PURE POINT DIFFRACTION AND POISSON SUMMATION

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ABSTRACT. We prove that the diffraction formula for regular model sets is equivalent to the Poisson Summation Formula for the underlying lattice. This is achieved using Fourier analysis of unbounded measures on locally compact abelian groups as developed by Argabright and de Lamadrid. We also obtain diffraction results for certain classes of non-regular so-called weak model sets.

1. INTRODUCTION

Research triggered by the experimental discovery of quasicrystals, see [2] for a recent mathematical monograph, provided examples of non-periodic structures with long-range order. Their diffraction spectrum consists of Bragg peaks only. A mathematical abstraction of these examples are so-called regular model sets, which are certain projections of a subset of a higher-dimensional lattice. In fact, model sets have been introduced and intensively studied before the discovery of quasicrystals by Meyer [23, 24], and they have later been re-investigated and advocated by Moody, see e.g. [26].

A central result in mathematical diffraction theory states that regular model sets have a pure point diffraction spectrum. This has been proved in the Euclidean setting by Hof [15] using the underlying lattice Poisson Summation Formula (PSF), see also [2, Lemma 9.3]. When it became clear that examples with a non-Euclidean embedding space exist such as limit-periodic model sets [5], their diffraction has been studied in general σ-compact locally compact abelian (LCA) groups. However the corresponding proofs did not rely on the PSF but instead used dynamical systems, see Schlottmann [33] for so-called repetitive regular model sets and [18] for recent results in that direction. A complementary approach uses almost periodic measures, see e.g. Solomyak [34], Baake–Moody [4] and the recent work [35]. These results have also been extended to weighted Dirac combs with weight functions on the embedding space of sufficiently fast decay, which are called admissible in [30, 19].

In this article, we will reprove the diffraction formula for regular model sets on general σ-compact LCA groups using the PSF of the underlying lattice. In fact we show that the lattice PSF and the diffraction formula for regular model sets can be derived from one another. We also show that the diffraction formula of regular model sets and the diffraction formula of the underying lattice can be derived from one another. Our proofs shed some new light on the Euclidean case. One interpretation of our results is that the lattice PSF induces a generalised PSF for the model set and vice versa. This clarifies an opinion sometimes expressed

by experimental physicists that diffraction properties of quasicrystals should be deducible from those of the underlying lattice.

Working beyond Euclidean space, we cannot use Hof's tempered distribution approach, but rely instead on Fourier theory of unbounded measures as in Argabright and de Lamadrid [1, 6]. Whereas working with measures only seems a severe restriction, this is in fact natural as diffraction may be described by a measure. Indeed, the diffraction measure of the infinite idealisation of a finite specimen decomposes into a discrete and a continuous part, which correspond to the Bragg peaks and to the continuous component in the diffraction picture.

We will extend elements of Hof's proof to the non-Euclidean setting. Hof used a certain uniform distribution result for regular model sets in his arguments. We will show that uniform distribution also follows from the underlying lattice PSF. In the Euclidean setting, this has already been argued by Meyer [23], see also [24, Sec. V.7.3], [22, Prop. 5.1]. Other proofs of uniform distribution in the general setting are based on geometric [32] or dynamical systems arguments [25]. Our approach indicates that problems equivalent to the PSF such as function reconstruction via sampling [8] may also be successfully analysed for model sets in the abstract setting. It may further be a starting point for extending cut-and-project schemes beyond the abelian case, such as to cover the affine group of Euclidean space.

Let us describe the structure of this article. After reviewing mathematical diffraction theory, we recall the Fourier analysis of unbounded measures in Section 3. Here we are particularly interested in generalised PSF for measures which extend the lattice case and in double transformability. In Section 4 we consider weighted model sets and discuss their Fourier analysis. We prove that, for certain weight functions, their generalized PSF is equivalent to the PSF of the underlying lattice, and we show uniform distribution using the lattice PSF. In Section 5, we will use the so-called autocorrelation measure to study the diffraction of regular model sets. We show that the diffraction formula for regular model sets can be obtained by combining the generalized PSF and the density formula. Thus the diffraction formula can be obtained by a double application of the PSF for the underlying lattice. We also show that the lattice PSF follows from the diffraction formula for regular model sets. We close with some remarks on pure point diffraction for non-regular model sets and Meyer sets, and by proving double transformability of translation bounded transformable measures with Meyer set support.

2. Elements of diffraction theory

We give a focussed introduction to diffraction theory, see [12, 9] for physical background and [2, Section 9.1.2] for mathematical background in the Euclidean case. Diffraction of X-rays by matter results from scattering by the individual atoms and interference between the scattering waves. For a finite sample with atom position set $\Lambda \subset \mathbb{R}^3$, one defines the structure factor $F(\boldsymbol{s}) = \sum_{\boldsymbol{p} \in \Lambda} f_{\boldsymbol{p}} e^{-2\pi i \, \boldsymbol{s} \cdot \boldsymbol{p}}$, where the so-called scattering factor $f_{\boldsymbol{p}}$ is a complex weight associated with an atom at $\boldsymbol{p}$. Assume that the incident beam is a plane wave with wave vector $\boldsymbol{k}_0$, and assume that one measures diffraction at a distance $\boldsymbol{r}$ very large in comparison to the sample size. Then the observed intensity $I(\boldsymbol{r})$ of diffraction at distance $\boldsymbol{r}$ is

approximately given by

$$I(\boldsymbol{r}) = \frac{A}{|\boldsymbol{r}|^2}|F(\boldsymbol{k} - \boldsymbol{k}_0)|^2,$$

where $\boldsymbol{k} = |\boldsymbol{k}_0| \cdot \boldsymbol{r}/|\boldsymbol{r}|$, and A is some positive normalisation constant.

For a measure-theoretic description, assume that $\Lambda \subset \mathbb{R}^d$ is uniformly discrete and consider the Dirac comb $\omega = \delta_\Lambda = \sum_{p \in \Lambda} \delta_p$ of Λ. We assume for simplicity that all atoms have equal scattering factors $f_p = 1$. We want to infer the diffraction of ω from finite samples $\omega_n = \omega|_{B_n}$, where we restrict to balls B_n of radius n. Diffraction of the finite measure ω_n can be rephrased using a so-called Wiener diagram

$$
\begin{array}{ccc}
\omega_n & \xrightarrow{\ *\ } & \omega_n * \widetilde{\omega_n} \\
{\scriptstyle\mathcal{F}}\big\downarrow & & \big\downarrow{\scriptstyle\mathcal{F}} \\
\widehat{\omega_n} & \xrightarrow{\ |\cdot|^2\ } & \widehat{\omega_n} \cdot \overline{\widehat{\omega_n}}
\end{array}
$$

Here $\mathcal{F}$ denotes the Fourier transform, $*$ denotes convolution, and the reflected measure $\widetilde{\omega}$ is defined via $\widetilde{\omega}(f) = \omega(\widetilde{f})$ with $\widetilde{f}(x) = \overline{f(-x)}$. The Wiener diagram commutes due to the convolution theorem of Fourier analysis. Hence the diffraction of ω_n may alternatively be computed as the Fourier transform of the so-called autocorrelation measure $\gamma_n = \omega_n * \widetilde{\omega_n}$. Note that the diffraction measure allows reconstruction of the autocorrelation γ_n but not of ω_n.

For ω unbounded instead of ω_n, the Wiener diagram has no direct measure-theoretic interpretation. As convolution is defined only if one measure is bounded, an autocorrelation γ of ω may however be interpreted as a vague limit of the finite autocorrelation measures, i.e.,

$$\gamma = \omega \circledast \widetilde{\omega} := \lim_{n \to \infty} \frac{1}{\theta(B_n)} \omega_n * \widetilde{\omega_n},$$

if this limit exists. Here θ denotes the Lebesgue measure. Such a limit exists at least on some subsequence of $(B_n)_{n \in \mathbb{N}}$ if the set $\Lambda - \Lambda$ of interatomic distances is uniformly discrete. The measure γ is also called the Eberlein convolution of ω, see e.g. [2]. It is a positive definite measure by construction. Secondly, a Fourier transform of ω may make sense via tempered distributions but not as a measure if ω is non-periodic. Indeed, if $\widehat{\omega}$ is supported on a uniformly discrete set, then ω must be supported on a finite union of lattice translates [21].

However for $\omega = \delta_\Lambda$ a lattice Dirac comb, one has $\gamma = \mathrm{dens}(\Lambda) \cdot \omega$. The Fourier transform of ω is the measure $\widehat{\omega} = \mathrm{dens}(\Lambda) \cdot \delta_{\Lambda_0}$, where Λ_0 is the lattice dual to Λ. Hence the modified Wiener diagram commutes in that situation. Note that the measure equation $\widehat{\omega} = \mathrm{dens}(\Lambda) \cdot \delta_{\Lambda_0}$ is a version of the classical PSF.

More generally, if ω is not Fourier transformable as a measure, it is still possible to analyse diffraction from a measure theoretic viewpoint if an autocorrelation γ of ω exists as a measure. This will be true in all examples below. In that situation, γ will be transformable due to positive definiteness, and its Fourier transform $\widehat{\gamma}$ will be a positive measure. One can then infer diffraction properties of Λ from the Lebesgue decomposition of $\widehat{\gamma}$. The discrete part describes the Bragg peaks, and the continuous part describes the diffuse background in the diffraction picture. Moreover, diffraction of Λ can indeed be inferred from finite samples as the Fourier transform is continuous, see [6, Thm. 4.16] and [27, Lemma 1.26]. From a physical viewpoint, this justifies why one may approximate a large finite sample by its infinite idealisation.

Our main result Theorem 5.2 states that Dirac combs of regular model sets, which includes lattice Dirac combs, are pure point diffractive. In that case, their diffraction amplitudes are computed as in the finite measure case by "squaring the Fourier-Bohr coefficients". Moreover a modified Wiener diagram holds for a large class of weighted model sets including lattice Dirac combs, see Remark 5.4.

3. Fourier transformability

Let us fix our notation. G stands for an arbitrary LCA group. A Haar measure on G will be denoted by θ_G. We denote by $C_c(G)$ the space of continuous, compactly supported functions on G, and by $C_U(G)$ the space of uniformly continuous and bounded functions on G. For $f \in L^1(G)$ we denote its Fourier transform by $\widehat{f}$ and its inverse Fourier transform by $\widecheck{f}$. Let $\widehat{G}$ denote the Pontryagin dual of G. Given any LCA group G with Haar measure θ_G, we always choose the Plancherel measure $\theta_{\widehat{G}}$ on the dual group $\widehat{G}$, i.e., the Haar measure such that the Plancherel theorem [10, Thm. 3.4.8] holds. Let $\mathcal{M}(G)$ denote the set of complex regular Radon measures on G. A measure $\mu \in \mathcal{M}(G)$ is *translation bounded* if $\sup\{|\mu|(t+K) \,|\, t \in G\} < \infty$ for every compact $K \subset G$, where $|\mu| \in \mathcal{M}(G)$ is the variation measure of μ. Let $\mathcal{M}^\infty(G) \subset \mathcal{M}(G)$ denote the set of translation bounded complex regular Radon measures on G. If for some $1 \le p \le \infty$ a function $f : G \to \mathbb{C}$ satisfies $f \in L^p(|\mu|)$, we write $f \in L^p(\mu)$ for convenience.

3.1. **Poisson Summation Formula for a lattice.** Let L be a lattice in G, i.e., a discrete, co-compact subgroup of G, and consider the lattice Dirac comb $\mu = \delta_L$. The Dirac comb δ_L is a translation bounded positive measure. Normalise the Haar measure on G/L such that the Weil formula [29, Eqn. (3.3.10)] holds. Let us denote by $L_0 \subset \widehat{G}$ the annihilator of L in $\widehat{G}$, i.e.,

$$L_0 = \{\chi \in \widehat{G} : \chi(x) = 1 \text{ for all } x \in L\}.$$

By Pontryagin duality, the annihilator $L_0 \cong \widehat{G/L}$ of L is a lattice in $\widehat{G}$. It is called the lattice dual to L. Its Dirac comb δ_{L_0} is a translation bounded positive measure. As Haar measure on L we choose the counting measure $\theta_L = \delta_L$, and on L_0 we choose the Plancherel measure θ_{L_0} with respect to G/L. It is given by $\theta_{L_0} = \mathrm{dens}(L) \cdot \delta_{L_0}$. Consider $KL(G) := \{f \in C_c(G) : \widehat{f} \in L^1(\widehat{G})\}$. The following result is well known, see e.g. [29, Thm. 5.5.2] and [10, Thm. 3.6.3].

Theorem 3.1 (lattice PSF). *Let $L \subset G$ be a lattice in G, and let $L_0 \subset \widehat{G}$ be its dual lattice. Then the Poisson summation formula*

$$\langle \delta_L, f \rangle = \mathrm{dens}(L) \cdot \langle \delta_{L_0}, \widecheck{f} \rangle$$

holds for all $f \in KL(G)$. □

Remark 3.2. In fact the lattice PSF also holds for sufficiently decaying f of unbounded support, but we will not consider such functions in this manuscript. One may regard the measure $\mathrm{dens}(L) \cdot \delta_{L_0}$ as the Fourier transform of the measure δ_L. Note that as a consequence of the lattice PSF, $f \in KL(G)$ has a lattice integrable Fourier transform, i.e., $\widehat{f}|_{L_0} \in L^1(L_0)$. These two observations motivate the definition of the Fourier transform of a measure in the following section, see also Proposition 3.9 (ii).

3.2. **Fourier transforms as measures.** As usual, convolution is for $f, g \in L^1(G)$ defined by $f * g(x) = \int f(y)g(x-y)d\theta_G(y)$. We have $f * g = g * f$ since G is unimodular. We also use $\widetilde{f}(x) = \overline{f(-x)}$, which defines a unitary representation of G on the Hilbert space $L^2(G)$. Hence $f \in L^2(G)$ satisfies $f * \widetilde{f} \in P(G)$, where $P(G)$ denotes the set of continuous positive definite functions on G, see [13] for background. This implies that $f * \widetilde{f}$ is Fourier transformable by Bochner's theorem [29, Thm. 4.4.19], and we have $\widehat{f * \widetilde{f}} = |\widehat{f}|^2$. We recall the definition of transformability of a measure [1, Sec. 2].

Definition 3.3 (Fourier transform). *A measure $\mu \in \mathcal{M}(G)$ is* transformable *if there exists a measure $\widehat{\mu} \in \mathcal{M}(\widehat{G})$ such that for all $f \in C_c(G)$ we have $\check{f} \in L^2(\widehat{\mu})$ and*

$$\langle \mu, f * \widetilde{f} \rangle = \langle \widehat{\mu}, |\check{f}|^2 \rangle.$$

In this case, $\widehat{\mu}$ is called the Fourier transform *of μ.*

Remark 3.4. In the Euclidean setting, the Fourier transform is often considered as an appropriate tempered distribution. Here the Fourier transform $\widehat{\mu}$ is even required to be a measure. Such $\widehat{\mu}$ is uniquely determined if it exists [1, Thm. 2.1]. Moreover $\widehat{\mu}$ is then translation bounded [1, Thm. 2.5].

Remark 3.5. The above definition generalises the Fourier transform of functions. Indeed, examples of transformable measures are given by $\mu = f \cdot \theta_G$, where $f \in P(G)$ or $f \in L^p(G)$ for $1 \le p \le 2$, see [1, Thm. 2.2]. Every finite measure is transformable. A measure $\mu \in \mathcal{M}(G)$ is called positive definite if $\int_G f * \widetilde{f}(x) \, d\mu(x) \ge 0$ for every $f \in C_c(G)$. As a consequence of Bochner's theorem, every positive definite measure is transformable [1, Thm. 4.1]. Any Haar measure on a closed subgroup of G is, as a measure on G, positive definite and hence transformable [1, Prop. 6.2, Cor. 6.2]. For the Haar measure on a closed subgroup of G, the definition of Fourier transform reduces to a version of the classical PSF, compare Section 3.1 and Proposition 3.9. Thus, transformability expresses that the measure satisfies some generalised PSF.

3.3. **Spaces of test functions.** We discuss transformability in terms of test functions in particular subclasses of $C_c(G)$. The above definition uses the function space

$$K_2(G) = \operatorname{span}\{f * \widetilde{f} : f \in C_c(G)\}.$$

Note that $f * g \in K_2(G)$ for $f, g \in C_c(G)$, which follows from polarisation. The space $K_2(G)$ is dense in $C_c(G)$, which may be seen by approximating $f \in C_c(G)$ by convolution with a Dirac net and by polarisation, see p. 9 and Eq. (4.6) in [1] for the argument.

We are interested in L^1-characterisations of transformability. Note that if $\mu \in \mathcal{M}(G)$ is transformable, then for $f \in C_c(G)$ such that $\widehat{f} \in L^1(\widehat{G})$ we even have $\widehat{f} \in L^1(\widehat{\mu})$, see [1, Prop. 3.1]. Thus the space of functions

$$KL(G) = \{f \in C_c(G) : \widehat{f} \in L^1(\widehat{G})\}$$

is important. As $C_c(G) \subset L^1(G)$, every $f \in KL(G)$ satisfies the inversion formula $f = \check{\widehat{f}}$, see [10, Thm. 3.5.8]. Often, positive definiteness will be important for our arguments. For this reason, we will sometimes deal with the function space

$$PK(G) := \operatorname{span}\{P(G) \cap KL(G)\}.$$

The requirement $\widehat{f} \in L^1(\widehat{G})$ is actually not needed in the definition of $PK(G)$.

Lemma 3.6. $f \in P(G) \cap C_c(G)$ *implies* $\widehat{f} \in L^1(\widehat{G})$. *Hence* $PK(G) = span\{P(G) \cap C_c(G)\}$.

Proof. Let $f \in C_c(G)$ be positive definite. Since f is continuous and positive definite, by Bochner's theorem, see e.g. [31, Sec. 1.4.3], there exists a finite measure $\sigma \in \mathcal{M}(\widehat{G})$ such that
$$f(x) = \int_{\widehat{G}} \chi(x) \, d\sigma(\chi) \, .$$
Then, by [1, Thm. 2.2], [27, Lemma 1.17], the measure $f \cdot \theta_G$ is transformable and its Fourier transform is σ. Again by [1, Thm. 2.2] or [27, Lemma 1.16], as $f \in L^1(G)$, the measure $f \cdot \theta_G$ is transformable and its Fourier transform is $\widehat{f} \cdot \theta_{\widehat{G}}$. Therefore, the uniqueness of the Fourier transform [1, Thm. 2.1] or [27, Thm. 1.13] yields $\sigma = \widehat{f} \cdot \theta_{\widehat{G}}$. As σ is a finite measure, it follows that $\widehat{f} \cdot \theta_{\widehat{G}}$ is a finite measure, and hence $\widehat{f} \in L^1(\widehat{G})$. $\qquad\square$

We thus have the following relationship among our spaces:
$$K_2(G) \subset PK(G) \subset KL(G) \subset C_c(G) \, .$$
As $K_2(G)$ is dense in $C_c(G)$, it follows that $PK(G)$ and $KL(G)$ are also dense in $C_c(G)$. Many examples of functions in $PK(G)$ are provided by the following lemma.

Lemma 3.7. *If* $f, g \in L^2(G)$ *have compact support, then* $f * g \in PK(G)$.

Proof. By polarisation, it suffices to prove the result in the case $g = \widetilde{f}$. By [31, Thm. on page 4, (d)] or [10, Lemma 3.4.1] we have $f * \widetilde{f} \in C_0(G)$. Moreover, as f has compact support, so has $f * \widetilde{f}$. This shows that $f * \widetilde{f} \in C_c(G)$. By construction $f * \widetilde{f}$ is positive definite, which completes the claim. $\qquad\square$

Remark 3.8. For later use we note $1_W * \widetilde{1_W} \in PK(G) \subset KL(G)$ for relatively compact measurable $W \subset G$.

We have the following characterisation of transformability by generalised PSF. For the Haar measure on a closed subgroup of G, part (ii) of the theorem is the classical PSF as in [29, Thm. 5.5.2].

Proposition 3.9. *For* $\mu \in \mathcal{M}(G)$ *and* $\nu \in \mathcal{M}(\widehat{G})$ *the following are equivalent:*
  (i) μ *is transformable and* $\widehat{\mu} = \nu$.
  (ii) *For every* $f \in KL(G)$ *we have* $\check{f} \in L^1(\nu)$ *and* $\langle \mu, f \rangle = \langle \nu, \check{f} \rangle$.
  (iii) *For every* $f \in PK(G)$ *we have* $\check{f} \in L^1(\nu)$ *and* $\langle \mu, f \rangle = \langle \nu, \check{f} \rangle$.
  (iv) *For every* $f \in K_2(G)$ *we have* $\check{f} \in L^1(\nu)$ *and* $\langle \mu, f \rangle = \langle \nu, \check{f} \rangle$.

Proof. (i) $\Rightarrow$ (ii) follows with [1, Prop. 3.1]. (ii) $\Rightarrow$ (iii) $\Rightarrow$ (iv) holds since $K_2(G) \subset PK(G) \subset KL(G)$. (iv) $\Rightarrow$ (i) holds trivially. $\qquad\square$

3.4. **Double transformability.** For $f \in L^1(G)$ define $f^\dagger \in L^1(G)$ by $f^\dagger(x) = f(-x)$. Similarly, for $\mu \in \mathcal{M}(G)$ define $\mu^\dagger \in \mathcal{M}(G)$ via $\langle \mu^\dagger, f \rangle = \langle \mu, f^\dagger \rangle$ for all $f \in C_c(G)$. If $\mu \in \mathcal{M}(G)$ and $\widehat{\mu} \in \mathcal{M}(\widehat{G})$ are both transformable, then the inversion theorem $\widehat{\widehat{\mu}} = \mu^\dagger$ holds, and any of the measures $\mu, \mu^\dagger$ and $\widehat{\mu}$ is translation bounded [1, Thm. 3.4]. This generalises the inversion theorem for integrable functions, see

e.g. [10, Thm. 3.5.8]. We characterise when a transformable measure is twice trans-
formable.

Theorem 3.10. *Let $\mu \in \mathcal{M}(G)$ be transformable. Then the following are equivalent.*

    (i) *$\widehat{\mu} \in \mathcal{M}(\widehat{G})$ is transformable.*

    (ii) *For every $g \in K_2(\widehat{G})$ we have $\check{g} \in L^1(\mu^\dagger)$.*

If any of the above conditions holds, then $\widehat{\widehat{\mu}} = \mu^\dagger$, and the measures $\mu, \mu^\dagger$ and $\widehat{\mu}$ are translation bounded.

Proof. (i) $\Rightarrow$ (ii) Since both $\mu \in \mathcal{M}(G)$ and $\widehat{\mu} \in \mathcal{M}(\widehat{G})$ are transformable, we have $\widehat{\widehat{\mu}} = \mu^\dagger \in \mathcal{M}(G)$. Now the claim follows from Proposition 3.9.

    (ii) $\Rightarrow$ (i) Consider any $g \in K_2(\widehat{G})$. Since by assumption $\widehat{g} \cdot \mu$ is a finite measure, its Fourier transform as a measure is the absolutely continuous measure with density function

$$I(\chi) := \int_G \overline{\chi}(s)\widehat{g}(s)\mathrm{d}\mu(s).$$

Thus, for all $f \in K_2(G)$ we have $\langle \widehat{g} \cdot \mu, f \rangle = \langle I \cdot \theta_{\widehat{G}}, \check{f} \rangle$. We also have $f \cdot \widehat{g} \in C_c(G)$ and $\widetilde{f \cdot \widehat{g}} = \check{f} * g \in L^1(\widehat{G})$. Therefore, as μ is transformable we get

$$\langle \mu, f \cdot \widehat{g} \rangle = \langle \widehat{\mu}, \check{f} * g \rangle = \langle (g^\dagger * \widehat{\mu}) \cdot \theta_{\widehat{G}}, \check{f} \rangle.$$

Combining these we obtain

$$\langle I \cdot \theta_{\widehat{G}}, \check{f} \rangle = \langle \widehat{g} \cdot \mu, f \rangle = \langle (g^\dagger * \widehat{\mu}) \cdot \theta_{\widehat{G}}, \check{f} \rangle.$$

This proves the measure equality $I \cdot \theta_{\widehat{G}} = (g^\dagger * \widehat{\mu}) \cdot \theta_{\widehat{G}}$. As I and $g * \widehat{\mu}$ are both continuous functions, they must be equal, and by evaluating at 0 we get $\langle \mu, \widehat{g} \rangle = \langle \widehat{\mu}, g \rangle$. Therefore, for all $g \in K_2(\widehat{G})$ we have $\check{g} \in L^1(\mu^\dagger)$ and $\langle \widehat{\mu}, g \rangle = \langle \mu^\dagger, \check{g} \rangle$. As $\mu^\dagger \in \mathcal{M}(G)$, the claim now follows from Proposition 3.9. $\square$

Remark 3.11. Reinspecting the above proof, we can formulate the following result. Let $\mu \in \mathcal{M}(G)$ be transformable. If there exists some $\nu \in \mathcal{M}(\widehat{G})$ such that $|\mu| \leq |\widehat{\nu}|$, then μ is twice transformable.

3.5. **Fourier-Bohr coefficients.** For a σ-compact LCA group G and a trans-
formable translation bounded measure μ, the discrete part of $\widehat{\mu}$ can be computed by a certain averaging procedure. To define suitable averaging sequences, consider for $U, W \subset G$ the *(generalised) van Hove boundary*

$$\partial^U W = ((U + \mathrm{cl}(W)) \cap \mathrm{cl}(W^c)) \cup ((U + \mathrm{cl}(W^c)) \cap \mathrm{cl}(W)),$$

which was introduced in [33, Eqn. (1.1)], see also [28, Sec. 2.2] for a discussion. As $\partial W = \partial^{\{e\}} W \subset \partial^U W$ for U any unit neighbourhood, the van Hove boundary may be considered as a thickened topological boundary in that case. A *(generalised) van Hove sequence* is a sequence $(A_n)_{n \in \mathbb{N}}$ of compact sets in G of positive (and finite) Haar measure, $0 < \theta(A_n) < \infty$, such that for all compact $K \subset G$ we have

$$(3.1) \qquad \lim_{n \to \infty} \frac{\theta(\partial^K A_n)}{\theta(A_n)} = 0.$$

Existence of van Hove sequences in G is discussed in [33]. In Euclidean space, any sequence of non-empty closed rectangular boxes of diverging inradius is a van Hove sequence. Also any sequence of non-empty closed balls of diverging radius is a van Hove sequence.

Proposition 3.12 (Fourier-Bohr coefficients)**.** *For a σ-compact LCA group G, let $\mu \in \mathcal{M}^\infty(G)$ be transformable and consider $\chi \in \widehat{G}$. Let $(A_n)_{n\in\mathbb{N}}$ be any van Hove sequence in G. Then for every $t \in G$ we have*

$$\widehat{\mu}(\{\chi\}) = \lim_{n\to\infty} \frac{1}{\theta(A_n)} \int_{t+A_n} \overline{\chi}(x)\,\mathrm{d}\mu(x).$$

The convergence is uniform in $t \in G$.

Remark 3.13. The above average is sometimes called the *Fourier-Bohr coefficient* of μ at χ, compare [7, Def. 2.1] or [17, Eq. 8.14]. The proposition extends Hof's result [15, Thm. 3.2] to the non-Euclidean setting. The proposition also gener- alises a result of Lenz [20, Cor. 5], which has been derived for positive definite measures using dynamical systems. The proposition can partly be deduced from [17, Thm. 11.3] when transformability of $\widehat{\mu}$ is granted. A statement about uniform convergence appears, in the Euclidean setting, in [7, Lemma 2.4]. A short proof based on almost periodicity may be given as in [27, Thm. 1.19].

Our proof is an adaption of Hof's arguments based on the PSF. Hence the statement is a rather direct consequence of transformability. Let us first recall a fundamental property of characters.

Lemma 3.14. *Consider any σ-compact LCA group G and let $\chi \in \widehat{G}$. Then for every van Hove sequence $(A_n)_{n\in\mathbb{N}}$ in G we have*

$$\lim_{n\to\infty} \frac{1}{\theta(A_n)} \int_{A_n} \chi(x)\,\mathrm{d}\theta(x) = \delta_{\chi,e}.$$

Proof. The conclusion of the lemma clearly holds for $\chi = e$. Consider any character $\chi \neq e$ and fix any $y \in G$ such that $\chi(y) \neq 1$. By left invariance of the Haar measure on G and $\chi(yx) = \chi(y)\chi(x)$ we have

$$\int_{A_n} \chi(x)\,\mathrm{d}\theta(x) = \int_G 1_{A_n}(yx)\chi(yx)\,\mathrm{d}\theta(x) = \chi(y) \int_{-y+A_n} \chi(x)\,\mathrm{d}\theta(x).$$

Due to the van Hove property of $(A_n)_{n\in\mathbb{N}}$, we have

$$\left| \int_{-y+A_n} \chi(x)\,\mathrm{d}\theta(x) - \int_{A_n} \chi(x)\,\mathrm{d}\theta(x) \right| \leq \theta((-y+A_n)\Delta A_n) \leq \theta(\partial^{\{-y\}}A_n),$$

which is $o(\theta(A_n))$ as $n \to \infty$ since $(A_n)_n$ is a van Hove sequence. Combining the above properties yields

$$|1 - \chi(y)| \cdot \left| \frac{1}{\theta(A_n)} \int_{A_n} \chi(x)\,\mathrm{d}\theta(x) \right| = o(1)$$

as $n \to \infty$. Since $\chi(y) \neq 1$, the statement of the lemma follows. $\square$

Proof of Proposition 3.12. We prove the proposition for $\chi = e$. The general case then follows from $\widehat{\mu}(\{\chi\}) = (\delta_{\chi^{-1}} * \widehat{\mu})(\{e\})$ and $(\delta_{\chi^{-1}} * \widehat{\mu}) = \widehat{\overline{\chi}\mu}$. We give an approx- imation argument using sufficiently smooth compactly supported functions.

Define $\varphi = \psi * \widetilde{\psi} \in C_c(G)$ for some $\psi \in C_c(G)$ such that $\int \psi\,\mathrm{d}\theta = 1$. Then also $\int \varphi\,\mathrm{d}\theta = 1$. Fix any van Hove sequence $(A_n)_{n\in\mathbb{N}}$ in G and define

$$f_n^t(x) := \frac{1}{\theta(A_n)} 1_{t+A_n}(x).$$

We will also denote $(f_n^t)_\varphi := \varphi * f_n^t$. Then $(f_n^t)_\varphi \in KL(G)$ by Lemma 3.7, and Proposition 3.9 (ii) yields $\widetilde{(f_n^t)_\varphi} \in L^1(\widehat{\mu})$ and

$$(3.2) \qquad \langle \mu, (f_n^t)_\varphi \rangle = \langle \widehat{\mu}, \widetilde{(f_n^t)_\varphi} \rangle.$$

We will identify the limit in the statement of the proposition from the rhs. The lhs will yield uniform convergence. Let us start with the rhs. We first note $\widetilde{(f_n^t)_\varphi}(\chi) \to \delta_{\chi,e}$. Indeed, $\widetilde{(f_n^t)_\varphi}(e) = \check{\varphi}(e) \cdot \widetilde{f_n^t}(e) = 1$ since φ is normalised. Furthermore for $\chi \neq e$ we have

$$\left| \widetilde{(f_n^t)_\varphi}(\chi) \right| = |\check{\varphi}(\chi)| \cdot \left| \check{f}_n^t(\chi) \right| \le \|\varphi\|_1 \cdot \left| \check{f}_n^t(\chi) \right| \to 0$$

by Lemma 3.14, as $(t + A_n)_{n \in \mathbb{N}}$ is a van Hove sequence. Since $\varphi \in KL(G)$ by Lemma 3.7, we have $\check{\varphi} \in L^1(\widehat{\mu})$ by [1, Prop. 3.1]. In fact $\check{\varphi}$ is an integrable majorant of $\widetilde{(f_n^t)_\varphi}$ as

$$\left| \widetilde{(f_n^t)_\varphi} \right| = |\check{\varphi}| \cdot \left| \widetilde{f_n^t} \right| \le |\check{\varphi}| \cdot \|f_n^t\|_1 = |\check{\varphi}|.$$

We can thus apply Lebesgue's dominated convergence theorem to obtain

$$\lim_{n \to \infty} \langle \widehat{\mu}, \widetilde{(f_n^t)_\varphi} \rangle = \langle \widehat{\mu}, \delta_{\chi,e} \rangle = \widehat{\mu}(\{e\}).$$

Now consider the limit $n \to \infty$ on the lhs of (3.2). Since f_n^t is proportional to the characteristic function of $t + A_n$, by a standard tedious computation which we omit, we have that $f_n^t(x) \neq (f_n^t)_\varphi(x)$ implies $x \in t + \partial^K A_n$, where $K = \mathrm{supp}(\varphi)$. Hence we have for all n the estimate

$$|\langle \mu, f_n^t \rangle - \langle \mu, (f_n^t)_\varphi \rangle| \le \|1 - \varphi\|_\infty \cdot \frac{|\mu|(t + \partial^K A_n)}{\theta(A_n)}.$$

The rhs vanishes as $n \to \infty$ uniformly in $t \in G$, by translation boundedness of μ and by the van Hove property of $(A_n)_{n \in \mathbb{N}}$. This may be seen by inspecting the proof of [19, Lemma 9.2 (b)]. Hence existence and uniformity of the limit follow. $\qquad \square$

4. FOURIER ANALYSIS OF WEIGHTED MODEL SETS

Let G, H be LCA groups and assume that $\mathcal{L}$ is a lattice in $G \times H$. We will consider measures on G supported on certain projected lattice subsets. The goal of this section is to prove that their Fourier transform formula follows from the PSF of the underlying lattice. A consequence is a certain averaging property of such measures which is also known as the density formula.

4.1. **Cut-and-project schemes and weighted model sets.** We recall the definitions of a cut-and-project scheme and of a model set.

Definition 4.1 (Cut-and-project scheme)**.** *Let G, H be LCA groups, and let $\mathcal{L}$ be a lattice in $G \times H$, i.e., a discrete co-compact subgroup of $G \times H$. We call $(G, H, \mathcal{L})$ a* cut-and-project scheme *if, with canonical projections $\pi^G : G \times H \to G$, $\pi^H : G \times H \to H$,*

(i) *the restriction $\pi^G|_\mathcal{L}$ of π^G to $\mathcal{L}$ is one-to-one,*
(ii) *$\pi^H(\mathcal{L})$ is dense in H.*

Remark 4.2. Note that condition (ii) may be assumed to hold without loss of generality by passing from H to $\overline{\pi^H(\mathcal{L})}$. Since $\pi^G|_\mathcal{L}$ is one-to-one, $\pi^G|_\mathcal{L}$ is a group isomorphism between $\mathcal{L}$ and $L = \pi^G(\mathcal{L})$, and hence invertible in that case. We thus get a map $\star : L \to H$ via the composition $L \xrightarrow{(\pi^G|_\mathcal{L})^{-1}} \mathcal{L} \xrightarrow{\pi^H} L^\star$, which is also called

the star map. It is readily checked that $\mathcal{L} = \{(x, x^\star) \mid x \in L\}$. We will not use the star map in the sequel, since a number of our results hold without assumption (i).

Remark 4.3. Assume that $(G, H, \mathcal{L})$ is a cut-and-project scheme. Then the annihilator $\mathcal{L}_0 \subset \widehat{G} \times \widehat{H}$ of $\mathcal{L}$ is a lattice, the lattice dual to $\mathcal{L}$. Let us write $\pi^{\widehat{G}} : \widehat{G} \times \widehat{H} \to \widehat{G}$, $\pi^{\widehat{H}} : \widehat{G} \times \widehat{H} \to \widehat{H}$ for the canonical projections and define $L_0 = \pi^{\widehat{G}}(\mathcal{L}_0)$. Pontryagin duality can be used to show that $\pi^{\widehat{G}}|_{\mathcal{L}_0}$ is one-to-one/dense if and only if $\pi^H|_{\mathcal{L}}$ is dense/one-to-one and $\pi^{\widehat{H}}|_{\mathcal{L}_0}$ is one-to-one/dense if and only if $\pi^G|_{\mathcal{L}}$ is dense/one-to-one, see e.g. [26, Sec. 5]. Hence $(\widehat{G}, \widehat{H}, \mathcal{L}_0)$ is also a cut-and-project scheme, and we have a star map $\star : L_0 \to \widehat{H}$ as in $(G, H, \mathcal{L})$. This dual cut-and-project scheme describes the diffraction of a model set in $(G, H, \mathcal{L})$.

Definition 4.4 (Model set). Let a cut-and-project scheme $(G, H, \mathcal{L})$ be given and assume that $W \subset H$ is relatively compact and measurable. Then $\wedge(W) = \pi^G(\mathcal{L} \cap G \times W)$ is called a *weak model set*, compare [25, 16]. If W has non-empty interior, then $\wedge(W)$ is called a *model set*. We say that $\wedge(W)$ is a *regular model set* if W relatively compact, measurable, has non-empty interior and $\theta_H(\partial W) = 0$.

Remark 4.5 (Delone sets). Recall that $D \subset G$ is uniformly discrete if there exists a non-empty open set $U \subset G$ such that $x + U$ contains at most one point of D for every $x \in G$. The set $D \subset G$ is called relatively dense in G if there is a compact set $K \subset G$ such that $D + K = G$. If $D \subset G$ is both uniformly discrete and relatively dense, then D is called a *Delone set*. If $W \subset H$ is relatively compact, then $\wedge(W)$ is uniformly discrete. This is a simple consequence of uniform discreteness of $\mathcal{L}$. If $W \subset H$ has non-empty interior, then $\wedge(W)$ is relatively dense. For details of the arguments see e.g. [26, Prop. 2.6 (i)].

Definition 4.6 (Weighted model set). *Let $(G, H, \mathcal{L})$ be cut-and-project scheme. Any function $h : H \to \mathbb{C}$ is called a* weight function *on H. Assume that h is a weight function such that*

$$\omega_h := \sum_{(x,y) \in \mathcal{L}} h(y) \delta_x$$

is a measure on G. Then $\omega_h \in \mathcal{M}(G)$ is called a weighted model set *from $(G, H, \mathcal{L})$.*

Remark 4.7. We will be interested in weight functions h such that ω_h is a translation bounded or transformable measure. Any weak model set $\wedge(W)$ leads to the weighted model set $\omega_h = \delta_{\wedge(W)}$ with $h = 1_W$. In fact ω_h is then a translation bounded measure since $\wedge(W)$ is uniformly discrete, but a non-periodic ω_h may not be transformable, see the example [15, p. 37].

We say that $\omega_h \in \mathcal{M}(G)$ is *uniformly translation bounded* if for every compact subset $K \subset G$ we have

$$\sup\{|\omega_{t+h}(s + K)| : (s, t) \in G \times H\} < \infty.$$

An important class of weighted model sets arise from Riemann integrable functions $h : H \to \mathbb{C}$.

Lemma 4.8. *Let $h : H \to \mathbb{C}$ be a bounded and compactly supported weight function. Then ω_h is a weighted model set. In fact ω_h is a uniformly translation bounded measure on G.*

Proof. Since h is bounded and of compact support, we find $0 \le c < \infty$ and compact $W \subset H$ such that $|h| \le c \cdot 1_W$. Fix arbitrary compact $K \subset G$ and $s \in G$, $t \in H$. We then have

$$|\omega_{t+h}(s+K)| = \left| \sum_{(x,y) \in \mathcal{L}} (t+h)(y) 1_{s+K}(x) \right| \le \sum_{(x,y) \in \mathcal{L}} c \cdot 1_{t+W}(y) 1_{s+K}(x)$$

$$\le c \cdot \sup_{t \in G} \sharp (\mathcal{L} \cap ((t+W) \times (s+K))) < \infty.$$

By uniform discreteness of the lattice $\mathcal{L}$, the term on the rhs is a finite constant which does not depend on $s \in G$ or $t \in H$. This shows that ω_h is a uniformly translation bounded measure and, in particular, a weighted model set. $\square$

4.2. **Generalised PSF for weighted model sets.** The theorems of this subsection form the heart of this paper. We would like to remark that conditions (i), (ii) of Definition 4.1 are not used in the proofs. We first consider weighted model sets with positive definite weight functions.

Theorem 4.9 (PSF for weighted model sets I)**.** *Let $(G, H, \mathcal{L})$ be a cut-and-project scheme with dual cut-and-project scheme $(\widehat{G}, \widehat{H}, \mathcal{L}_0)$. Then the following are equivalent.*

(i) *The lattice Dirac comb $\delta_{\mathcal{L}} \in \mathcal{M}^{\infty}(G \times H)$ is transformable and satisfies the PSF*

$$\widehat{\delta_{\mathcal{L}}} = \mathrm{dens}(\mathcal{L}) \cdot \delta_{\mathcal{L}_0}.$$

(ii) *For every $h \in PK(H)$, the weighted model set $\omega_h \in \mathcal{M}^{\infty}(G)$ is strongly translation bounded, transformable and satisfies, with $\omega_{\check{h}} \in \mathcal{M}^{\infty}(\widehat{G})$, the generalised PSF*

$$\widehat{\omega_h} = \mathrm{dens}(\mathcal{L}) \cdot \omega_{\check{h}}.$$

(iii) *For every $h \in K_2(H)$, the weighted model set $\omega_h \in \mathcal{M}^{\infty}(G)$ is strongly translation bounded, transformable and satisfies, with $\omega_{\check{h}} \in \mathcal{M}^{\infty}(\widehat{G})$, the generalised PSF*

$$\widehat{\omega_h} = \mathrm{dens}(\mathcal{L}) \cdot \omega_{\check{h}}.$$

The following remark serves as a preparation for the proof of Theorem 4.9.

Remark 4.10 (test functions in product spaces)**.** For given functions $g : G \to \mathbb{C}$ and $h : H \to \mathbb{C}$, we will denote by $g \odot h$ the function $G \times H \to \mathbb{C}$ given by $(g \odot h)(s,t) = g(s) \cdot h(t)$. It is easy to see that $g \in C_c(G)$ and $h \in C_c(H)$ imply $g \odot h \in C_c(G \times H)$, and that $g \in K_2(G)$ and $h \in K_2(H)$ imply $g \odot h \in K_2(G \times H)$. Similarly, $g \in KL(G)$ and $h \in KL(H)$ imply $g \odot h \in KL(G \times H)$, and $g \in PK(G)$ and $h \in PK(H)$ imply $g \odot h \in PK(G \times H)$ by [6, Lemma 3.2].

Proof of Theorem 4.9. "(i) $\Rightarrow$ (ii)" Without loss of generality, fix any positive definite $h \in PK(H)$. Then ω_h is a uniformly translation bounded measure since $\delta_{\mathcal{L}}$ is translation bounded, see Lemma 4.8. For arbitrary positive definite $g \in PK(G)$ we have $g \odot h \in PK(G \times H)$, by assumption and Theorem 3.1 we have $\check{g} \odot \check{h} \in L^1(\delta_{\mathcal{L}_0})$ and hence

$$0 \le \langle \delta_{\mathcal{L}}, g \odot h \rangle = \mathrm{dens}(\mathcal{L}) \cdot \langle \delta_{\mathcal{L}_0}, \check{g} \odot \check{h} \rangle < \infty$$

By definition of ω_h we have $\langle \omega_h, g \rangle = \langle \delta_{\mathcal{L}}, g \odot h \rangle$. For the rhs of the above equation we note that by definition of $\omega_{\breve{h}}$ we have

$$\langle \delta_{\mathcal{L}_0}, \breve{g} \odot \breve{h} \rangle = \sum_{(\chi, \eta) \in \mathcal{L}_0} \breve{h}(\eta) \cdot \breve{g}(\chi) = \langle \omega_{\breve{h}}, \breve{g} \rangle.$$

Therefore we have for arbitrary $g \in PK(G)$ the equality

$$(4.1) \qquad\qquad \langle \omega_h, g \rangle = \mathrm{dens}(\mathcal{L}) \cdot \langle \omega_{\breve{h}}, \breve{g} \rangle.$$

Next we show that the linear functional $\omega_{\breve{h}}$ is a measure, which will follow from positive definiteness of h. Note that $\breve{h} \in C(\widehat{G})$ is a positive function since h is positive definite. Now consider any compact set $K \subset \widehat{G}$. Then there exists some $f \in C_c(G)$ such that $\left| \breve{f} \right|^2 \geq 1_K$, see e.g. [10, Lemma 3.4.5]. Hence for all $\phi \in C_c(\widehat{G})$ with $\mathrm{supp}(\phi) \subset K$ we have

$$\left| \langle \omega_{\breve{h}}, \phi \rangle) \right| = \left| \sum_{(\chi, \eta) \in \mathcal{L}_0} \phi(\chi) \breve{h}(\eta) \right| \leq \sum_{(\chi, \eta) \in \mathcal{L}_0} |\phi(\chi)| \breve{h}(\eta) \leq \sum_{(\chi, \eta) \in \mathcal{L}_0} \|\phi\|_\infty 1_K(\chi) \breve{h}(\eta)$$

$$\leq \sum_{(\chi, \eta) \in \mathcal{L}_0} \|\phi\|_\infty \left| \breve{f} \right|^2 (\chi) \breve{h}(\eta) = \left(\sum_{(\chi, \eta) \in \mathcal{L}_0} \left| \breve{f} \right|^2 (\chi) \breve{h}(\eta) \right) \|\phi\|_\infty.$$

Here the term in brackets is finite as $g := f * \widetilde{f} \in PK(G)$ and hence Eqn. (4.1) holds. Defining $C_K := \sum_{(\chi, \eta) \in \mathcal{L}_0} \left| \breve{f} \right|^2 (\chi) \breve{h}(\eta)$, we have for every $\phi \in C_c(\widehat{G})$ with $\mathrm{supp}(\phi) \subset K$ the estimate

$$\left| \omega_{\breve{h}}(\phi) \right| \leq C_K \|\phi\|_\infty.$$

This shows that $\phi \mapsto \sum_{(\chi, \eta) \in \mathcal{L}_0} \phi(\chi) \breve{h}(\eta)$ defines a measure on H, and it is straightforward to see that this measure is exactly $\omega_{\breve{h}}$. This measure is positive by definition, and for any positive definite $g \in PK(G)$ we have seen above that $\langle \omega_{\breve{h}}, \breve{g} \rangle < \infty$. This implies $\breve{g} \in L^1(\omega_{\breve{h}})$ for every $g \in PK(G)$, which together with (4.1) gives that ω_h is transformable by Proposition 3.9. Translation boundedness of $\omega_{\breve{h}}$ follows from Remark 3.4.

"(ii) $\Rightarrow$ (iii)" Follows immediately from $K_2(G) \subset PK(G)$.

"(iii) $\Rightarrow$ (i)" The claim $\delta_{\mathcal{L}} \in \mathcal{M}^\infty(G \times H)$ follows from strong translation boundedness of the measures ω_h for $h \in K_2(H)$ by elementary estimates. Let $g \in K_2(G)$ and $h \in K_2(H)$. As before, from (iii) it is immediate that

$$(4.2) \qquad\qquad \langle \delta_{\mathcal{L}}, g \odot h \rangle = \mathrm{dens}(\mathcal{L}) \cdot \langle \delta_{\mathcal{L}_0}, \breve{g} \odot \breve{h} \rangle.$$

By (iii) we have $\breve{g} \in L^1(\omega_{\breve{h}})$, which means $\breve{g} \odot \breve{h} \in L^1(\delta_{\mathcal{L}_0})$. Hence the PSF holds for all functions in $K_2(G) \odot K_2(H) := \{ g \odot h \,|\, g \in K_2(G), h \in K_2(H) \}$. We split the proof for general functions from $K_2(G \times H)$ in four steps.

Step 1: We show for any $g \in K_2(G)$ and $h \in K_2(H)$ that $\widehat{(g \odot h)}$ is convolvable with $\delta_{\mathcal{L}_0}$ and that the function $\mathrm{dens}(\mathcal{L}) \cdot \widehat{(g \odot h)} * \delta_{\mathcal{L}_0}$ is the Fourier transform of the finite measure $(g \odot h) \cdot \delta_{\mathcal{L}}$. In particular, this implies that $\widehat{(g \odot h)} * \delta_{\mathcal{L}_0} \in C_U(\widehat{G} \times \widehat{H})$.

Let $(\chi, \psi) \in \widehat{G} \times \widehat{H}$. As $K_2(G)$ and $K_2(H)$ are closed under multiplication by characters, $(\overline{\chi} g) \odot (\overline{\psi} h) \in K_2(G) \odot K_2(H)$. Therefore, by the above we have $\widetilde{\overline{\chi} g} \odot \widetilde{\overline{\psi} h} \in L^1(\delta_{\mathcal{L}_0})$ and $\langle \delta_{\mathcal{L}}, (\overline{\chi} g) \odot (\overline{\psi} h) \rangle = \mathrm{dens}(\mathcal{L}) \cdot \langle \delta_{\mathcal{L}_0}, \widetilde{\overline{\chi} g} \odot \widetilde{\overline{\psi} h} \rangle$. Therefore, we

have

$$\int_{G \times H} \overline{\psi(s)\chi(t)} \, \mathrm{d}[(g \odot h) \cdot \delta_{\mathcal{L}}](s,t) = \langle \delta_{\mathcal{L}}, (\overline{\chi}g) \odot (\overline{\psi}h) \rangle$$

$$= \mathrm{dens}(\mathcal{L}) \cdot \langle \delta_{\mathcal{L}_0}, \widetilde{\overline{\chi}g} \odot \widetilde{\overline{\psi}h} \rangle = \mathrm{dens}(\mathcal{L}) \cdot \langle \delta_{\mathcal{L}_0}, T_{\chi,\psi}(\check{g} \odot \check{h}) \rangle$$

$$= \mathrm{dens}(\mathcal{L}) \cdot \delta_{\mathcal{L}_0} * (\widehat{g} \odot \widehat{h})(\chi,\psi),$$

where the convolution makes sense as $T_{\chi,\psi}(\check{g} \odot \check{h}) = \widetilde{\overline{\chi}g} \odot \widetilde{\overline{\psi}h} \in L^1(\delta_{\mathcal{L}_0})$. This shows that the function $\mathrm{dens}(\mathcal{L}) \cdot \widehat{(g \odot h)} * \delta_{\mathcal{L}_0}$ is the Fourier transform of the finite measure $(g \odot h) \cdot \delta_{\mathcal{L}}$.

Step 2: For any $g \in K_2(G)$, $h \in K_2(H)$ and $f \in K_2(G \times H)$ we have $\check{f} \in L^1(\widehat{(g \odot h)} * \delta_{\mathcal{L}_0})$ and

$$\langle \delta_{\mathcal{L}}, f \cdot (g \odot h) \rangle = \mathrm{dens}(\mathcal{L}) \cdot \langle \widehat{(g \odot h)} * \delta_{\mathcal{L}_0} \cdot \theta_{\widehat{G} \times \widehat{H}}, \check{f} \rangle.$$

This follows immediately from $\langle \delta_{\mathcal{L}}, f \cdot (g \odot h) \rangle = \langle (g \odot h) \cdot \delta_{\mathcal{L}}, f \rangle$ and from the fact that the Fourier transforms of a finite measure as a measure and as a finite measure coincide [1, Thm. 2.2].

Step 3: We show that for any $g \in K_2(G)$, $h \in K_2(H)$ and $f \in K_2(G \times H)$, all positive definite, we have $\widetilde{(g \odot h)} * \check{f} \in L^1(\delta_{\mathcal{L}_0})$ and

$$\langle \widehat{(g \odot h)} * \delta_{\mathcal{L}_0} \cdot \theta_{\widehat{G} \times \widehat{H}}, \check{f} \rangle = \langle \delta_{\mathcal{L}_0}, \check{f} * \widetilde{(g \odot h)} \rangle.$$

By Step 2 we know that $\check{f} \in L^1(\widehat{(g \odot h)} * \delta_{\mathcal{L}_0})$, while by Step 1 we know that $\widehat{(g \odot h)} * \delta_{\mathcal{L}_0}$ is given by the continuous function

$$\widehat{(g \odot h)} * \delta_{\mathcal{L}_0}(x) = \int_{\widehat{G} \times \widehat{H}} \widehat{(g \odot h)}(x-y) \, \mathrm{d}\delta_{\mathcal{L}_0}(y).$$

Therefore we have by positive definiteness

$$0 \le \langle \widehat{(g \odot h)} * \delta_{\mathcal{L}_0} \cdot \theta_{\widehat{G} \times \widehat{H}}, \check{f} \rangle = \int_{\widehat{G} \times \widehat{H}} \check{f}(x) \int_{\widehat{G} \times \widehat{H}} \widehat{(g \odot h)}(x-y) \mathrm{d}\delta_{\mathcal{L}_0}(y) \, \mathrm{d}\theta_{\widehat{G} \times \widehat{H}}(x) < \infty.$$

By positivity, we can use Tonelli's theorem to exchange the order of integration. This results in

$$\langle \delta_{\mathcal{L}_0}, \check{f} * \widetilde{(g \odot h)} \rangle = \int_{\widehat{G} \times \widehat{H}} \check{f}(x) * \widetilde{(g \odot h)}(x) \, \mathrm{d}\delta_{\mathcal{L}_0}(y)$$

$$= \int_{\widehat{G} \times \widehat{H}} \int_{\widehat{G} \times \widehat{H}} \check{f}(x) \widetilde{(g \odot h)}(x-y) \, \mathrm{d}\theta_{\widehat{G} \times \widehat{H}}(x) \, \mathrm{d}\delta_{\mathcal{L}_0}(y)$$

$$= \int_{\widehat{G} \times \widehat{H}} \check{f}(x) \int_{\widehat{G} \times \widehat{H}} \widehat{(g \odot h)}(x-y) \, \mathrm{d}\delta_{\mathcal{L}_0}(y) \, \mathrm{d}\theta_{\widehat{G} \times \widehat{H}}(x) < \infty,$$

which proves Step 3.

Step 4: We prove the PSF for general functions in $K_2(G \times H)$. Consider without loss of generality $f \in K_2(G \times H)$ positive definite. As f has compact support, we can find compact sets $K_1 \subset G, K_2 \subset H$ such that $\mathrm{supp}(f) \subset K_1 \times K_2$. Next, pick two functions $g \in K_2(G)$ and $h \in K_2(H)$ such that $g \equiv 1$ on K_1 and $h \equiv 1$ on K_2. For example, one may pick a continuous function $g_1 \in C_c(G)$ with $\int_G g_1(t) \mathrm{d}\theta_G(t) = 1$ and then some $g_2 \in C_c(G)$ which is 1 on $K_1 - \mathrm{supp}(g_1)$. Then $g = g_1 * g_2 \in K_2(G)$ and $g \equiv 1$ on K_1. We choose $h \in K_2(H)$ in the same way. Then by construction $g \odot h \equiv 1$ on $\mathrm{supp}(f)$, and we therefore have $f \cdot (g \odot h) = f$. As both $\check{f}$ and $\widetilde{g \odot h}$ are elements of $L^1(\widehat{G} \times \widehat{H}) \cap L^2(\widehat{G} \times \widehat{H})$, by taking the inverse Fourier transform we also get

$$\check{f} * \widetilde{(g \odot h)} = \check{f}.$$

In order to apply Step 3, we use depolarisation to find $a_i \in \mathbb{C}$ and $g_i \in K_2(G), h_i \in K_2(H)$ positive definite such that $g \odot h = \sum_{i=1}^{N} a_i \cdot (g_i \odot h_i)$ for some N. By Step 3 we have $\widetilde{(g_i \odot h_i)} * \check{f} \in L^1(\delta_{\mathcal{L}_0})$ and

$$\langle \widetilde{(g_i \odot h_i)} * \delta_{\mathcal{L}_0} \cdot \theta_{\widehat{G} \times \widehat{H}}, \check{f} \rangle = \langle \delta_{\mathcal{L}_0}, \check{f} * \widetilde{(g_i \odot h_i)} \rangle.$$

Therefore we have

$$\check{f} = \check{f} * \widetilde{(g \odot h)} = \sum_{i=1}^{N} a_i \cdot \check{f} * \widetilde{(g_i \odot h_i)} \in L^1(\delta_{\mathcal{L}_0})$$

and

$$\langle \delta_{\mathcal{L}}, f \rangle = \langle \delta_{\mathcal{L}}, f \cdot (g \odot h) \rangle = \mathrm{dens}(\mathcal{L}) \cdot \langle \widetilde{(g \odot h)} * \delta_{\mathcal{L}_0} \cdot \theta_{\widehat{G} \times \widehat{H}}, \check{f} \rangle$$

$$= \mathrm{dens}(\mathcal{L}) \cdot \sum_{i=1}^{N} a_i \cdot \langle \widetilde{(g_i \odot h_i)} * \delta_{\mathcal{L}_0} \cdot \theta_{\widehat{G} \times \widehat{H}}, \check{f} \rangle = \mathrm{dens}(\mathcal{L}) \cdot \sum_{i=1}^{N} a_i \cdot \langle \delta_{\mathcal{L}_0}, \check{f} * \widetilde{(g_i \odot h_i)} \rangle$$

$$= \mathrm{dens}(\mathcal{L}) \cdot \langle \delta_{\mathcal{L}_0}, \check{f} * \widetilde{(g \cdot h)} \rangle = \mathrm{dens}(\mathcal{L}) \cdot \langle \delta_{\mathcal{L}_0}, \check{f} \rangle.$$

This completes the proof. $\qquad\square$

The weighted Dirac combs ω_h in the previous theorem are in fact twice Fourier transformable.

Theorem 4.11 (Double transformability for weighted model sets)**.** *Let $(G, H, \mathcal{L})$ be a cut-and-project scheme with dual cut-and-project scheme $(\widehat{G}, \widehat{H}, \mathcal{L}_0)$. Then for every $h \in PK(H)$, the weighted model set $\omega_h \in \mathcal{M}^\infty(G)$ is twice transformable, and $\omega_{\check{h}} \in \mathcal{M}^\infty(\widehat{G})$ satisfies the generalised PSF*

$$\widehat{\omega_{\check{h}}} = \mathrm{dens}(\mathcal{L}_0) \cdot \omega_{h^\dagger}.$$

Proof. Recalling Theorem 4.9, it remains to be shown that $\omega_{\check{h}}$ is transformable with transform $\mathrm{dens}(\mathcal{L}_0) \cdot \omega_{h^\dagger}$. Noting $(\omega_h)^\dagger = \omega_{h^\dagger}$ and $\mathrm{dens}(\mathcal{L}) \cdot \mathrm{dens}(\mathcal{L}_0) = 1$, by Theorem 3.10 it suffices to show that $\check{g} \in L^1(\omega_{h^\dagger})$ for all $g \in K_2(\widehat{G})$. As h is compactly supported, there exists some $f \in C_c(H)$ such that $\left| \check{f} \right|^2 \geq |h^\dagger|$. Let $g \in K_2(\widehat{G})$. Then, as $g \odot (f * \widetilde{f}) \in K_2(\widehat{G} \times \widehat{H})$, by the PSF for $\mathcal{L}_0$ we get $\check{g} \odot \left| \check{f} \right|^2 \in L^1(\delta_{\mathcal{L}})$ and

$$0 \leq \mathrm{dens}(\mathcal{L}_0) \cdot \langle \delta_{\mathcal{L}}, \check{g} \odot \left| \check{f} \right|^2 \rangle = \langle \delta_{\mathcal{L}_0}, g \odot (f * \widetilde{f}) \rangle < \infty.$$

Using $\left| \check{f} \right|^2 \geq |h^\dagger|$ we thus get $\sum_{(x,y) \in \mathcal{L}} |\check{g}(x)| |h^\dagger(y)| < \infty$, which means $\check{g} \in L^1(\omega_{h^\dagger})$. $\qquad\square$

We have the following result for the test function space $KL(G)$. With respect to transformability, it emphasises the condition that $\omega_{\check{h}}$ needs to be a measure.

Theorem 4.12 (PSF for weighted model sets II)**.** *Let $(G, H, \mathcal{L})$ be a cut-and-project scheme and let $h \in KL(G)$. Then $\omega_h \in \mathcal{M}^\infty(G)$, and the following holds.*

(i) *For all $g \in KL(G)$ the sum $\sum_{(\chi, \eta) \in \mathcal{L}_0} \check{g}(\chi) \check{h}(\eta) =: \langle \omega_{\check{h}}, \check{g} \rangle$ is absolutely convergent and we have*

$$\langle \omega_h, g \rangle = \mathrm{dens}(\mathcal{L}) \cdot \langle \omega_{\check{h}}, \check{g} \rangle.$$

(ii) *The measure ω_h is transformable if and only if $\omega_{\check{h}}$ is a measure. In this case*

$$\widehat{\omega_h} = \mathrm{dens}(\mathcal{L}) \cdot \omega_{\check{h}}.$$

$\qquad\square$

Proof. The claim $\omega_h \in \mathcal{M}^{\infty}(G)$ for $h \in KL(G)$ is Lemma 4.8. Part (i) is proved by rethinking the arguments in the proof of Theorem 4.9. Here we use that $g \cdot h \in KL(G \times H)$ by Remark 4.10, and hence we can apply the lattice PSF Theorem 3.1.

As to part "(ii) $\Rightarrow$", consider for $h \in KL(H)$ and $g_1, g_2 \in C_c(G)$ the equations

$$\langle \omega_h, g_1 * g_2 \rangle = \langle \delta_{\mathcal{L}}, (g_1 * g_2) \odot h \rangle = \mathrm{dens}(\mathcal{L}) \cdot \langle \delta_{\mathcal{L}_0}, (\check{g}_1 \cdot \check{g}_2) \odot \check{h} \rangle = \mathrm{dens}(\mathcal{L}) \cdot \langle \omega_{\check{h}}, \check{g}_1 \cdot \check{g}_2 \rangle.$$

Here the second equation uses that $(g_1 * g_2) \odot h \in KL(G \times H)$, such that the PSF for the lattice $\mathcal{L}$ can be applied. By denseness of $\widehat{C_c(G)}$ in $C_0(\widehat{G})$ and by the Riesz representation theorem for $C_0(\widehat{G})$, we have that the bounded linear functional $\check{g}_1 \mathrm{d}\omega_{\check{h}}$ is a finite Radon measure. This can be used to define a linear functional $\widehat{\mu}$ by

$$\widehat{\mu}(\varphi) = \int_{\widehat{G}} \frac{\varphi}{\check{g}_1} \check{g}_1 \mathrm{d}\omega_{\check{h}},$$

where $\varphi \in C_c(\widehat{G})$ and $g_1 \in C_c(G)$ is chosen such that $\check{g}_1$ is positive on the support of φ. It is easy to see that $\widehat{\mu}$ is well-defined and a bounded linear functional. Hence $\widehat{\mu}$ is a measure, which concides with $\omega_{\check{h}}$, as is seen by direct calculation.

For "(ii) $\Leftarrow$", fix $h \in KL(H)$ and consider for arbitrary $g \in K_2(G)$ the equation

$$\langle \omega_h, g \rangle = \langle \delta_{\mathcal{L}}, g \odot h \rangle = \mathrm{dens}(\mathcal{L}) \cdot \langle \delta_{\mathcal{L}_0}, \check{g} \odot \check{h} \rangle = \mathrm{dens}(\mathcal{L}) \cdot \langle \omega_{\check{h}}, \check{g} \rangle.$$

Here the second equation uses $g \odot h \in KL(G \times H)$, such that the PSF for the lattice $\mathcal{L}$ can be applied. In particular $\check{g} \in L^1(\omega_{\check{h}})$ since $\check{g} \odot \check{h} \in L^1(\delta_{\mathcal{L}_0})$. Hence ω_h is transformable with $\widehat{\omega_h} = \mathrm{dens}(\mathcal{L}) \cdot \omega_{\check{h}}$. $\qquad\square$

4.3. Density formula for weighted model sets.

A consequence of the lattice PSF is a certain averaging property which is known as the density formula for regular model sets. See [16, Sec. 3] for a discussion of its history. Note that condition (i) of Definition 4.1 is not used in the following proofs.

Proposition 4.13 (Density formula for weight functions in $PK(H)$)**.** *Let $(G, H, \mathcal{L})$ be a cut-and-project scheme with σ-compact G, and let $(A_n)_{n \in \mathbb{N}}$ be any van Hove sequence in G. Then for all $h \in PK(H)$ and for all $t \in G$ we have*

$$\lim_{n \to \infty} \frac{\omega_h(t + A_n)}{\theta_G(A_n)} = \mathrm{dens}(\mathcal{L}) \cdot \int_H h \, \mathrm{d}\theta_H$$

The convergence is uniform in $t \in G$.

Proof. This follows from the generalised PSF Theorem 4.9. As $\omega_{\check{h}}$ is a measure, we have $\omega_{\check{h}}(\{0\}) = \check{h}(0)$. Here we used that $\pi^{\widehat{G}}|_{\mathcal{L}_0}$ is one-to-one, which follows from denseness of $\pi^H(\mathcal{L})$ in H by Pontryagin duality. Moreover, as ω_h is a translation bounded measure by Lemma 4.8 and transformable, we can apply Proposition 3.12 to obtain

$$\widehat{\omega_h}(\{0\}) = \lim_{n \to \infty} \frac{\omega_h(t + A_n)}{\theta_G(A_n)}$$

uniformly in $t \in G$. The claim follows now from Theorem 4.9. $\qquad\square$

The range of the density formula can be extended to Riemann integrable weight functions $h : H \to \mathbb{C}$ by a standard approximation argument, see e.g. [4]. For the convenience of the reader, we repeat the short argument.

Theorem 4.14 (Density formula for Riemann integrable weight functions). *Let $(G, H, \mathcal{L})$ be a cut-and-project scheme with σ-compact G. If $h : H \to \mathbb{C}$ is Riemann integrable, then for every van Hove sequence $(A_n)_{n \in \mathbb{N}}$ in G the density formula holds, i.e., for every $t \in G$ we have*

$$\lim_{n \to \infty} \frac{\omega_h(t + A_n)}{\theta_G(A_n)} = \operatorname{dens}(\mathcal{L}) \cdot \int_H h \, d\theta_H.$$

The convergence is uniform in $t \in G$.

Proof. We assume without loss of generality that h is real valued. Let $\varepsilon > 0$ and define $c = \operatorname{dens}(\mathcal{L}) > 0$. Since h is Riemann integrable, by the density of $K_2(H)$ in $C_c(H)$, there exists two functions $g_1, g_2 \in K_2(G)$ such that $g_1 \le h \le g_2$ and $\int (g_2 - g_1) \, d\theta_H \le \frac{\varepsilon}{2c}$. By the density formula Theorem 4.13 there exists an N such that for all $n \ge N$, all $t \in G$ and $i \in \{1, 2\}$ we have

$$\left| \frac{\omega_{g_i}(t + A_n)}{\theta_G(A_n)} - c \int g_i \, d\theta_H \right| \le \frac{\varepsilon}{2}.$$

Thus, as $\omega_{g_1} \le \omega_h \le \omega_{g_2}$, for all $n \ge N$ and all $t \in G$ we have

$$c \int h \, d\theta_H - \frac{\omega_h(t + A_n)}{\theta_G(A_n)} \le \frac{\varepsilon}{2} + c \int g_2 \, d\theta_H - \frac{\omega_{g_1}(t + A_n)}{\theta_G(A_n)} \le \varepsilon$$

and similarly

$$c \int h \, d\theta_H - \frac{\omega_h(t + A_n)}{\theta_G(A_n)} \ge -\frac{\varepsilon}{2} + c \int g_1 \, d\theta_H - \frac{\omega_{g_2}(t + A_n)}{\theta_G(A_n)} \ge -\varepsilon$$

Hence the claim of the theorem follows. $\square$

5. Diffraction of weighted model sets

5.1. **Autocorrelation of weighted model sets.** The following result is well-known, see e.g. [4]. For the convenience of the reader, we revisit its proof and note that condition (i) of Definition 4.1 does not enter in the arguments.

Proposition 5.1. *Let $(G, H, \mathcal{L})$ be a cut-and-project scheme with σ-compact G. Let $h : H \to \mathbb{C}$ be Riemann integrable. Then the weighted model set $\omega_h \in \mathcal{M}^\infty(G)$ has a unique autocorrelation measure $\gamma = \omega_h \circledast \widetilde{\omega_h} \in \mathcal{M}^\infty(G)$ which is given by*

$$\gamma = \operatorname{dens}(\mathcal{L}) \cdot \omega_{h * \widetilde{h}}$$

Proof. Fix any van Hove sequence $(A_n)_{n \in \mathbb{N}}$ in G. According to Section 2, the autocorrelation of $\omega_h \in \mathcal{M}^\infty(G)$ is defined as the vague limit of the finite autocorrelation measures γ_n given by

$$\gamma_n = \frac{1}{\theta_G(A_n)} \, \omega_h|_{A_n} * \widetilde{\omega_h|_{A_n}} = \frac{1}{\theta_G(A_n)} \, \omega_h|_{A_n} * \omega_{\widetilde{h}}|_{-A_n} = \sum_{(z, z') \in \mathcal{L}} \eta_n'(z') \delta_z,$$

where $|_{A_n}$ denotes restriction to A_n, and where $\eta_n'(z')$ is given by

$$\eta_n'(z') = \frac{1}{\theta_G(A_n)} \sum_{(x, x') \in \mathcal{L} \cap (A_n \cap (z + A_n)) \times H)} h(x') \overline{h(x' - z')}.$$

For fixed n, the above sum is finite since ω_h is a measure and h is bounded. Also note

$$\left| \sum_{(x, x') \in \mathcal{L} \cap (A_n \Delta (z + A_n)) \times H} h(x') \overline{h(x' - z')} \right| \le \|h\|_\infty \cdot |\omega_h|(\partial^{\{z\}} A_n) = o(\theta_G(A_n))$$

as $n \to \infty$ since ω_h is translation bounded and A_n is a van Hove sequence, see [19, Lemma 9.2 (b)]. This shows that vaguely $\gamma_n = \sum_{(z,z') \in \mathcal{L}} \eta_n(z') \delta_z + o(1)$ as $n \to \infty$ where

$$\eta_n(z') = \frac{1}{\theta_G(A_n)} \sum_{(x,x') \in \mathcal{L} \cap A_n \times H} h(x') \overline{h(x' - z')}.$$

Since the function $y \mapsto h(y) \overline{h(y - z')}$ is Riemann integrable on H, we can apply the density formula Theorem 4.14 and obtain

$$\eta(z') = \lim_{n \to \infty} \eta_n(z') = \mathrm{dens}(\mathcal{L}) \cdot \int_H h(y) \overline{h(y - z')} \, \mathrm{d}\theta_H(y)$$
$$= \mathrm{dens}(\mathcal{L}) \cdot (h * \widetilde{h})(z').$$

Since $\omega_{h*\widetilde{h}}$ is uniformly discrete, this implies that γ_n converges vaguely to γ, and the claim follows. $\qquad \square$

5.2. **Pure point diffraction in regular model sets.** The following theorem is our main result. The implication "(i) $\Rightarrow$ (iii)" is the well-known diffraction formula as in [15, 33, 4].

Theorem 5.2 (Pure point diffraction of weighted model sets)**.** *Let $(G, H, \mathcal{L})$ be a cut-and-project scheme with σ-compact G and denote by $(\widehat{G}, \widehat{H}, \mathcal{L}_0)$ its dual. Then the following are equivalent.*

(i) *The lattice Dirac comb $\delta_{\mathcal{L}} \in \mathcal{M}^\infty(G \times H)$ is transformable and satisfies the PSF*

$$\widehat{\delta_{\mathcal{L}}} = \mathrm{dens}(\mathcal{L}) \cdot \delta_{\mathcal{L}_0}.$$

(ii) *The lattice Dirac comb $\delta_{\mathcal{L}} \in \mathcal{M}^\infty(G \times H)$ has autocorrelation $\gamma \in \mathcal{M}^\infty(G \times H)$ and diffraction $\widehat{\gamma} \in \mathcal{M}^\infty(\widehat{G} \times \widehat{H})$ given by*

$$\gamma = \mathrm{dens}(\mathcal{L}) \cdot \delta_{\mathcal{L}}, \qquad \widehat{\gamma} = \mathrm{dens}(\mathcal{L})^2 \cdot \delta_{\mathcal{L}_0}.$$

(iii) *For every Riemann integrable function $h : H \to \mathbb{C}$, the weighted model set $\omega_h \in \mathcal{M}^\infty(G)$ is uniformly translation bounded, with autocorrelation $\gamma \in \mathcal{M}^\infty(G)$ and diffraction $\widehat{\gamma} \in \mathcal{M}^\infty(\widehat{G})$ given by*

$$\gamma = \mathrm{dens}(\mathcal{L}) \cdot \omega_{h*\widetilde{h}}, \qquad \widehat{\gamma} = \mathrm{dens}(\mathcal{L})^2 \cdot \omega_{|\widecheck{h}|^2}.$$

In particular, ω_h has pure point diffraction for every Riemann integrable function $h : H \to \mathbb{C}$.

Remark 5.3. The above theorem applies to regular model sets, as for any relatively compact measurable $W \subset H$ such that $\theta_H(\partial W) = 0$, its characteristic function $h = 1_W : H \to \mathbb{R}$ is Riemann integrable.

Proof of Theorem 5.2. "(i) $\Rightarrow$ (ii)" rests on an explicit computation of γ that can be inferred from Proposition 5.1. The reverse implication "(ii) $\Rightarrow$ (i)" is trivial. "(i) $\Rightarrow$ (iii)" Uniform translation boundedness of ω_h is Lemma 4.8. The explicit form of the autocorrelation γ is Proposition 5.1, which relies on Theorem 4.12 or Theorem 4.9 (i) $\Rightarrow$ (ii). The statement about $\widehat{\gamma}$ now follows from Theorem 4.9 (i) $\Rightarrow$ (iii). The implication "(iii) $\Rightarrow$ (i)" is Theorem 4.9 (iii) $\Rightarrow$ (i) applied to the autocorrelation measure. $\qquad \square$

Remark 5.4 (Modified Wiener diagram). For any weighted model set ω_h with weight function $h \in PK(H)$ the modified Wiener diagram

$$
\begin{array}{ccc}
\omega_h & \xrightarrow{\;\;\circledast\;\;} & \mathrm{dens}(\mathcal{L}) \cdot \omega_{h*\widetilde{h}} \\[2pt]
{\scriptstyle\mathcal{F}}\big\downarrow & & \big\downarrow{\scriptstyle\mathcal{F}} \\[2pt]
\mathrm{dens}(\mathcal{L}) \cdot \omega_{\widecheck{h}} & \xrightarrow{\;\;|\cdot|^2\;\;} & \mathrm{dens}(\mathcal{L})^2 \cdot \omega_{|\widecheck{h}|^2}
\end{array}
$$

commutes, as $\omega_{\widecheck{h}}$ is a measure in that case by Theorem 4.9. This includes lattice Dirac combs, as one may choose H trivial in that case. The diagram may no longer commute for a general Riemann integrable weight function h, as $\omega_{\widecheck{h}}$ might not be a measure in that case, and as ω_h might not be a transformable measure. However the upper right path is still well defined in that case, such that the diffraction of ω_h is a pure point measure and may be computed by "squaring the Fourier-Bohr coefficients".

5.3. **Pure point diffraction in weak model sets.** By definition, the window $W \subset H$ of a weak model set is relatively compact and measurable. Hence ω_h where $h = 1_W$ is a weighted model set in that case by Lemma 4.8. But ω_h may not be pure point diffractive. On the other hand $h * \widetilde{h} \in PK(G)$ by Lemma 3.7, which means that the measure $\omega_{h*\widetilde{h}}$ is transformable by Theorem 5.2. Thus the question arises which weighted model sets ω_h have an autocorrelation given by $\mathrm{dens}(\mathcal{L}) \cdot \omega_{h*\widetilde{h}}$. As argued by Moody [25], this property is typical when one considers the ensemble of weak model sets with all shifts of a given window together with the uniform measure on this ensemble [25, Theorem 1]. For compact windows, it is related to maximal density of the weak model set [16, Prop. 3.4]. The following result extends [25, Cor. 1].

Theorem 5.5. [3] *Let $(G, H, \mathcal{L})$ be a cut-and-project scheme with σ-compact G and let ω_h be the Dirac comb of a weak model set, i.e., $h = 1_W$ for some relatively compact measurable $W \subset H$. Assume that there exists a van Hove sequence $(A_n)_{n\in\mathbb{N}}$ in G such that ω_h has maximal density with respect to $(A_n)_n$, i.e.,*

$$
\lim_{n\to\infty} \frac{1}{\theta_G(A_n)} \omega_h(A_n) = \mathrm{dens}(\mathcal{L}) \cdot \theta_H(\overline{W}).
$$

Then, with respect to the given van Hove sequence $(A_n)_n$, the weak model set ω_h has autocorrelation γ and diffraction $\widehat{\gamma}$ given by

$$
\gamma = \mathrm{dens}(\mathcal{L}) \cdot \omega_{g*\widetilde{g}}, \qquad \widehat{\gamma} = \mathrm{dens}(\mathcal{L})^2 \cdot \omega_{|\widecheck{g}|^2},
$$

where $g = 1_{\overline{W}}$. In particular, ω_h has pure point diffraction. $\qquad\square$

Remark 5.6. The above result reduces to the diffraction formula for regular model sets, since any regular model set has maximal density [16, Prop. 3.4]. For a model set with window satisfying $\theta_H(\partial W) > 0$, its diffraction spectrum may contain a non-trivial continuous component. In that case lack of maximal density may be interpreted as introducing some randomness into the system. Note however that the maximal density condition is not necessary for pure point diffraction. For example one may take a window with empty interior and consider a shift of the window which has empty intersection with the projected lattice. The existence of such a shift is seen by a Baire argument, compare e.g. [5] or [16, Prop. 2.12]. This will result in an empty weak model set, which is pure point diffractive.

5.4. **Bragg peaks in Meyer sets.** Next, let $\Lambda \subset G$ be a Meyer set [35, Def. 7.2], i.e., Λ and $\Lambda - \Lambda - \Lambda$ are both uniformly discrete and relatively dense. Since any autocorrelation γ of Λ is positive definite, it is weakly almost periodic [27, Sec. 11] and admits an Eberlein decomposition [17, Eqn. (8.28)]. Let γ_S denote the strongly almost periodic part of γ. Then $(\widehat{\gamma})_{pp} = \widehat{\gamma_S}$, see [27, Sec. 10]. Since Λ is a Meyer set, there exists a cut-and-project scheme $(G, H, \mathcal{L})$ and a positive and positive definite $h \in C_c(H)$ such that $\gamma_S = \omega_h$, see [35, Prop. 12.1]. Since h is positive and positive definite, $\widehat{h}$ is a finite measure and thus $\widehat{h} \in L^1(\widehat{H})$. Hence $h \in PK(H)$, and thus Theorem 4.12 yields an alternative proof of the following result.

Theorem 5.7. [35, Thm. 12.2] *Let $\Lambda \subset G$ be a Meyer set with autocorrelation γ, with σ-compact G. Then there exists a cut-and-project scheme $(G, H, \mathcal{L})$ such that*

$$\gamma_S = \omega_h, \qquad (\widehat{\gamma})_{pp} = \omega_{\breve{h}}$$

for some $h \in PK(H)$. □

Remark 5.8. Hence the formula for the pure point part of the diffraction of an arbitrary Meyer set Λ is a consequence of the PSF for some cut-and-project scheme in which Λ is a subset of a model set. We note that the above arguments can also be applied to the pure point part of the diffraction of an arbitrary weighted Dirac comb with Meyer set support, which reproves [35, Prop. 12.1] using the PSF.

5.5. **Double transformability for measures with Meyer set support.** Finally, let $\Lambda \subset G$ be a Meyer set and let μ be a measure supported inside Λ. Note that μ does not need to be pure point diffractive. We prove that if μ is transformable, then it is automatically twice transformable. This extends Theorem 4.11.

Theorem 5.9. *Let G be a σ-compact LCA group, let $\Lambda \subset G$ be a Meyer set and let $\mu \in \mathcal{M}^\infty(G)$ be supported inside Λ. If μ is transformable, then $\widehat{\mu}$ is also transformable, and we have $\widehat{\widehat{\mu}} = \mu^\dagger$.*

Proof. We check the integrability condition in Theorem 3.10. Since Λ is a Meyer set, there exists a cut-and-project scheme $(G, H, \mathcal{L})$ and a window W such that $\Lambda \subset \curlywedge(W)$ by [35, Thm. 1.8]. Also, as μ is translation bounded, there exists some finite positive constant c such that $|\mu(\{x\})| \leq c$ for all $x \in \Lambda$. Next, we pick some $h \in K_2(H)$ such that $h \geq c \cdot 1_W$. Then $|\mu| \leq c \cdot \omega_h$. Now, by Theorem 4.11, the measure ω_h is twice transformable. Therefore, for all $g \in K_2(\widehat{G})$ we have $\breve{g} \in L^1(\omega_{h^\dagger})$. Hence, as $|\mu^\dagger| \leq c \cdot \omega_{h^\dagger}$ we get $\breve{g} \in L^1(\mu^\dagger)$. □

Remark 5.10. Our validation of the integrability condition in Theorem 3.10 relies on the lattice PSF: we embed the Meyer set into a regular model set coming from a cut-and-project scheme $(G, H, \mathcal{L})$, and then the integrability condition follows from the PSF applied to the dual lattice $\mathcal{L}_0$.

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