof. Readers who prefer a more concrete base can replace G by $\mathbb{R}^n$ and the measure ω by a discretely supported Dirac comb throughout.

2 General setup and class of measures

Let G be a σ-compact, locally compact Abelian (LCA) group, which we always understand to include the Hausdorff property. The group action will be written additively. The group G is equipped with a fixed Haar measure θ which is unique up to a scalar multiple. If necessary, we will write θ_G to link the Haar measure to its group. Later on, we will need the *dual group*, denoted by $\hat{G}$, and we will then assume that it is equipped with a matching Haar measure $\theta_{\hat{G}}$ such that the generalized Plancherel formula holds, see [9, Thm. 2.5]. In this paper, the word 'measure' will always mean a linear functional (possibly complex valued) on the space of continuous functions on G with compact support, which we identify with a regular Borel measure according to the Riesz-Markov representation theorem [32].

Recall that G, when seen as a locally compact space, is *σ-compact* (or countable at infinity) if and only if a countable family

$$\mathcal{A} \; = \; \{A_n \mid n \in \mathbb{N}\} \tag{1}$$

of relatively compact open sets A_n exists with $A_1 \neq \varnothing$, $\bar{A_n} \subset A_{n+1}$ for all $n \in \mathbb{N}$, and $G = \bigcup_{n\in\mathbb{N}} A_n$, see [31, Thm. 8.22]. In particular, $0 < \theta(A_n) < \infty$ for all $n \in \mathbb{N}$. This property of σ-compactness facilitates the calculation with volume averages which we will need throughout. We assume that such a sequence $\mathcal{A}$ has been selected and fixed.

Let $S \subset G$ be a countable set and $w \colon S \to \mathbb{C}$ a function such that the corresponding *weighted Dirac comb*

$$\omega \; = \; \sum_{x\in S} w(x)\, \delta_x \tag{2}$$

defines a complex regular Borel measure on G. Here, δ_x is the unit point (or Dirac) measure located at x. The measure ω need not be bounded, and the unbounded ones are those of particular interest to us here. However, we will assume:

Axiom 1 The measure ω of (2) is translation bounded.

Recall that a measure ω is called *translation bounded* (or shift-bounded) if, for all compact $K \subset G$, $\sup_{t\in G} |\omega|(t + K) \leq C_K < \infty$ for some constant C_K which only depends on K. Here, $|\omega|$ denotes total variation measure and $t + K := \{t + x \mid x \in K\}$. If ω is of the form (2), the condition translates into $\sup_{t\in G}\sum_{x\in S\cap(t+K)}|w(x)|\le C_K<\infty$. Following [19], we will denote the space of translation bounded complex measures on G by $\mathcal{M}^\infty(G)$. For most of this paper, we consider $\mathcal{M}^\infty(G)$ equipped with the *vague topology.* This means that we identify a translation bounded measure with the corresponding linear functional on $\mathcal{K}(G)$, the space of complex valued continuous functions with compact support, which is justified by the Riesz-Markov representation theorem [32, Thm. IV.18]. Later on, we will also need different topologies on $\mathcal{M}^\infty(G)$, but we postpone details to Section 9.

Next, we have to approach the autocorrelation measure attached to ω. With $\omega(g) := \int_G g\,\mathrm{d}\omega$ for $g\in\mathcal{K}(G)$, we can define a partner measure, $\tilde{\omega}$, via $\tilde{\omega}(g)=\overline{\omega(\tilde{g})}$ where $\tilde{g}(x):=\overline{g(-x)}$. For the measure ω of (2), this means $\tilde{\omega}=\sum_{x\in S}\overline{w(x)}\,\delta_{-x}$.

Consider the fixed sequence $\mathcal{A}$ of (1). Set $\omega_n=\omega|_{A_n}$ and $\tilde{\omega}_n=(\omega_n)\tilde{}$. Then, the measure

$$\gamma_\omega^{(n)} \;:=\; \frac{\omega_n*\tilde{\omega}_n}{\theta(A_n)} \tag{3}$$

is well defined, since it is the (volume averaged) convolution of two *finite* measures. It reads $\gamma_\omega^{(n)}=\sum_{z\in\varDelta}\eta_n(z)\,\delta_z$ where $\varDelta=S-S$ (which is still countable) and

$$\eta_n(z) \;=\; \frac{1}{\theta(A_n)}\sum_{\substack{x,y\in S\cap A_n\\ x-y=z}} w(x)\overline{w(y)}\,. \tag{4}$$

For $z\notin\varDelta$, we set $\eta_n(z)=0$. By construction, η_n is then a *positive definite function* on G (see [9, Ch. I.3] for background material). Next, recall that a measure μ is called *positive definite* iff $\mu(g*\tilde{g})\ge 0$ for all $g\in\mathcal{K}(G)$. So, the measures $\gamma_\omega^{(n)}$ are positive definite, as follows from [9, Prop. 4.4].

Axiom 2 The pointwise limit $\eta(z):=\lim_{n\to\infty}\eta_n(z)$ exists for all $z\in\varDelta$.

Of course, $\eta(z)=0$ unless $z\in\varDelta$, so that Axiom 2 guarantees the existence of $\eta(z)$ for all $z\in G$. Also, $\eta(z)$ is positive definite, and hence satisfies $|\eta(z)|\le\eta(0)$ for all $z\in G$.

REMARK: Let us add a few comments on Axiom 2. Since ω is translation bounded by Axiom 1, the family of finite volume approximations $\gamma_\omega^{(n)}$ of (3) are uniformly translation bounded [22, Prop. 2.2]. This means that they always have points of accumulation in the vague topology. For any such limit point γ, we can select a suitable subsequence $\gamma_\omega^{(n_i)}$ which converges to γ. Since $\varDelta$ is countable, this can be done in such a way that also $\eta_{n_i}(z)$

pointwise converges for all $z \in \varDelta$. This argument shows that Axiom 2 is basically a convention because we can always achieve it a posteriori by properly thinning out the (averaging) sequence $\mathcal{A}$ of (1).

The next Axiom comes in two forms. The first part of the paper requires only the weaker (first) version of the Axiom. When we come to the diffraction results, we shall need the stronger version.

Axiom 3 The set $\varDelta^{\rm ess} := \{z \in G \mid \eta(z) \neq 0\} \subset \varDelta$ is closed and discrete.

Axiom 3$^+$ The set $\varDelta^{\rm ess}$ is uniformly discrete.

Recall that a set $P \subset G$ is called *uniformly discrete* if an open neighbourhood V of $0 \in G$ exists such that $(t+V) \cap P = \{t\}$ for all $t \in P$.

After Axiom 2 and either Axiom 3 or the stronger Axiom 3^+, we see that the sequence $\big(\gamma_\omega^{(n)}\big)_{n\in\mathbb{N}}$ converges, in the vague topology, to

$$\gamma_\omega \;=\; \sum_{z\in\varDelta} \eta(z)\delta_z \;=\; \sum_{z\in\varDelta^{\rm ess}} \eta(z)\delta_z \tag{5}$$

which is a pure point measure. The limit is called the *autocorrelation measure*, or autocorrelation for short, of the Dirac comb ω of (2) w.r.t. the sequence $\mathcal{A}$ of (1). It is a translation bounded measure, a consequence of Axiom 1; compare [22, Prop. 2.2].

Note that different sequences $\mathcal{A}$ can, and generally will, lead to different autocorrelations. Nonetheless, the development of our ideas depends only on the fixed sequence $\mathcal{A}$. The effect of changing sequences will be discussed in the Appendix.

Since the positive definite measures are closed in the vague topology, γ_ω is positive definite and $\eta(z)$ is a positive definite function on all of G. Let us assume that the $\mathcal{A}$-density of the set S is positive, i.e. $\eta(0) > 0$, to exclude the trivial case that $\gamma_\omega = 0$.
REMARK: In general, $\eta(z)$ will not be a continuous function on G, but, by the Riesz-Segal-von Neumann theorem [20, p. 104], it always admits a unique decomposition into a continuous positive definite function and another positive definite function which vanishes θ-almost everywhere on G. In most cases of interest to us, the continuous part will be absent, and it is the remaining part that matters.

The support of γ_ω (which is the support of $\eta(z)$) plays a special rôle in this article, and we will in particular need the group generated by it,

$$L \;:=\; \langle \varDelta^{\rm ess} \rangle_{\mathbb{Z}} \tag{6}$$

which is a subgroup of G.

Our next goal is the introduction of a suitable uniformity that allows us to form the (Hausdorff) completion of L. Since $\eta(z)$ is a positive definite function on G (and hence certainly also on the subgroup L), the function

$$m(z) \;:=\; 1 - \frac{\eta(z)}{\eta(0)}$$

is negative definite [9, Cor. 7.7]. In particular, it satisfies $m(0) = 0$ and $\tilde{m} = m$, see [9, Prop. 7.5]. Moreover, the function $\sqrt{|m(z)|}$ is subadditive, i.e.

$$\sqrt{|m(z+z')|} \;\leq\; \sqrt{|m(z)|} + \sqrt{|m(z')|}$$

for all $z, z' \in G$, see [9, Prop. 7.15]. Let us now define

$$\varrho(s,t) \;=\; \big|m(s-t)\big|^{1/2} \tag{7}$$

which is non-negative, symmetric (due to $\tilde{m} = m$) and satisfies the triangle inequality (due to the above subadditivity property). Also, it is immediate that $\varrho(s+r, t+r) = \varrho(s,t)$ for all $r \in G$. Hence we have

Fact 1 *The function ϱ of* (7) *defines a translation invariant pseudo-metric, both on G and on L.* □

Remark: If $w(x) \equiv 1$ in the definition (2) of ω, one could alternatively work directly with $\varrho'(s,t) := \eta(0) - \eta(s-t)$. This is then also a pseudo-metric, called *variogram* in geostatistics, see [28, Thm. 1]. However, it is not true in general that negative definite functions themselves define a pseudo-metric; $g(x) = 1 - \exp(-x^2)$ is a counterexample on $\mathbb{R}$.

The pseudo-metric ϱ of (7) defines a uniformity, both on G and on L, and hence a topology, which we call the *autocorrelation topology*, or AC topology for short. This topology is, in general, different from the topology that came with G in the beginning.

Next we define, for $\varepsilon > 0$, a set P_ε of ε*-almost periods* of the autocorrelation γ_ω through

$$P_\varepsilon \;=\; \{t \in G \mid \varrho(t,0) < \varepsilon\}\,. \tag{8}$$

We clearly have $P_\varepsilon \subset P_{\varepsilon'}$ for $\varepsilon < \varepsilon'$. Note also that $P_1 = \varDelta^{\rm ess}$ and $P_\varepsilon = G$ for all $\varepsilon > 1$, so that the interesting range of ε is $0 < \varepsilon \leq 1$. For such ε, we have $P_\varepsilon \subset \varDelta^{\rm ess}$, because $t \in P_\varepsilon$ implies $0 < |\eta(t)| \leq \eta(0)$, hence $t \in \varDelta^{\rm ess}$. From the symmetry of ϱ, we know that $t \in P_\varepsilon$ implies $-t \in P_\varepsilon$, while the triangle inequality shows that $t \in P_\varepsilon$ and $t' \in P_{\varepsilon'}$ results in $t + t' \in P_{\varepsilon+\varepsilon'}$. Thus:

Fact 2 *The sets P_ε are symmetric, and $P_\varepsilon + P_{\varepsilon'} \subset P_{\varepsilon+\varepsilon'}$.* $\square$

Axiom 4 For all $\varepsilon > 0$, the set P_ε is relatively dense.

Recall that a set $P \subset G$ is called *relatively dense* if there exists a compact set $K \subset G$ such that, for all $x \in G$, $(x+K) \cap P \neq \varnothing$. Equivalently, there exists a compact set $K \subset G$ with $P+K = G$, where $P+K := \{p+k \mid p \in P,\, k \in K\}$. Note that, together with Axiom 3^+, we will have that the P_ε are actually *Delone sets* if $0 < \varepsilon \leq 1$, i.e. they are both uniformly discrete and relatively dense.

Lemma 1 *If $t \in P_\varepsilon$, then $|\eta(x) - \eta(x+t)| < \eta(0)\,\sqrt{2}\,\varepsilon$, for all $x \in G$.*

Proof: If $t \in P_\varepsilon$, then $\left|1 - \frac{\eta(t)}{\eta(0)}\right|^{1/2} < \varepsilon$ by definition, which is equivalent to $|\eta(0) - \eta(t)| < \eta(0)\,\varepsilon^2$. This implies $0 \leq \eta(0) - \mathrm{Re}(\eta(t)) < \eta(0)\,\varepsilon^2$ where the positivity of the middle expression follows from $|\eta(t)| \leq \eta(0)$.

Recall that η is a positive definite function on all of G, so for arbitrary $x \in G$, we can invoke Krein's inequality, see [9, p. 12, Eq. (4)] or [20, p. 103]:

$$\big|\eta(x) - \eta(x+t)\big|^2 \;\leq\; 2\,\eta(0)\,\big(\eta(0) - \mathrm{Re}(\eta(t))\big).$$

Together with the previous estimate, this establishes the assertion. $\square$

The situation which we have outlined has a number of variations. It is not essential that the original measure ω be a Dirac comb. We do require that it be translation bounded and that its autocorrelation be a point measure supported on a closed discrete set. Certainly, ω could have some density 0 deviation from a Dirac comb without making any difference to the outcome. In fact, there is an entire class of measures ω, the so-called homometry class, all with the same autocorrelation. They cannot be distinguished by diffraction.

An important type of situation that we wish to point out is that in which S itself is a Delone subset of G with finite local complexity, i.e. $S - S$ is closed and discrete. In this case, we can associate with S the Dirac comb $\omega = \delta_S = \sum_{x \in S} \delta_x$, which obviously satisfies Axiom 1. If it also satisfies Axiom 2, we say that is has a well-defined autocorrelation (relative to the sequence $\mathcal{A}$). Axiom 3 is then already implicit in the finite local complexity, which has the geometric meaning that for any compact set $K \subset G$ there are only finitely many types of point sets $S \cap (a+K)$, up to translation, as a runs over G. Furthermore, in this case, it is possible to replace ϱ by the topologically equivalent but simpler pseudo-metric ϱ' which was mentioned in the Remark after Fact 1. We also say, by slight abuse of language, that S is ε-almost periodic if Axiom 4 holds. The results of Section 3 below apply to point sets S which satisfy these conditions.

Let us close this part with a basic result on the diffraction measure attached to an arbitrary $\omega \in \mathcal{M}^\infty(G)$ for a specified sequence $\mathcal{A}$ of (1). If the autocorrelation measure γ_ω exists as the limit of the $\gamma_\omega^{(n)}$ defined in (3), then $\gamma_\omega \in \mathcal{M}^\infty(G)$, see [22, Prop. 2.2] and our above Remark after Axiom 2. It is also positive definite because the positive definite measures are closed in the vague topology [9, p. 18]. As such, the measure γ_ω is transformable, i.e. there is a uniquely determined positive measure $\hat{\gamma}_\omega$ on $\hat{G}$ such that

$$\gamma_\omega(g * \tilde{g}) \;=\; \hat{\gamma}_\omega(|\tilde{\hat{g}}|^2)$$

for all $g \in \mathcal{K}(G)$, where $\hat{g}$ denotes ordinary Fourier transform on $L^1(G)$, compare [9, Thm. 4.7 and Cor. 4.8]. What is more, $\hat{\gamma}_\omega$ is also translation bounded [9, Prop. 4.9]. To summarize:

Fact 3 *Let G be a σ-compact LCA group, and $\omega \in \mathcal{M}^\infty(G)$. Let an averaging sequence $\mathcal{A}$ be fixed. If the corresponding autocorrelation γ_ω exists, it is a positive definite, translation bounded measure on G. Moreover, its Fourier transform $\hat{\gamma}_\omega$ exists and is a positive, translation bounded measure on $\hat{G}$, the dual group of G.* □

3 Construction of a cut and project scheme

The goal of this section is to establish how L is related, in a natural way, to a lattice in an appropriate extension of the LCA group G, and to use this connection to construct a cut and project scheme that will ultimately help us to prove the pure point diffractivity. Our assumptions in this Section are Axioms 1 – 4, but not Axiom 3^+.

An essential ingredient of our approach is the precompactness of certain sets. Recall that a subset P of the LCA group G is *precompact* (or totally bounded) if, for any open neighbourhood U of $0 \in G$, there is a *finite* set F so that $P \subset U + F$. Note that P is precompact if and only if the closure of its image in the Hausdorff completion is compact, compare [31, Ch. 13 A] and [12, Ch. II.4.2].

Lemma 2 *For all $0 < \varepsilon < 1$, the set P_ε is precompact in the AC topology.*

PROOF: In view of the above remark, it suffices to show that, for any $\varepsilon' > 0$, P_ε can be covered by finitely many translates of the set $P_{\varepsilon'}$ because the latter form a fundamental system of neighbourhoods. Let $0 < \varepsilon < 1$ be fixed, and choose any ε' with $0 < \varepsilon' < 1 - \varepsilon$. Since $P_{\varepsilon'}$ is relatively dense, there exists a compact set $K \subset G$ such that $P_{\varepsilon'} + K = G$.

Let $t \in P_\varepsilon$ and write $t = s + k$ with $s \in P_{\varepsilon'}$ and $k \in K$. Then we get

$$t - s \;\in\; P_\varepsilon - P_{\varepsilon'} \;=\; P_\varepsilon + P_{\varepsilon'} \;\subset\; P_{\varepsilon+\varepsilon'}$$

from Fact 2. We conclude that $k = t - s \in F := (K \cap P_{\varepsilon+\varepsilon'}) \subset L$ which is a *finite* set because $\varepsilon + \varepsilon' < 1$ by construction, so we know that $P_{\varepsilon+\varepsilon'} \subset \varDelta^{\mathrm{ess}}$ which is discrete and closed. So, $t \in P_{\varepsilon'} + F$, and hence $P_\varepsilon \subset P_{\varepsilon'} + F$. This being true for all $0 < \varepsilon' < 1 - \varepsilon$, it is clearly true for all $\varepsilon' > 0$ and our assertion follows. □

Note that the proof does *not* extend to $\varepsilon = 1$. In fact, we presently see no general reason for $P_1 = \varDelta^{\mathrm{ess}}$ to be precompact. However, it is precompact if S (the support of ω) is a model set, or the set of visible lattice points.

Let us now define H to be the (Hausdorff) completion of L of (6) in the AC topology. We then know that a uniformly continuous mapping $\varphi\colon L \to H$ exists with the following properties:

C1 The image $\varphi(L)$ is dense in H.

C2 The mapping φ is an open mapping from L onto $\varphi(L)$, the latter with the induced topology of the completion H.

C3 We have $\ker(\varphi) =$ closure of $\{0\}$ in L.

In fact, these three properties characterize (H, φ) as *the* completion of L, in the sense that it is unique up to isomorphism. Note that the condition for φ to be an embedding is

$$\ker(\varphi) \;=\; \bigcap_{\varepsilon>0} P_\varepsilon \;=\; \{0\}\,.$$

Since this characterization of the completion is not entirely standard, we add a few comments. Since the Hausdorff completion is unique up to isomorphism, the three properties follow rather directly from the universal characterization in [12, Thm. II.3.3] (recall that a bijection π between two uniform spaces is an isomorphism if and only if both π and its inverse are uniformly continuous [12, Prop. I.2.2 (b)]). Conversely, given φ with the three properties, one compares with the Hausdorff completion, which now brings in another mapping, $\psi\colon L \to \hat{L}$ say. Then, the existence of a uniformly continuous mapping $\pi\colon \hat{L} \to H$ with $\pi \circ \psi = \varphi$ is assured. Comparing kernels, one concludes that π is one-to-one on $\psi(L)$. So, with the open mapping property of φ, we may conclude that the dense subsets $\varphi(L)$ and $\psi(L)$ are isomorphic (via π), and this then extends to an isomorphism between H and $\hat{L}$ by the Corollary of [12, Thm. II.3.2].

Proposition 1 *The completion H is a locally compact Abelian group.*

Proof: That H is a topological group and Abelian is an immediate consequence of the completion procedure. For the local compactness, it is sufficient to show that $0 \in H$ has a compact neighbourhood. Fix some $0 < \varepsilon < 1$. The set P_ε is precompact (Lemma 2), hence $\overline{\varphi(P_\varepsilon)} \subset H$ is compact, compare [31, Thm. 13.2]. It is, in fact, a neighbourhood of $0 \in H$.

To see this, observe that $\varphi(P_\varepsilon) = \varphi(L) \cap V$ for some open set $V \subset H$ because of property C2. If $v \in \overline{V}$, for every open neighbourhood N of v, $N \cap V \neq \varnothing$, hence also $N \cap V \cap \varphi(L) = N \cap \varphi(P_\varepsilon) \neq \varnothing$. Consequently, $v \in \overline{\varphi(P_\varepsilon)}$ and $\overline{V} = \overline{\varphi(P_\varepsilon)}$. □

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

Lemma 3 *The set $\tilde{L}$ is uniformly discrete in $G \times H$.*

Proof: Fix some ε with $0 < \varepsilon < 1$ and choose an open set $V \subset H$ such that $V \cap \varphi(L) = \varphi(P_\varepsilon)$, which is always possible due to property C2. Let U be a compact neighbourhood of $0 \in G$ and assume that $(t, \varphi(t)) \in U \times V$ for some $t \in L$. Then $\varphi(t) \in V \cap \varphi(L) = \varphi(P_\varepsilon)$ which implies $t \in P_\varepsilon$, hence also $t \in U \cap P_\varepsilon = F$ where F is a finite set. Consequently, $\tilde{L} \cap (U \times V)$ is finite, too.

Since $U \times V$ is a neighbourhood of $(0,0) \in G \times H$, $(0,0)$ is isolated in $\tilde{L}$, and by translation this is true of all points of $\tilde{L}$. The Hausdorff property of H then implies that $\tilde{L}$ is discrete, with a uniform separating neighbourhood, hence also uniformly discrete. □

For any subset $X \subset H$, we define

$$\Lambda(X) \; := \; \{x \in L \mid \varphi(x) \in X\}\,. \tag{9}$$

This type of construction of subsets in G plays an important role in the sequel.

Lemma 4 *For all $0 < \varepsilon < 1$, the compact set $W := \overline{\varphi(P_\varepsilon)}$ has non-empty interior, i.e. $\overset{\circ}{W} \neq \varnothing$.*

PROOF: From Lemma 2, P_ε is precompact (in L), so W, and also ∂W, is compact in the Hausdorff completion. Then $\varLambda(W)$ clearly contains P_ε and is thus relatively dense in G. The strategy will now be to show that $\varLambda(\partial W)$ is *not* relatively dense in G, hence $W \neq \partial W$, and $\overset{\circ}{W} \neq \varnothing$.

We employ Baire's theorem [31, Thm. 13.29 (b)] which applies to locally compact spaces, so H is of second category as a consequence of Proposition 1. Recall that $\varDelta = S - S$ is countable, so also $L = \langle \varDelta^{\text{ess}} \rangle_{\mathbb{Z}}$ is still countable, and $\varphi(L)$ is then a meagre subset of H. Since ∂W is nowhere dense, we know that a $c \in H$ exists such that $(c + \partial W) \cap \varphi(L) = \varnothing$. Let $K \subset G$ be any non-empty compact set. We then clearly have $\big(K \times (c + \partial W)\big) \cap \tilde{L} = \varnothing$.

If V_1 is a compact neighbourhood of 0, then $K \times (c + \partial W + V_1)$ is compact and $\big(K \times (c + \partial W + V_1)\big) \cap \tilde{L}$ is finite. We can then find a neighbourhood V of $0 \in H$ such that $\big(K \times (c + \partial W + V)\big) \cap \tilde{L} = \varnothing$.

Finally, since $\varphi(L)$ is dense in H, there exists $t \in L$ with $-\varphi(t) \in c + V$, so that $\big(K \times (-\varphi(t) + \partial W)\big) \cap \tilde{L} = \varnothing$. This implies $\big((t + K) \times \partial W\big) \cap \tilde{L} = \varnothing$ and hence $(t + K) \cap \varLambda(\partial W) = \varnothing$, where t depends on K. Since the compact set $K \subset G$ was arbitrary, this means $\varLambda(\partial W)$ is not relatively dense and our assertion follows. $\square$

Lemma 5 *The set $\tilde{L}$ is relatively dense in $G \times H$.*

PROOF: Fix some $0 < \varepsilon < 1$ and set $W = \overline{\varphi(P_\varepsilon)}$ as in Lemma 4. Since $P_\varepsilon \subset L$ is relatively dense in G by Axiom 4, there is a compact set $K \subset G$ such that $G = P_\varepsilon + K$. Consequently, $G \times \{0\} \subset \tilde{L} + \big(K \times (-W)\big)$, because any $x \in G$ now admits the decomposition

$$(x, 0) \;=\; (t + k, 0) \;=\; (t, \varphi(t)) + (k, -\varphi(t))$$

for some $t \in P_\varepsilon$ and $k \in K$, where $(t, \varphi(t)) \in \tilde{L}$.

Furthermore, $G \times H = \tilde{L} + (G \times W)$ since $\varphi(L)$ is dense in H by property C1 and $\overset{\circ}{W} \neq \varnothing$ by Lemma 4. With $G \times W = (G \times \{0\}) + (\{0\} \times W)$, we get

$$\begin{aligned} G \times H \;&=\; \tilde{L} + (G \times W) \;\subset\; \tilde{L} + \tilde{L} + \big(K \times (-W)\big) + (\{0\} \times W) \\ &=\; \tilde{L} + \big(K \times (W - W)\big) \;\subset\; G \times H. \end{aligned}$$

Consequently, $G \times H = \tilde{L} + \big(K \times (W - W)\big)$, and since $K \times (W - W)$ is compact, $\tilde{L}$ is relatively dense. $\square$

So, $\tilde{L}$ is a discrete subgroup of H, hence closed, and it is also relatively dense, hence co-compact. Thus:

Corollary 1 *The factor group $\mathbb{T} := (G \times H)/\tilde{L}$ is compact.* $\square$

In what follows, we give G the structure of a topological group in a new way that mixes its standard topology with the AC topology on L. The main result will be that the completion of G with respect to this new topology is precisely the group $\mathbb{T}$.

Consider $G \times L$ with the product topology, where G is given the standard topology it came with and L is given the AC topology that was introduced in Section 2. Let

$$\alpha : L \longrightarrow G \times L$$

be the diagonal map, i.e. $\alpha(t) = (t, t)$. For any open neighbourhood U of $0 \in G$ and any $\varepsilon > 0$, we then have

$$\alpha(L) \cap (U \times P_\varepsilon) \;=\; \{(t,t) \mid t \in U \cap P_\varepsilon\}$$

which is finite. Thus $\alpha(0)$ is isolated in $G \times L$ and $\alpha(L)$ is a closed discrete subgroup of $G \times L$.

Consequently, $(G \times L)/\alpha(L)$ is a topological group with the natural quotient topology. The natural map

$$\psi : G \times L \longrightarrow (G \times L)/\alpha(L)$$

is continuous and also open. Furthermore, $G \simeq (G \times L)/\alpha(L)$ through the mapping $x \mapsto (x, 0) \bmod \alpha(L)$, and in this way we obtain a new "mixed" topology on G. With $\varphi \colon L \to H$ as before, we have the following diagram:

$$\begin{tikzcd}
0 \arrow[r] & L \arrow[r, "\alpha"] \arrow[d, "\mathrm{id}"'] & G \times L \arrow[r, "\psi"] \arrow[d, "\mathrm{id}\times\varphi"'] & (G \times L)/\alpha(L) \arrow[r] \arrow[d, "\overline{\varphi}"] & 0 \\
0 \arrow[r] & L \arrow[r, "\mathrm{id}\times\varphi"] & G \times H \arrow[r, "\pi"] & \mathbb{T} = (G \times H)/\tilde{L} \arrow[r] & 0
\end{tikzcd}$$

Here, π is the natural map from $G \times H$ to $\mathbb{T}$, so that the two horizontal sequences are exact, and $\overline{\varphi}$ is the unique (continuous) homomorphism which makes the central block of the diagram commutative.

Proposition 2 *The mapping* $\overline{\varphi}\colon (G\times L)/\alpha(L) \longrightarrow \mathbb{T}$ *defines a completion of* $(G\times L)/\alpha(L)$*. In particular,* $\mathbb{T}$ *may be regarded as the Hausdorff completion of* G *with respect to the mixed topology.*

PROOF: Since $\mathbb{T}$ is a compact group, it is complete [12, Cor. II.3.1]. It suffices to establishes the three properties (C1)–(C3) for $(G\times L)/\alpha(L)$, $\mathbb{T}$, and $\overline{\varphi}$.

(I) $\mathrm{im}(\overline{\varphi})$ is dense in $\mathbb{T}$:
The closure of the image of $G\times L$ in $\mathbb{T}$ has a closed preimage in $G\times H$ which contains $G\times\varphi(L)$ and hence also $G\times H$.

(II) $\ker(\overline{\varphi})$ is the closure of $\{0\}$ in $(G\times L)/\alpha(L)$:
Certainly, $\ker(\overline{\varphi})$ is closed. Let $\psi(x,t)\in\ker(\overline{\varphi})$. This implies $(x,\varphi(t))\in\tilde{L}$, so $x\in L$ and $\varphi(x)=\varphi(t)$. Then $(t-x)\in\ker(\varphi)$ and $\psi(x,t)=\psi(0,t-x)$ is contained in $\psi\big(\{0\}\times\ker(\varphi)\big)$. Since $\ker(\varphi)$ is the closure of $\{0\}$ in L, each neighbourhood of $(t-x)$ in L contains 0. So, each neighbourhood of $\psi(x,t)$ must contain $\psi(0,0)$.

(III) $\overline{\varphi}$ is an open mapping onto $\mathrm{im}(\overline{\varphi})$, the latter equipped with the topology induced from $\mathbb{T}$:
Let $U\subset G$, $V\subset L$ be non-empty open sets. Then $\varphi(V)=W\cap\varphi(L)$ for some open set $W\subset H$ and

$$\begin{array}{ccc}
U\times V & \xrightarrow{\ \psi\ } & \psi(U\times V)\\
{\scriptstyle \mathrm{id}\times\varphi}\big\downarrow & & \big\downarrow{\scriptstyle\overline{\varphi}}\\
\begin{array}{c}U\times\varphi(V)=\\ (U\times W)\cap(G\times\varphi(L))\end{array} & \xrightarrow{\ \pi\ } & \begin{array}{c}\pi\big((U\times W)\cap(G\times\varphi(L))\big)=\\ \pi(U\times W)\cap\pi(G\times\varphi(L))\end{array}
\end{array}$$

The only part of this diagram which needs explanation is the equation in the bottom right hand corner. With the obvious notation, one gets

$$\begin{aligned}
\pi(u,w) &= \pi(x,\varphi(t)) \qquad \text{(for some } x\in G \text{ and } t\in L)\\
\Longrightarrow\ (u,w) &= (x,\varphi(t))+(s,\varphi(s)) \qquad \text{(for some } s\in L)\\
\Longrightarrow\ (u,w) &= (x+s,\varphi(t+s)) \in (U\times W)\cap\big(G\times\varphi(L)\big).
\end{aligned}$$

This completes the proof. □

REMARK: In plainer language, the new mixed topology on G can be described by saying that $x,y\in G$ are close if, for some small $v\in G$ and some $t\in P_\varepsilon$ with small $\varepsilon>0$, we have the relation $y=x+v+t$.

4 Diffraction

In this Section, we will be assuming Axioms 1, 2, 3^+, and 4. In particular, the constructions and results of Section 3 are in force.

The plan is now to use the relation between G and $\mathbb{T}$ to derive the nature of the Fourier transform of the autocorrelation γ_ω. This will be achieved by first regularizing it through the convolution with suitable continuous functions, then studying the properties of their Fourier transforms, and later transfering them to $\hat{\gamma}_\omega$ via appropriate limits.

So, let $c \in \mathcal{K}(G)$ be a real valued and non-negative function. Then also $c * \tilde{c} \in \mathcal{K}(G)$, i.e. it has compact support. Consequently, $g_c = (c * \tilde{c}) * \gamma_\omega$ is a well-defined bounded continuous function, see [9, Prop. 1.12], because γ_ω is translation bounded. It is also a positive definite function by construction, hence transformable, i.e. its Fourier transform exists and is a finite positive measure on the dual group, $\hat{G}$, by Bochner's theorem [9, Thm. 3.12]. Using the convolution theorem [9, Prop. 4.10], we see that

$$\hat{g}_c \; = \; |\hat{c}|^2 \, \hat{\gamma}_\omega$$

where $\hat{c}$ is a continuous function on $\hat{G}$.

Let us find out more about $\hat{g}_c$. Observe first that g_c is a positive definite function which is real and certainly continuous at $0 \in G$. By [9, Prop. 3.10], it is then automatically a uniformly continuous function on G in the original topology. But in view of our assumptions, we can show more:

Lemma 6 *The function g_c is uniformly continuous in the mixed topology.*

PROOF: It is sufficient to show that, for all $\varepsilon > 0$, $t \in P_\varepsilon$ implies the estimate $|g_c(x) - g_c(x+t)| \le C\varepsilon$ for all $x \in G$ and for some $C = C(c)$. A direct calculation shows

$$g_c(x) \; = \sum_{z \in \Delta^{\mathrm{ess}}} \eta(z) \, \big(c * \tilde{c}\big)(x - z) \; = \; \sum_{z \in L} \eta(z) \, \big(c * \tilde{c}\big)(x - z) \, .$$

Consequently, for $t \in P_\varepsilon$, where $P_\varepsilon \subset L$, one obtains

$$\begin{aligned}
\big|g_c(x) - g_c(x+t)\big| \; &= \; \Big| \sum_{z \in L} \big(\eta(z) - \eta(z+t)\big) \, \big(c * \tilde{c}\big)(x - z) \Big| \\
&\le \; \|c * \tilde{c}\|_\infty \sum_{z \in F_x} \big|\eta(z) - \eta(z+t)\big| \\
&\le \; \|c * \tilde{c}\|_\infty \, \sqrt{2} \, \eta(0) \, \mathrm{card}(F_x) \, \varepsilon
\end{aligned}$$

where Lemma 1 was used in the last step and F_x is given by

$$F_x = \big(\varDelta^{\mathrm{ess}} \cap (x - \mathrm{supp}(c * \tilde{c}))\big) \cup \big((-t + \varDelta^{\mathrm{ess}}) \cap (x - \mathrm{supp}(c * \tilde{c}))\big).$$

This is a finite set because $\varDelta^{\mathrm{ess}}$ is closed and discrete by Axiom 3 and $(c * \tilde{c})$ has compact support. In fact, by Axiom 3^+, the cardinality of F_x is uniformly bounded in x by a constant that is independent of t, so our above estimate is uniform in x and the assertion follows. $\square$

The purpose of this exercise is that we can now extend g_c to a uniquely defined uniformly continuous function on $\mathbb{T}$, the completion of G with the mixed topology. We will call this new function $g_c^{\mathbb{T}}$.

As the uniformly continuous extension of g_c, also $g_c^{\mathbb{T}}$ is a continuous positive definite function, this time on all of $\mathbb{T}$. By Bochner's theorem, see [9, Thm. 3.12] or [33, Thm. 1.4.3], there is a uniquely defined finite positive measure μ_c on the dual group, $\hat{\mathbb{T}}$, so that

$$g_c^{\mathbb{T}}(x) \;=\; \int_{\hat{\mathbb{T}}} \langle k, x\rangle \,\mathrm{d}\mu_c(k)$$

for all $x \in G$. Here, $\langle k, \cdot\rangle$ denotes the continuous character on $\mathbb{T}$ attached to $k \in \hat{\mathbb{T}}$. Furthermore, since $\mathbb{T}$ is compact, $\hat{\mathbb{T}}$ is discrete, and we thus get a representation of $g_c^{\mathbb{T}}$ as an absolutely convergent Fourier series, i.e.

$$g_c^{\mathbb{T}}(x) \;=\; \sum_{k \in \hat{\mathbb{T}}} a_c(k)\, \langle k, x\rangle \tag{10}$$

where equality holds for all $x \in \mathbb{T}$, compare [15, Thm. 2.8.4 (ii)]. Here, the $a_c(k)$ are the non-negative numbers

$$a_c(k) \;=\; \int_{\mathbb{T}} \overline{\langle k, x\rangle}\, g_c^{\mathbb{T}}(x)\, \mathrm{d}\theta_{\mathbb{T}}(x) \;=\; \mu_c(\{k\}) \;\geq\; 0$$

with $\sum_{k\in\hat{\mathbb{T}}} a_c(k) = g_c^{\mathbb{T}}(0) < \infty$.

We have already proved that the canonical homomorphism $\beta \colon G \to \mathbb{T} = (G \times H)/\tilde{L}$ is given by

$$x \;\mapsto\; (x, 0) \bmod \tilde{L}\,.$$

This leads to a mapping $C(\mathbb{T}, \mathbb{C}) \to C(G, \mathbb{C})$ where $h^{\mathbb{T}} \mapsto h^{\mathbb{T}} \circ \beta$ and, in particular, to an injective mapping $\hat{\beta} \colon \hat{\mathbb{T}} \simeq \tilde{L}^{\circ} \to \hat{G}$. Here, $\tilde{L}^{\circ}$ is the dual of the lattice $\tilde{L}$, i.e. the space of all continuous homomorphisms of $G \times H \to \mathbb{C}$ that are trivial on $\tilde{L}$. Since $\beta(G)$ is dense in $\mathbb{T}$, $\hat{\beta}$ is one-to-one.

For $k \in \hat{\mathbb{T}}$, we write ℓ_k for the corresponding character on G attached to $\hat{\beta}(k)$, i.e. $\ell_k(x) = \langle k, \beta(x)\rangle$. Thus, with (10), we now obtain for the function g_c the expansion

$$g_c(x) \; = \; \sum_{k\in\hat{\mathbb{T}}} a_c(k)\, \ell_k(x)$$

which is convergent for all $x \in G$. Consequently, for all $h \in \mathcal{K}(\hat{G})$,

$$\begin{aligned}
\big(\hat{g}_c, h\big) \; &= \; \big(g_c, \hat{h}\big) \; = \; \int_G \hat{h}(x) \sum_{k\in\hat{\mathbb{T}}} a_c(k)\, \ell_k(x)\, \mathrm{d}\theta_G(x) \\
&= \; \sum_{k\in\hat{\mathbb{T}}} a_c(k) \int_G \hat{h}(x)\, \ell_k(x)\, \mathrm{d}\theta_G(x) \; = \; \sum_{k\in\hat{\mathbb{T}}} a_c(k)\, h(\hat{\beta}(k)) \\
&= \; \Big(\sum_{k\in\hat{\mathbb{T}}} a_c(k)\, \delta_{\hat{\beta}(k)}, h \Big)
\end{aligned}$$

where the interchange of the sum and the integral is justified by the summability of $\sum_{k\in\hat{\mathbb{T}}} a_c(k)$. This shows that $\hat{g}_c$ is a positive pure point measure,

$$\hat{g}_c \; = \; \sum_{\ell\in L^\circ} a_c\big(\hat{\beta}^{-1}(\ell)\big)\, \delta_\ell\,, \tag{11}$$

with $L^\circ = \hat{\beta}(\tilde{L}^\circ)$.

The next step consists in choosing a net of functions $(c_U)_{U\in\mathcal{U}}$ that constitutes an *approximate unit*, compare [9, Def. 1.6], where $\mathcal{U}$ is a basis for the neighbourhood filter of $0 \in G$.

So, let $c_U \in \mathcal{K}(G)$ be a non-negative function, with $\mathrm{supp}(c_U) \subset U$ and normalization according to $\int_G c_U(x)\, \mathrm{d}\theta_G = 1$, and let the net of probability measures $c_U\, \theta_G$ converge to δ_0 in the vague topology. Such a net exists for all LCA groups. Then also $(c_U * \tilde{c}_U)\, \theta_G \to \delta_0$ vaguely, and the 'forward version' of Levy's continuity theorem [9, Thm. 3.13] gives us compact convergence of $|\hat{c}_U|^2$ towards $\hat{\delta}_0 \equiv 1$ on $\hat{G}$. For simplicity of notation, we now write

$$\gamma_U \; := \; g_{c_U} \; = \; c_U * \tilde{c}_U * \gamma_\omega\,.$$

By what we have just seen, $\hat{\gamma}_U$ is a positive pure point measure on $\hat{G}$, supported on L°. Also, $\hat{\gamma}_U = |\hat{c}_U|^2\, \hat{\gamma}_\omega$ by the convolution theorem.

Proposition 3 *Let $(c_U)_{U\in\mathcal{U}}$ be a normalized regularization net of δ_0 as described above, and let ω be the Dirac comb of* (2). *Then the measures $\hat{\gamma}_U$ converge to $\hat{\gamma}_\omega$, both in the vague and in the local norm topology.*[1]

[1]For all compact $K \subset \hat{G}$, $\|(\hat{\gamma}_U - \hat{\gamma}_\omega)|_K\| \to 0$, where $\|.\|$ is the usual variation norm.

PROOF: The vague convergence is a direct consequence of the continuity of the Fourier transform. To show the second assertion, we have to demonstrate that the restriction of $\hat{\gamma}_U$ to any compact set $K \subset \hat{G}$ norm converges to the restriction of $\hat{\gamma}_\omega$ to K.

Let $K \subset \hat{G}$ be compact and fix $\varepsilon > 0$. From the above, we know that $\sup_{x\in K} \big| |\hat{c}_U(x)|^2 - 1 \big| < \varepsilon$, for all sufficiently small neighbourhoods U of $0 \in G$. Since $\hat{\gamma}_\omega$ is a positive measure, we then also have

$$\big\| \big(\hat{\gamma}_U - \hat{\gamma}_\omega\big)\big|_K \big\| \;=\; \int_K \big| |\hat{c}_U|^2 - 1 \big| \,\mathrm{d}\hat{\gamma}_\omega \;\leq\; \int_K \sup_{x\in K} \big| |\hat{c}_U(x)|^2 - 1 \big| \,\mathrm{d}\hat{\gamma}_\omega \;\leq\; \varepsilon\, \hat{\gamma}_\omega(K)$$

from which the assertion follows. □

Proposition 3 is an important cornerstone because both the absolutely continuous and the pure point measures are norm closed subsets in the cone of positive measures, compare [32, Ch. IV.5]. This rests upon the equation $|\nu_1 + \nu_2| = |\nu_1| + |\nu_2|$ which is valid if $\nu_1 \perp \nu_2$, i.e. for measures which are mutually singular. In particular, this applies if ν_1 is pure point and ν_2 continuous. If a sequence of pure point measures μ_n norm converges to $\mu = \mu_{\rm pp} + \mu_{\rm cont}$, one can then show that, for any compact set K and any $\varepsilon > 0$, $|\mu_{\rm cont}|(K) < \varepsilon$, hence $\mu_{\rm cont} = 0$. By construction, the $\hat{\gamma}_n$ are all pure point measures and form a norm-converging sequence. The limit $\hat{\gamma}_\omega$ is thus also a positive pure point measure, and translation bounded by Fact 3. To summarize:

Theorem 1 *Let G be a σ-compact LCA group. If the Dirac comb ω of* (2)*, seen as a complex measure on G, and its autocorrelation γ_ω relative to the averaging sequence $\mathcal{A}$ of* (1) *satisfy Axioms* 1, 2, 3^+*, and* 4*, then the corresponding diffraction measure $\hat{\gamma}_\omega$ on the dual group $\hat{G}$ is a translation bounded, positive pure point measure.* □

5 Diffraction in model sets

A *cut and project scheme* is a triple $(G, J, \tilde{M})$ consisting of a pair of LCA groups G, J and a lattice $\tilde{M} \subset G \times J$ for which the canonical projections $\pi_G : G \times J \longrightarrow G$ and $\pi_J : G \times J \longrightarrow J$ satisfy

1. $\pi_G|_{\tilde{M}}$ is one-to-one and

2. $\pi_J(\tilde{M})$ is dense in J.

We write $M := \pi_G(\tilde{M})$, so M is a subgroup of G and note that the mapping

$$(\ )^* \ := \ \pi_J \circ (\pi_G|_{\tilde{M}})^{-1} : \ M \longrightarrow J \tag{12}$$

has dense image in J. Note that, for $x \in \tilde{M}$, $(\pi_G|_{\tilde{M}})^{-1}(x) = (\pi_G)^{-1}(x) \cap \tilde{M}$ which is a single point by our assumption on π_G. We will denote by θ_G and θ_J a fixed pair of Haar measures on G and J.

Let us summarize our findings of Section 3 for later use.

Proposition 4 *Let G, J be LCA groups, and assume that G is also σ-compact. Then $(G, H, \tilde{L})$ with $\tilde{L}$ as constructed in Section 3 constitutes a cut and project scheme, where H is the Hausdorff completion of $L = \langle \varDelta^{\mathrm{ess}} \rangle_{\mathbb{Z}}$ in the AC topology. Moreover, $\pi_G(\tilde{L}) = L$ and φ is the $*$-mapping of* (12), *hence $\pi_H(\tilde{L}) = \varphi(L)$.* □

A set $\varLambda \subset G$ is a *regular model set* for the cut and project scheme $(G, J, \tilde{M})$ if there is a relatively compact set $W \subset J$ with non-empty interior and with boundary of Haar measure 0 such that

$$\varLambda \ = \ \varLambda(W) \ := \ \{\pi_G(y) \mid y \in \tilde{M}, \, \pi_J(y) \in W\} \ = \ \{x \in M \mid x^* \in W\} \, . \tag{13}$$

The word *regular* refers to the assumption on W that its boundary, ∂W, has measure 0. The assumption that W has non-empty interior is the non-trivial case of what we are about to consider, and assures that the set $\varLambda$ is relatively dense in G (though this is not necessary for what follows).

A *weighted subset* of G is a subset $\varLambda$ of G together with a (bounded) mapping $w : \varLambda \longrightarrow \mathbb{C}$, which we will assume to be bounded throughout this paper.

Theorem 2 *Let $(G, J, \tilde{M})$ be a cut and project scheme with LCA groups G and J, where G is also σ-compact. Let $W \subset J$ be relatively compact with boundary of Haar measure* 0. *Let f be any complex-valued function on J which is supported and continuous on $\overline{W}$. Define a weighting w on $\varLambda(W)$ by $w(x) := f(x^*)$. Let ω be the Dirac comb $\omega = \sum_{x \in \varLambda} w(x) \delta_x$. Then, for any van Hove sequence $\{A_n\}$ in G, the corresponding diffraction measure $\hat{\gamma}_\omega$ is translation bounded, positive and pure point. In particular, the weighted model set $(\varLambda(W), w)$ is pure point diffractive.*

This result, in various degrees of generality, has been proved by A. Hof [22], B. Solomyak [37], and M. Schlottmann [36]. These proofs are all based upon the pointwise ergodic theorem for uniformly ergodic dynamical systems, following or extending Dworkin's argument [14]. Below, we present an alternative derivation which rests on our above results. To our knowledge, this is the first proof that links Theorem 2 directly back to almost periodicity rather than dynamical systems and ergodic theory. For more on van Hove sequences, see the Appendix.

The strategy of the proof is to show that the hypotheses of Theorem 1 are satisfied. For this, the main ingredient is a version of Weyl's theorem on uniform projection. In the form stated here, it is [6, Thm. 6.2], and the explicit proof given there is based on the version of Weyl's theorem in [35]. A new direct proof and a variant without the assumption $\theta_J(\partial W) = 0$ is derived in [30].

Theorem 3 (Weyl) *Assuming the notation and prerequisites of Theorem 2,*

$$\lim_{n\to\infty} \frac{1}{\theta_G(A_n)} \sum_{x\in\varLambda(W)\cap A_n} f(x^*) \; = \; C \int_W f \, \mathrm{d}\theta_J \, , \tag{14}$$

where C is a positive contstant that depends only on the choice of the Haar measures on G and J and on the lattice $\tilde{M}$. □

Proof of Theorem 2: We fix, once and for all, a van Hove sequence $\{A_n\}$ in G. It is clear that ω is a translation bounded measure since the set $\varLambda$ is uniformly discrete and the values of f are bounded in absolute value. Furthermore,

$$\eta_n(z) \; = \; \frac{\big(\omega_n * \tilde{\omega}_n\big)(\{z\})}{\theta_G(A_n)} \; = \; \frac{1}{\theta_G(A_n)} \sum_{\substack{x,y\in\varLambda\cap A_n \\ x-y=z}} f(x^*)\overline{f(y^*)} \, . \tag{15}$$

Note that z^* is well-defined since z lies in M. Using the function $f\,\overline{T_{z^*}(f)}$ in Weyl's theorem (where T_a denotes the shift by a) we obtain

$$\eta(z) \; = \; \lim_{n\to\infty} \frac{\big(\omega_n * \tilde{\omega}_n\big)(\{z\})}{\theta_G(A_n)} \; = \; C \int_W f(u)\overline{f(u-z^*)} \, \mathrm{d}\theta_J(u) \, . \tag{16}$$

In particular, the autocorrelation exists. Also, since $\varLambda - \varLambda \subset \varLambda(W-W)$ and $W-W$ has compact closure, we obtain that $\varLambda - \varLambda$ is uniformly discrete, and the essential support of the autocorrelation of ω is thus uniformly discrete.

It remains to prove the ε-almost periodicity. For this it suffices to show that, for all $\varepsilon > 0$, the set of points $z \in M$ for which $|\eta(0) - \eta(z)| < \varepsilon$ is relatively dense. Choose $\varepsilon > 0$. Then

$$\begin{aligned} |\eta(0) - \eta(z)| &= \left| C \int_W f(u) \overline{\bigl(f(u) - f(u - z^*)\bigr)} \, \mathrm{d}\theta_J(u) \right| \\ &\leq C \int_W |f(u)| \, |f(u) - f(u - z^*)| \, \mathrm{d}\theta_J(u) \, . \end{aligned}$$

Write $W = (W \cap (z^* + W)) \cup (W \backslash (z^* + W))$ and split the integral accordingly. Using the uniform continuity of f on $W \cap (z^* + W)$ we can find a neighbourhood V_1 of 0 so that, for all $z^* \in V_1$, the term with the integral over $W \cap (z^* + W)$ is bounded by $\varepsilon/2$. Using the boundedness of f and the uniform continuity of

$$\int_{W \backslash (u+W)} 1 \, \mathrm{d}\theta_J = \theta_J(W) - \bigl(\mathbf{1}_W * \tilde{\mathbf{1}}_W\bigr)(u) \qquad (17)$$

as a function of u, we can find a second neighbourhood V_2 of 0 on which the term with the integral over $W \backslash (z^* + W)$ is bounded by $\varepsilon/2$. Thus we obtain $|\eta(0) - \eta(z)| < \varepsilon$ for all $z \in \varLambda(V_1 \cap V_2)$. Since this set is relatively dense ($V_1 \cap V_2$ is open) and a subset of P_ε, the latter is also relatively dense. $\square$

Let us now come back to the discussion of Section 3, more precisely to the structure of the sets P_ε of ε-almost periods. If $0 < \varepsilon < 1$, the set $W = \overline{\varphi(P_\varepsilon)}$ has non-empty interior according to Lemma 4. This now has the immediate consequence that each such P_ε is a subset of a model set, i.e. $P_\varepsilon \subset \varLambda(W)$ in the setting of Eq. (9). Since we also have

$$\overline{\varphi(P_\varepsilon)} \subset \{ t \in H \mid \bar{\varrho}(t, 0) \leq \varepsilon \} \, ,$$

where $\bar{\varrho}$ means the (pseudo-)metric on H induced by ϱ, the difference between $\varLambda(W)$ and P_ε is a subset of $\{ t \in L \mid \varrho(t, 0) = \varepsilon \}$. If our original set S itself is a model set, then this property of the P_ε relates to the fact that also $S - S$ is a model set [29], which, in turn, contains the P_ε for all $0 < \varepsilon < 1$. Moreover, since L is countable, a difference between $\varLambda(W)$ and P_ε is possible for at most countably many values of ε. For all other values, the sets P_ε *are* the model sets determined by their closures, so that $\varDelta^{\mathrm{ess}}$ is actually the union of an ascending sequence of model sets.

6 Diffraction from visible lattice points

Let $\varGamma$ be a lattice in $\mathbb{R}^n$. If a basis is chosen, we can write the points of $\varGamma$ as $t = (t_1, \ldots, t_n)$ with $t_i \in \mathbb{Z}$, abbreviating the corresponding linear combination. Such a point is called *visible* if $\gcd(t_1, \ldots, t_n) = 1$. The property of visibility does not depend on the lattice basis chosen. The set $V = V(\varGamma)$ of visible points of $\varGamma$ is uniformly discrete in $\mathbb{R}^n$, but it is not relatively dense. In fact, as follows from [7, Prop. 4], relative denseness cannot be restored by adding points of density 0. Nonetheless, if we fix a natural sequence $\mathcal{A}$, e.g. an increasing sequence of balls around the origin of $\mathbb{R}^n$, we have:

Proposition 5 *The set $V(\varGamma)$ is pure point diffractive, i.e. the Fourier transform of the autocorrelation of the Dirac comb $\omega_V := \sum_{x \in V(\varGamma)} \delta_x$ is a positive pure point measure.*

Proposition 5 was established in [7]. Here, we offer an alternative proof based on the fact that Axioms 1, 2, 3^+, and 4 are satisfied by ω_V. The visible points thus show that the regime of our axioms goes considerably beyond ordinary model sets (which are always relatively dense).

We need the fact, established in [7, Thms. 1 and 2], that the autocorrelation of ω_V, for the sequence $\mathcal{A}$ of increasing balls around 0, exists and is a pure point measure γ_{ω_V} supported on $\varGamma$. Its coefficient at $t \in \varGamma$ is

$$\eta(t) \; = \; \gamma_{\omega_V}\big(\{t\}\big) \; = \; \mathrm{dens}(\varGamma)\, \xi(n) \prod_{p \,|\, \mathrm{cont}(t)} \Big(1 + \frac{1}{p^n - 2}\Big) \tag{18}$$

where $\mathrm{dens}(\varGamma)$ is the density of $\varGamma$, $\mathrm{cont}(t) := \max\{k \in \mathbb{Z} \mid t \in k\varGamma\}$, and

$$\xi(n) \; = \; \prod_{p \text{ prime}} \Big(1 - \frac{2}{p^n}\Big).$$

We also note that

$$\mathrm{dens}(V) \; = \; \eta(0) \; = \; \mathrm{dens}(\varGamma)\, \xi(n) \prod_{p \text{ prime}} \Big(1 + \frac{1}{p^n - 2}\Big) \; = \; \frac{\mathrm{dens}(\varGamma)}{\zeta(n)}$$

where $\zeta(n)$ is Riemann's zeta function [7, Prop. 6].

In the notation of Section 2, we obtain $\varDelta^{\mathrm{ess}} = \varDelta = V - V = \varGamma$, and Axioms 1, 2, and 3^+ clearly hold. To establish Axiom 4, choose any $\varepsilon > 0$.

Then

$$\begin{aligned} t \in P_\varepsilon \quad &\Longleftrightarrow \quad 1 - \frac{\eta(t)}{\eta(0)} \, < \, \varepsilon^2 \\ &\Longleftrightarrow \quad \eta(t) > \eta(0)(1-\varepsilon^2) = \mathrm{dens}(V)(1-\varepsilon^2) \end{aligned}$$

Since $\zeta(n)\xi(n)\prod_{p \text{ prime}}\bigl(1+\frac{1}{p^n-2}\bigr) = 1$, we may choose N so that

$$\zeta(n)\,\xi(n) \prod_{\substack{p \text{ prime}\\ p\leq N}} \Bigl(1+\frac{1}{p^n-2}\Bigr) \; > \; 1-\varepsilon^2 \, .$$

If $p_1,\dots,p_k$ are all the primes $\leq N$ then it is immediate from (18) that, for all $t \in p_1\cdot\ldots\cdot p_k\varGamma$, we have

$$\eta(t) \; = \; \mathrm{dens}(V)\,\zeta(n)\,\xi(n) \prod_{p\,|\,\mathrm{cont}(t)} \Bigl(1+\frac{1}{p^n-2}\Bigr) \; > \; \mathrm{dens}(V)\,(1-\varepsilon^2)$$

so that $P_\varepsilon \supset p_1\cdot\ldots\cdot p_k\varGamma$ is relatively dense. □

The set $F(k)$ of integers in $\mathbb{R}$ which are free of kth power factors for some fixed k are also shown in [7] to form a pure point diffractive set. We can again see that this situation is covered by our present setup. This time, the key piece of information is that the autocorrelation for $F(k)$ is supported on $\mathbb{Z}$, and the coefficients are given by [7, Thm. 4]

$$\gamma_{\omega_F}(t) \; = \; \xi(k) \prod_{p^k\,|\,t} \Bigl(1+\frac{1}{p^k-2}\Bigr). \tag{19}$$

Otherwise, the argument is similar.

Let us mention that neither of the two examples of this Section is a model set as defined in Section 5, even though both can be described in a cut and project scheme with the adele ring over $\mathbb{Z}$ as internal space. The special situation met here is that, in each case, the corresponding window W is compact, but happens to be the boundary of another set, i.e. $W = \partial W'$. As such, W has empty interior, which lines up with the set of visible points (or the set of k-free integers) not being relatively dense. To make matters worse, W has positive measure, see [7] for details. The concept of *weak model set* introduced in [30] includes such sets, but the original diffraction results of [22, 36] do not apply and the original proof of pure point diffraction in [7] is rather painful. It is thus somewhat astonishing to observe that, in our present setting with almost periodicity, examples such as the visible points turn out to be relatively harmless.

7 Fibonacci chain as model set

For many tilings and point sets of importance, an explicit cut and project scheme is known, or even is the only known way to define it. However, perhaps the most famous ones, such as the Penrose tiling, are defined through substitution rules or through perfect matching rules, and the additional possibility to describe it by projection is still somewhat mysterious. In particular, it is not clear what the intrinsic properties are which lead to the projection picture. Our above approach, at least in principle, allows to determine the internal group and thus the most natural cut and project scheme for a given pattern. We will explain this for the one-dimensional example of the Fibonacci chain, which already shows the key features. Strictly speaking, we will make use of the known cut and project scheme for it and only use the AC topology to justify the choice of internal space *a posteriori*. It is possible to avoid this, but then we would have to use the full machinery of substitution systems to evaluate the autocorrelation, which is not really enlightening.

The Fibonacci chain can be defined by means of the primitive two-letter substitution rule σ which sends $a \to ab$ and $b \to a$. A bi-infinite sequence can easily be obtained as a fixed point of σ^2,

$$a|a \xrightarrow{\sigma^2} aba|aba \xrightarrow{\sigma^2} \ldots \xrightarrow{\sigma^2} w$$

where $|$ denotes the origin or reference point, and convergence is in the obvious product topology. Both letters occur with positive frequency in the word w. A natural choice for a geometric realization is an interval of length $\tau = \big(1+\sqrt{5}\,\big)/2$ for a and another of length 1 for b. Let us now consider the set $\varLambda$ of left endpoints of this arrangement which is the ubiquitous Fibonacci point set. Its difference set $\varDelta = \varLambda - \varLambda$ is a subset of the ring $\mathbb{Z}[\tau]$ of integers in the quadratic field $\mathbb{Q}\big(\sqrt{5}\,\big)$. On the other hand, $\langle 1, \tau\rangle_{\mathbb{Z}} = \mathbb{Z}[\tau]$, whence we get $L = \mathbb{Z}[\tau]$ because 1 and τ are certainly in $\varDelta^{\mathrm{ess}}$.

It is known that $\varLambda$ is a model set [29]. It can be described as

$$\varLambda \;=\; \varLambda(W) \;=\; \{x \in \mathbb{Z} \mid x^* \in W\}$$

where $W = (-1, \tau - 1]$ is a half-open interval and $*$ denotes algebraic conjugation in $\mathbb{Q}\big(\sqrt{5}\,\big)$ as defined by $\sqrt{5} \mapsto -\sqrt{5}$. Also, $\varLambda - \varLambda$ is a model set, this time with window $[-\tau, \tau]$. Using this and Weyl's theorem on uniform distribution, see Theorem 3 above, one obtains a closed formula for the autocorrelation of $\varLambda$. If $z \in \mathbb{Z}[\tau]$, one has

$$\eta(z) \;=\; \frac{\operatorname{dens}(\varLambda)}{\operatorname{vol}(W)} \int_{\mathbb{R}} 1_W(\xi) 1_{W-z^*}(\xi) \,\mathrm{d}\xi \,, \tag{20}$$

where 1_W denotes the characteristic function of the set W, and $\eta(z) = 0$ otherwise. So, $\varrho(z,0)$ small means $\eta(z)$ close to $\eta(0)$, and the latter is tantamount to saying that z^* is small in the usual topology of $\mathbb{R}$. In other words, the Hausdorff completion of $L = \mathbb{Z}[\tau]$ in the AC topology is $\mathbb{R}$, and φ is nothing but the star map in this setting. This gives the promised a posteriori justification for the standard cut and project setup used for the Fibonacci chain.

It is perhaps remarkable that the star map is totally discontinuous in the original topology of $G = \mathbb{R}$, while it becomes uniformly continuous in the new AC topology, and, with hindsight, this could have been a guide to finding the extra topology much earlier.

Let us add that very much the same procedure works for many of the famous standard examples, see [2] and references given there for the zoo tamed so far. The above approach will always yield a setting that is equivalent to what is called the minimal embedding case in previous works. One particularly interesting case is the rhombic Penrose tiling, whose vertex set is commonly described either in terms of a projection from four or from 5 dimensions. The former is the minimal embedding case, but one then has to view the set as a multiple component model set. In our new setting, this would be reflected by H being the direct product $\mathbb{R}^2 \times C_5$ where C_5 is the cyclic group of order 5. If one insists on a Euclidean internal space, one can then embed C_5 into another copy of $\mathbb{R}$ which gives the common description with 3-space as internal group. However, this is not a cut and project scheme in the strict sense because the projection of the lattice into internal space is no longer dense, see [29] for details.

8 Period doubling chain as model set

Not all model sets in Euclidean space (i.e. with $G = \mathbb{R}^n$) can be desribed with an internal group H that is also Euclidean, and there are relevant examples [8] where one has to go beyond. With our above setting, one is able to actually determine the internal space also in this situation. We will now illustrate this for the example of the period doubling point set, where H will turn out to be 2-adic. The resulting point set is an example of a Toeplitz sequence and has been studied before, see [17] and references therein. What is new here is the derivation of the 2-adic integers from intrinsic data, extracted via the autocorrelation topology.

Let σ be the primitive two-letter substitution defined by $a \to ab$ and $b \to aa$. This is the well-known period doubling substitution [1, p. 301]. As above, a bi-infinite sequence can be obtained as fixed point of σ^2,

$$b|a \xrightarrow{\sigma^2} abab|abaa \xrightarrow{\sigma^2} \dots \xrightarrow{\sigma^2} w$$

where $|$ denotes again the origin or reference point. Note that this infinite word w is a so-called singular 2-cycle of σ because w and $\sigma(w)$ differ only at the position to the left of the marker, although they are locally indistinguishable. This is, however, of no relevance to our analysis because both w and $\sigma(w)$ are repetitive.

Let us realize the symbolic sequence as a 'coloured' point set in $\mathbb{R}$ by using an interval of length 1 for both symbols, a and b, but different types (colours) of endpoints. Let Λ_a and Λ_b denote the sets of left endpoints of all a- and b-intervals, so that $\Lambda_a \cup \Lambda_b = \mathbb{Z}$. Since σ^2 maps a to $abaa$ and b to $abab$, we obtain the equations

$$\begin{aligned} \Lambda_a &= 4\Lambda_a \cup (4\Lambda_a + 2) \cup (4\Lambda_a + 3) \cup 4\Lambda_b \cup (4\Lambda_b + 2) \\ \Lambda_b &= (4\Lambda_a + 1) \cup (4\Lambda_b + 1) \cup (4\Lambda_b + 3)\,. \end{aligned}$$

This can be simplified to the decoupled equations

$$\begin{aligned} \Lambda_a &= 2\mathbb{Z} \cup (4\Lambda_a + 3) \\ \Lambda_b &= (4\mathbb{Z} + 1) \cup (4\Lambda_b + 3) \end{aligned}$$

which, by iteration, leads to the solution

$$\Lambda_a = \bigcup_{n\geq 0} \big(2 \cdot 4^n\mathbb{Z} + (4^n - 1)\big) \tag{21}$$

$$\Lambda_b = \bigcup_{n\geq 1} \big(4^n\mathbb{Z} + (2 \cdot 4^{n-1} - 1)\big) \,\cup\, \{-1\}, \tag{22}$$

The rôle of $\{-1\}$ is exceptional since the other fixed point of σ^2 (where the b at -1 is replaced by an a, see above) has $-1 \in \Lambda_a$ rather than in Λ_b. Fortunately, this is of no relevance to the autocorrelation, and we will simply suppress the point (-1) in the following calculations. Since both point sets consist of disjoint unions of translates of lattices whose lattice constants increase as powers of 4, they are examples of what is usually called a limit periodic point set [18, p. 160].

We are ultimately interested in understanding Λ_a and Λ_b in terms of our above concepts, which needs the knowledge of the autocorrelation. We will sketch how this can be calculated in this case, without going too much into detail. The idea is to approximate the sets by periodic point sets obtained from *finite* unions in (21) and (22), and to use Poisson's summation formula for the approximants to determine their diffraction measures via the usual intensity formula, i.e. by the fact that the diffraction intensities of a periodic structure are the absolute square of the corresponding amplitudes (or Fourier-Bohr coefficients). The autocorrelation is then obtained by inverse Fourier transform, and each step can easily be made rigorous because all approximations involved here are appropriately convergent.

So, let $\omega_a = \sum_{x\in\Lambda_a} \delta_x$ be the Dirac comb attached to Λ_a, and similarly for ω_b, however with the point measure at $x = -1$ removed. In view of the terms in (21) and (22), Poisson's summation formula gives

$$\begin{aligned}
\hat{\omega}_a &= \sum_{n\geq 0} \frac{e^{-2\pi i k(4^n-1)}}{2\cdot 4^n}\, \delta_{\mathbb{Z}/2\cdot 4^n} \\
\hat{\omega}_b &= \sum_{n\geq 1} \frac{e^{-2\pi i k(2\cdot 4^{n-1}-1)}}{4^n}\, \delta_{\mathbb{Z}/4^n}
\end{aligned}$$

where δ_Γ is the uniform Dirac comb of a lattice Γ and k is the wave number, i.e. the variable of the function in front of the point measures. A short reflection shows that the point measures are supported on the set

$$F \;=\; \Big\{ \frac{m}{2^r} \mid (r=0,\, m\in\mathbb{Z}) \text{ or } (r\geq 1,\, m \text{ odd}) \Big\} \tag{23}$$

which we will use as a parametrization of the support from now on.

For a superposition $\omega = \alpha\,\omega_a + \beta\,\omega_b$, the diffraction would then be

$$\hat{\gamma}_\omega \;=\; \sum_{k\in F} |\alpha A(k) + \beta B(k)|^2\, \delta_k \tag{24}$$

where the amplitudes, after a straightforward though somewhat lengthy calculation, turn out to be

$$A(k) \;=\; \frac{2}{3}\,\frac{(-1)^r}{2^r}\, e^{2\pi i k} \tag{25}$$

$$B(k) \;=\; \delta_{r,0} - A(k) \tag{26}$$

for any $k \in F$ of (23), and with $\delta_{r,0}$ being Kronecker's function. Choosing $\beta = 0$ and $\alpha = 1$ in (24), one obtains, by inverse Fourier transform, the autocorrelation of ω_a as

$$\gamma_a \; = \; \sum_{z\in\mathbb{Z}} \eta_a(z)\, \delta_z$$

with the autocorrelation coefficients

$$\eta_a(z) \; = \; \frac{2}{3} \cdot \begin{cases} 1 & \text{if } z = 0, \\ \left(1 - \frac{1}{2^{\ell+1}}\right) & \text{if } z = (2m+1)2^{\ell},\, \ell \geq 0. \end{cases} \tag{27}$$

For completeness, let us add that the other autocorrelation coefficients are

$$\eta_b(z) \; = \; \eta_a(z) - \frac{1}{3}$$

for all $z \in \mathbb{Z}$, while those for the correlation between the two types of points turn out to be

$$\eta_{ab}(z) \; = \; \eta_{ba}(z) \; = \; \frac{2}{3} - \eta_a(z)$$

because we have $\eta_a(z) + \eta_b(z) + \eta_{ab}(z) + \eta_{ba}(z) = 1$ and the general inversion symmetry follows from the palindromicity of the period doubling sequence, see [3].

Let us return to $\eta_a(z)$ of (27). If $\varepsilon > 0$ is given, then we have

$$\left|\, \eta_a(0) - \eta_a\big((2m+1)2^{\ell}\big) \,\right| \; < \; \varepsilon$$

for all $\ell \geq \ell_0$ (with suitable ℓ_0), and the ε-almost periods of γ_a are thus relatively dense. This shows, without using the model set description, that the set Λ_a (and also Λ_b) conforms to Axiom 4, and hence to all Axioms needed to apply Theorem 1, so the set is pure point diffractive. We have actually already seen the explicit diffraction formula in (24).

The translation invariant pseudo-metric (7) on $\mathbb{Z}$ is given by

$$\varrho_a(z,0) \; = \; \left| 1 - \frac{\eta_a(z)}{\eta_a(0)} \right|^{1/2} \; = \; \begin{cases} 0 & \text{if } z = 0, \\ 2^{-(\ell+1)/2} & \text{if } z = (2m+1)2^{\ell},\, \ell \geq 0. \end{cases}$$

This clearly defines the 2-adic topology on $L = \mathbb{Z}$ and we conclude that the internal group H of Section 3 is the 2-adic completion $\overline{\mathbb{Z}}_2$ of $\mathbb{Z}$. The autocorrelation coefficient $\eta_b(z)$ leads to the same conclusion.

In this setting, $\bar{\varLambda}_a$ and $\bar{\varLambda}_b$ are compact subsets of $\overline{\mathbb{Z}}_2$ which satisfy

$$\begin{aligned} \bar{\varLambda}_a \cup \bar{\varLambda}_b &= \overline{\mathbb{Z}}_2 \\ \bar{\varLambda}_a \cap \bar{\varLambda}_b &= \{-1\}. \end{aligned}$$

From this, we can obtain the model set description

$$\varLambda_a \;=\; \varLambda(W_a)\;, \quad \varLambda_b \;=\; \varLambda(W_b)$$

with $W_a = \bar{\varLambda}_a \setminus \{-1\}$ and $W_b = \bar{\varLambda}_b$. If we had chosen the other fixed point of σ^2, $\{-1\}$ would have gone to W_a instead of W_b.

9 Extensions: Almost periodic measures

Our restriction so far to Dirac combs ω with an autocorrelation that is a pure point measure supported on a closed and discrete set (or on a uniformly discrete set, if we invoke Axiom 3^+) was motivated by the possibility of a constructive, direct proof of the diffraction results, and on the explicit construction of an internal space for the corresponding cut and project scheme. In the physical applications, such Dirac combs are valid idealizations, but one would also like to know the nature of the diffraction measure for more general translation bounded measures.

The first (and rather obvious) extension concerns the case that ω has the form

$$\omega \;=\; g * \delta_S \tag{28}$$

where δ_S is a Dirac comb of the original form considered in Eq. (2) and g is any finite measure, e.g. a (possibly continuous) L^1-function. This would describe a situation where the measure ω emerges from adding up 'local' contributions at the positions of the set S. In this case, the autocorrelation exists whenever that for δ_S does, and one obtains the convolution

$$\gamma_\omega \;=\; (g * \tilde{g}) * \gamma_S\,.$$

The diffraction measure, by the convolution theorem, reads

$$\hat{\gamma}_\omega \;=\; |\hat{g}|^2 \cdot \hat{\gamma}_S\,.$$

So, if a translation bounded measure ω admits a factorization as in (28), we can apply our previous analysis directly to the discrete part of it, δ_S, and obtain the result on the basis of the properties of S. So, if δ_S satisfies Axioms 1, 2, 3^+ and 4, also the diffraction measure $\hat{\gamma}_\omega$ is pure point. In particular, this situation applies to all lattice periodic measures which can always be written as in (28).

More interesting, however, is the question for a complete characterization of translation bounded measures ω with pure point diffraction measure. Such a characterization can be given on the basis of [19], however for the price of losing the constructive part of our above analysis.

For this, we have to work with the space $\mathcal{M}^\infty(G)$, but equipped with other topologies. Let us first introduce the (local) norm topology. Let K be a compact neighbourhood of $0 \in G$, which we assume fixed from now on. For $\omega \in \mathcal{M}^\infty(G)$, we set

$$\|\omega\|_K \;:=\; \sup_{x\in G} |\omega|(x+K) \tag{29}$$

where $|\omega|$ denotes the absolute value of ω, which is also translation bounded. In our setting, a measure ω is translation bounded iff $\|\omega\|_K < \infty$, see the remarks in [36, p. 145]. It is clear that $\|.\|_K$ defines a norm, and any other compact neighbourhood, K' say, would lead to an equivalent one, and hence to the same topology, because K' can be covered by finitely many translates of K and vice versa. Note that $\mathcal{M}^\infty(G)$ with this norm is actually a Banach space, see [19, Ex. 2.13 and Thm. 2.3].

In general, as was pointed out by Bochner [11], almost periodicity is better defined through a relative compactness criterion than through relative denseness of almost periods. So we say that a measure ω is *norm almost periodic* if the set of translates, $M_\omega := \{\delta_t * \omega \mid t \in G\}$, is relatively compact in the norm topology. In a Banach space, however, this is equivalent to saying that, for all $\varepsilon > 0$, the set $\{\, t \mid \|\delta_t * \omega - \omega\|_K < \varepsilon\}$ of norm ε-almost periods is relatively dense, compare [39, Thm. 7.1].

Proposition 6 *Let ω conform to Axioms* 1, 2, *and* 3^+. *Then its autocorrelation, γ_ω, satisfies Axiom* 4 *if and only if it is norm almost periodic.*

PROOF: We have $\omega \in \mathcal{M}^\infty(G)$ (Axiom 1) and $\gamma_\omega = \sum_{z\in\varDelta^{\rm ess}} \eta(z)\delta_z$ exists (Axiom 2), with $\varDelta^{\rm ess}$ uniformly discrete (Axiom 3^+). There is nothing to be shown if $\eta(0) = \gamma_\omega(\{0\}) = 0$, so let us assume $\eta(0) > 0$ from now on. If

$t \in L$, we have $t + L = L$. For arbitrary $x \in G$, we then obtain

$$
\begin{aligned}
|\delta_t * \gamma_\omega - \gamma_\omega| (x+K) \;&=\; \Big| \sum_{z\in L} \big(\eta(z-t) - \eta(z)\big)\, \delta_z \Big| (x+K) \\
&\leq\; \sum_{z\in L} \big|\eta(z-t) - \eta(z)\big|\, \delta_z(x+K) \\
&=\; \sum_{z\in F_x} \big|\eta(z-t) - \eta(z)\big|
\end{aligned}
$$

where $F_x = \big(\varDelta^{\mathrm{ess}} \cup (t + \varDelta^{\mathrm{ess}})\big) \cap (x+K)$ is a *finite* set. Its cardinality is bounded by a constant C, uniformly in x, due to the uniform discreteness of the set $\varDelta^{\mathrm{ess}}$. Let us choose C so that $\sup_{x\in G} \big(\mathrm{card}(F_x)\big) < C$.

Assume that Axiom 4 is in force. Fix $\varepsilon > 0$ and set $\varepsilon' = \varepsilon / \big(C\eta(0)\sqrt{2}\,\big)$. For any $t \in P_{\varepsilon'}$, we then obtain from Lemma 1 that $|\eta(z \pm t) - \eta(z)| < \varepsilon / C$ for all $z \in G$, where we have used the symmetry of $P_{\varepsilon'}$ (see Fact 2). Consequently,

$$
\|\delta_t * \gamma_\omega - \gamma_\omega\|_K \;<\; C \sup_{z\in L} \big|\eta(z-t) - \eta(z)\big| \;\leq\; \varepsilon\,.
$$

But $P_{\varepsilon'}$ is relatively dense according to Axiom 4, and then so are the norm ε-almost periods of γ_ω, for all $\varepsilon > 0$, which proves one direction.

Conversely, let γ_ω be norm almost periodic and set

$$
Q_\varepsilon \;:=\; \{t \in L \mid \|\delta_t * \gamma_\omega - \gamma_\omega\|_K < \varepsilon\}.
$$

This is again a symmetric set because $\|\delta_x * \mu\|_K = \|\mu\|_K$ for all $\mu \in \mathcal{M}^\infty(G)$ and $x \in G$. Observe that, for all $z \in G$, we have

$$
|\eta(z \pm t) - \eta(z)| \;\leq\; \|\delta_{\mp t} * \gamma_\omega - \gamma_\omega\|_K \;=\; \|\delta_t * \gamma_\omega - \gamma_\omega\|_K\,.
$$

Fix $\varepsilon > 0$ and set $\varepsilon' = \eta(0)\varepsilon^2$ which is still positive. For all $t \in Q_{\varepsilon'}$, we get

$$
\varrho(t,0) \;=\; \left(\frac{|\eta(t) - \eta(0)|}{\eta(0)}\right)^{1/2} \;\leq\; \left(\frac{\|\delta_t * \gamma_\omega - \gamma_\omega\|_K}{\eta(0)}\right)^{1/2} \;<\; \varepsilon
$$

The set $Q_{\varepsilon'}$ is relatively dense which implies that also P_ε is relatively dense. This being true for all $\varepsilon > 0$, Axiom 4 is satisfied. $\square$

To be able to use the results of [19], we have yet to introduce another topology on $\mathcal{M}^\infty(G)$, called the *product topology* in [19, Ex. 2.15]. If $C_U(G)$ denotes the space of bounded, uniformly continuous functions on G, a measure $\mu \in \mathcal{M}^\infty(G)$ is identified with an element of the Cartesian product space $\big[C_U(G)\big]^{\mathcal{K}(G)}$ via

$$
\mu \;=\; \{g * \mu\}_{g\in\mathcal{K}(G)}
$$

where each $g * \mu$ is uniformly continuous and bounded by $\|g * \mu\|_\infty \leq \|g\|_\infty \sup_{t\in G} |\mu|\big(t + \mathrm{supp}(g)\big)$, hence an element of $C_U(G)$. This way, we have $\mathcal{M}^\infty(G) \subset \big[C_U(G)\big]^{\mathcal{K}(G)}$ which makes $\mathcal{M}^\infty(G)$ into a locally convex topological vector space, in the relative topology. A fundamental system of semi-norms is provided by $\|\mu\|_g := \|g*\mu\|_\infty$, with $g \in \big[C_U(G)\big]^{\mathcal{K}(G)}$. Unfortunately, $\mathcal{M}^\infty(G)$ is not a complete subspace of $\big[C_U(G)\big]^{\mathcal{K}(G)}$, but it is *bounded closed*, i.e. every closed and bounded subset of $\mathcal{M}^\infty(G)$ is also complete in $\big[C_U(G)\big]^{\mathcal{K}(G)}$, see [19, Thm. 2.4 and Cor. 2.1]. Let us add that, due to the product structure, a subset M of $\mathcal{M}^\infty(G)$ is bounded iff, for all $g \in \mathcal{K}(G)$, we have $\|g * \mu\|_\infty \leq C$ for all $\mu \in M$, with a constant $C = C(g)$ which does not depend on μ, compare [12, Ex. II.4.7 c].

A measure $\omega \in \mathcal{M}^\infty(G)$ is then called *strongly almost periodic* if the set $\{\delta_t * \omega \mid t \in G\}$ is relatively compact in this product topology.

Lemma 7 *If $\omega \in \mathcal{M}^\infty(G)$ is a norm almost periodic measure, it is also strongly almost periodic.*

PROOF: First, let $g \in \mathcal{K}(G)$ and $\mu \in \mathcal{M}^\infty(G)$. Then we obtain, with $V := \mathrm{supp}(g)$,

$$\begin{aligned}
\left| \int_G g(x-y)\,\mathrm{d}\mu(y) \right| \;&\leq\; \int_G \big|g(x-y)\big|\,\mathrm{d}|\mu|(y) \\
&\leq\; \int_G \mathbf{1}_V(x-y)\,\|g\|_\infty\,\mathrm{d}|\mu|(y) \\
&=\; \|g\|_\infty \cdot |\mu|(x-V) \\
&\leq\; \|g\|_\infty \sup_{x\in G} |\mu|\big(x + (-V)\big) \\
&\leq\; C_g\,\|g\|_\infty\,\|\mu\|_K
\end{aligned}$$

where $C_g > 0$ is a constant which emerges from the observation that the support of g is compact and can thus be covered by finitely many translates of K. So, we have

$$\|g * \mu\|_\infty \;=\; \sup_{x\in G} \left| \int_G g(x-y)\,\mathrm{d}\mu(y) \right| \;\leq\; C_g\,\|g\|_\infty\,\|\mu\|_K\,.$$

Let us now choose an arbitrary finite family $\mathcal{F} = \{g_1, \ldots, g_n\}$ of non-zero functions $g_i \in \mathcal{K}(G)$. Then,

$$V_\varepsilon^{\mathcal{F}}(0) \;:=\; \{\mu \in \mathcal{M}^\infty(G) \mid \sup_{1\leq i\leq n} \|g_i * \mu\|_\infty < \varepsilon\}$$

is a neighbourhood of the 0-measure in $\mathcal{M}^\infty(G)$ in the product topology. The neighbourhoods of this kind form a fundamental system of neighbourhoods of the 0-measure. Choose $\varepsilon' = \varepsilon / \max\{C_{g_i} \|g_i\|_\infty \mid 1 \leq i \leq n\}$. If $\mu \in B_{\varepsilon'}(0)$, the ε'-ball in the $\|.\|_K$-norm, then

$$\|g_i * \mu\|_\infty \;\leq\; \varepsilon$$

for all $1 \leq i \leq n$, hence $B_{\varepsilon'}(0) \subset V_\varepsilon^{\mathcal{F}}(0)$, and also $B_{\varepsilon'}(\nu) \subset V_\varepsilon^{\mathcal{F}}(\nu)$ for an arbitrary $\nu \in \mathcal{M}^\infty(G)$.

Finally, consider the norm almost periodic measure ω. For any $\varepsilon > 0$ and any finite family $\mathcal{F}$, we know that $\varepsilon' > 0$ and that $M_\omega := \{\delta_t * \omega \mid t \in G\}$ can be covered by finitely many translates of $B_{\varepsilon'}(0)$, and hence, by the above argument, also by finitely many translates of $V_\varepsilon^{\mathcal{F}}(0)$. This shows that M_ω is precompact. Since $\mathcal{M}^\infty(G)$ with the product topology is bounded closed as explained above, M_ω is also relatively compact, i.e. ω is strongly almost periodic. □

Let us now recall the following result from [19], which is proved on the basis of the Bohr compactification of G, see [19, Ch. 7].

Proposition 7 *Let $\mu \in \mathcal{M}^\infty(G)$ be a transformable measure, with associated measure $\hat{\mu} \in \mathcal{M}^\infty(\hat{G})$. Then $\hat{\mu}$ is a pure point measure if and only if μ is strongly almost periodic.*

PROOF: This follows from [19, Thm. 11.2 and Cor. 11.1] by an application of the inverse Fourier transform. □

Combining Proposition 7 with Fact 3, we obtain:

Theorem 4 *Let ω be a translation bounded complex measure on the σ-compact, locally compact Abelian group G and assume that, w.r.t. an averaging sequence $\mathcal{A}$, its autocorrelation measure γ_ω exists. Then γ_ω is a translation bounded positive definite measure, whose Fourier transform, $\hat{\gamma}_\omega$, exists and is a translation bounded positive measure on $\hat{G}$.*

Moreover, $\hat{\gamma}_\omega$ is a pure point measure (i.e. ω has pure point diffraction) if and only if γ_ω is strongly almost periodic. □

Consequently, together with Proposition 6 and Lemma 7, we get an independent derivation of our main Theorem 1.

It is not clear to what extent norm and strong almost periodicity coincide, as the product topology is weaker then the norm topology. The demarkation apparently is connected with the difference between Axioms 3 and 3^+. It is possible though to come to a partial converse of Lemma 7. For that, we first need a technical result.

Lemma 8 *Let u, v be two arbitrary complex numbers which satisfy the simultaneous inequalities $|u - bv| < \varepsilon$ and $|au - v| < \varepsilon$, with real numbers $0 \leq a, b \leq 1$. Then they also satisfy $|u - v| < 3\,\varepsilon$.*

PROOF: If $u = 0$ or $v = 0$, the statement is trivial. So, we may assume $u \neq 0$ and $v \neq 0$ from now on. Write $v = au + w$, so $|w| < \varepsilon$, and we obtain

$$\big|\, |u(1-ab)| - |bw| \,\big| \;\leq\; |u - abu - bw| \;=\; |u - bv| \;<\; \varepsilon\,.$$

This implies $|u(1-ab)| \,<\, |bw| + \varepsilon \,<\, 2\,\varepsilon$. By an analogous argument, we also get $|v(1-ab)| < 2\,\varepsilon$, hence $(1-ab)\max(|u|,|v|) < 2\,\varepsilon$. By assumption, $0 \leq (1-b) \leq (1-ab)$, and this gives

$$0 \;\leq\; (1-b) \;<\; \frac{2\,\varepsilon}{\max(|u|,|v|)}\,.$$

With this, we can estimate:

$$\begin{aligned} |u - v| \;&=\; |u - bv + bv - v| \;<\; \varepsilon + (1-b)|v| \\ &<\; \varepsilon + \frac{2\,|v|\,\varepsilon}{\max(|u|,|v|)} \;\leq\; 3\,\varepsilon \end{aligned}$$

which proves the assertion. □

Before we state the partial converse, let us make one further observation. Strong almost periodicity of a measure $\mu \in \mathcal{M}^\infty(G)$ means relative compactness of the set $M_\mu = \{\delta_t * \mu \mid t \in G\}$ in the product topology, which coincides with precompactness here. So, for every finite family $\mathcal{F}$ of functions and for every $\varepsilon > 0$, there are *finitely* many measures $\{\nu_1, \ldots, \nu_n\}$ such that

$$M_\mu \;\subset\; \bigcup_{i=1}^{n} V_\varepsilon^{\mathcal{F}}(\nu_i) \tag{30}$$

with the neighbourhoods $V_\varepsilon^{\mathcal{F}}$ defined in analogy to above, i.e. they are translates of those around 0. Without loss of generality, we may assume that all the ν_i are actually translates of μ, i.e. of the form $\nu_i = \delta_{t_i} * \mu$ for some $t_i \in G$. Observing now that

$$V_\varepsilon^{\mathcal{F}}(\delta_t * \mu) \;=\; \delta_t * V_\varepsilon^{\mathcal{F}}(\mu)$$

we can rephrase the relative compactness condition and (30) by saying that there are finitely many translations $\{t_1, \dots, t_n\}$ in G such that

$$M_\mu \subset \bigcup_{i=1}^{n} \big(\delta_{t_i} * V_\varepsilon^{\mathcal{F}}(\mu)\big).$$

This formulation is of advantage for the next result, and can also be used to see that strong almost periodicity of μ implies that all functions $g * \mu \in C_U(G)$, with $g \in \mathcal{K}(G)$, are (uniformly) almost periodic functions on G, see [39, p. 20] for a definition.

Proposition 8 *Let $\mu \in \mathcal{M}^\infty(G)$ be a pure point measure that is supported on a uniformly discrete set $\varDelta$. If μ is strongly almost periodic, it is also norm almost periodic.*

PROOF: We can assume $\mu = \sum_{z\in\varDelta} \eta(z)\delta_z$ with $\eta(z) \neq 0$ for all $z \in \varDelta$, i.e. we assume $\varDelta = \varDelta^{\mathrm{ess}}$. Since $\varDelta$ is uniformly discrete, we can choose a compact neighbourhood S of $0 \in G$ such that $(x + S) \cap (y + S) = \varnothing$ for all $x, y \in \varDelta$ with $x \neq y$. Without loss of generality, we may also assume that S is symmetric, i.e. $S = -S$, which simplifies some of the calculations.

Let us fix a function $g \in \mathcal{K}(G)$ with values in the interval $[0, 1]$, support S, and $g(0) = 1$. We can now apply our above reasoning on strong almost periodicity to neighbourhoods of type $V_{\varepsilon/3}^{\{g\}}$, i.e., for all $\varepsilon > 0$, there exist *finitely* many translations $\{t_1, \dots, t_n\}$ such that, for all $t \in G$, we have

$$\|g * (\mu - \delta_{t-t_i} * \mu)\|_\infty \; < \; \varepsilon/3 \tag{31}$$

for (at least) one of the t_i. Here, the supremum is taken over the function

$$\begin{aligned}
&\big|\big(g * (\mu - \delta_{t-t_i} * \mu)\big)(x)\big| \\
&= \Big|\sum_{z\in\varDelta} \eta(z) g(x - z) - \sum_{z\in\varDelta} \eta(z) g(x - z - (t - t_i))\Big| \\
&= \Big|\sum_{z\in\varDelta\cap(x+S)} \eta(z) g(x - z) - \sum_{z\in\varDelta\cap(x-(t-t_i)+S)} \eta(z) g(x - z - (t - t_i))\Big|
\end{aligned}$$

where we made use of the symmetry of S in the last step. This equation means that, for each value of x, there is at most one term from each of the sums. As x varies over G, one glides a g-shaped 'dumb-bell' over G with centres at distance $t - t_i$. The latter is locally constant and changes only if another t_i has to be chosen.

If only one term is caught, $\eta(z)$ in the first sum say, then we may choose $x = z$ to see that $|\eta(z)| < \varepsilon/3$. So, let us assume that z_1, z_2 are the two points of $\varDelta$ which are covered by the dumb-bell. Choosing first $x = z_1$ and then $x = z_2$, we obtain the simultaneous inequalities

$$\big|\eta(z_1) - b\,\eta(z_2)\big| \;<\; \varepsilon/3\,, \qquad \big|a\,\eta(z_1) - \eta(z_2)\big| \;<\; \varepsilon/3$$

where a, b are the corresponding values of the function g, hence numbers in the unit interval. Invoking Lemma 8, we get $\big|\eta(z_1) - \eta(z_2)\big| < \varepsilon$.

From this argument we conclude that for $\{t_1, \dots, t_m\}$ as chosen for (31) and for all $t \in G$, there is a $t_i \in \{t_1, \dots, t_m\}$ for which

$$\Big| \sum_{z \in \varDelta \cap (x+S)} \eta(z) \;-\; \sum_{z \in \varDelta \cap (x-(t-t_i)+S)} \eta(z) \Big| \;<\; \varepsilon \tag{32}$$

for all $x \in G$.

We have to show that M_μ is norm almost periodic. Since $\|.\|_K$ and $\|.\|_S$ are equivalent norms, they define the same topology. So, we have to show that, for all $\varepsilon > 0$, there are finitely many translations $\{t_1, \dots, t_m\}$ such that M_μ is covered by $\bigcup_{i=1}^m B_\varepsilon(\delta_{t_i} * \mu)$. This means that, for all $t \in G$, there must be (at least) one t_i so that

$$\|\mu - \delta_{t-t_i} * \mu\|_S \;<\; \varepsilon\,. \tag{33}$$

But this is equivalent to

$$\sup_{x \in G} \Big| \sum_{z \in \varDelta \cap (x+S)} \eta(z) \;-\; \sum_{z \in \varDelta \cap (x-(t-t_i)+S)} \eta(z) \Big| \;<\; \varepsilon\,,$$

which is precisely what happens if $\{t_1, \dots t_m\}$ are chosen as for (31).

Since $\varepsilon > 0$ was arbitrary, we conclude that M_μ is also norm almost periodic, which was our assertion. $\square$

Finally, to wrap up the results of this paper, we formulate:

Theorem 5 *Let ω be a translation bounded measure on the σ-compact LCA group G whose autocorrelation γ_ω exists (relative to an averaging sequence $\mathcal{A}$) and is a pure point measure with uniformly discrete support $\varDelta$ (in other words, ω conforms to Axioms* 1, 2, *and* 3^+*). Then the corresponding diffraction measure $\hat{\gamma}_\omega$ exists and the following statements are equivalent.*

(a) *Axiom* 4 *holds, i.e. the set* P_ε *of* (8) *is relatively dense for all* $\varepsilon > 0$.

(b) *The autocorrelation* γ_ω *is norm almost periodic.*

(c) *The autocorrelation* γ_ω *is strongly almost periodic.*

(d) *The diffraction measure* $\hat{\gamma}_\omega$ *is pure point.*

Proof: We have (a) $\Longleftrightarrow$ (b) by Proposition 6, while (c) $\Longleftrightarrow$ (d) follows from Proposition 7. Next, (b) $\Rightarrow$ (c) results from Lemma 7, and the converse direction is Proposition 8. □

Appendix: Averages and limits

So far, we have fixed one averaging sequence $\mathcal{A}$ out of a huge class of possible sequences. This is not entirely satisfactory because the resulting diffraction measure can, and generally will, depend on this choice. Let us thus indicate how to restrict the choice of $\mathcal{A}$ in order to get rid of this problem, at least to some extent. The method of choice is the use of so-called *van Hove sequences* which were introduced long ago in statistical mechanics to deal with a similar problem [34, Ch. 2.1].

The key idea here is the following. If the Dirac comb (or measure) ω is sufficiently 'homogeneous' and if the sets of the sequence $\mathcal{A}$ grow in such a way that their boundaries are suitably negligible (in measure) when compared to the full sets, one should expect independence of the autocorrelation of the actual choice of $\mathcal{A}$. This is certainly the case for lattices and general periodic structures in Euclidean spaces, where a sequence of balls (with arbitrary centres) is as good as one with cubes or similar shapes. To formalize this, consider two *compact* subsets B, K of G and define the K-boundary of B as

$$\partial^K B \;:=\; \big((B+K)\setminus \mathring{B}\big) \,\cup\, \big((\,\overline{G\setminus B} - K)\cap B\,\big). \tag{34}$$

This can be understood as some sort of K-thickening of ∂B. In particular, $\partial^{\{0\}} B = \partial B$. With this, $\mathcal{A}$ of (1) is called a (nested) *van Hove sequence* if, for every compact $K \subset G$,

$$\lim_{n\to\infty} \frac{\theta_G(\partial^K \bar{A}_n)}{\theta_G(A_n)} \;=\; 0\,. \tag{35}$$

The meaning of (35) is that the boundary/bulk ratio goes to zero (in measure) as $n \to \infty$, see [36, Sec. 1] for further details and consequences of this concept in the setting of translation bounded measures. Note that general van Hove sequences need not be nested, i.e. need not satisfy $\bar{A_n} \subset A_{n+1}$, but, since G is σ-compact, a general van Hove sequence always has a subsequence of the form $\mathcal{A}' = \big(a_n + A_n\big)_{n\in\mathbb{N}_0}$ with $\mathcal{A}$ of (1) and arbitrary $a_n \in G$.

Proposition 9 *Let Λ be a regular model set in the sense of Section* 5*, and let $\omega = \delta_\Lambda$ be its uniform Dirac comb. Then, for any general van Hove sequence $\mathcal{A}'$, the corresponding autocorrelation measure γ_ω exists. Furthermore, it is independent of $\mathcal{A}'$.*

PROOF: The result is true for point sets that lead to uniformly ergodic dynamical systems under the action of G, see [36, Thm. 3.4]. A regular model set is such a point set according to [36, Thm. 4.5 (1)]. □

This result contains the cases of lattices and periodic point sets. It can be extended to weighted model sets as we introduced them above, but we will not expand upon this here.

Although the stated independence of the van Hove sequence chosen is very plausible (or at least desirable) for many if not most physical applications, the situation is not always as nice as with regular model sets. Already in the case of the visible lattice points, the above statement is clearly false because of the existence of holes of arbitrary size. A sequence of balls centred around the origin would give a different answer than one that moves around chasing the holes. In other words, a certain degree of uniformity of the limit is lost. Nevertheless, some partial result remains true. If one restricts again to the *nested* form $\mathcal{A}$ of the van Hove sequence, existence of the autocorrelation and independence of $\mathcal{A}$ is regained, see [7] for details.

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