

Diffraction of fully Euclidean model sets

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Chapter 1

Introduction

Aperiodic order is the mathematical study of non-periodically ordered structures. It is a combination of several, seemingly disparate, areas of mathematics; primarily consisting of algebra, analysis, geometry, and number theory. This field was born out of the 1980's discovery of physical quasicrystals by Daniel Schectman [31], for which he was later awarded the 2011 Nobel Prize in Chemistry. The most fundamental model of aperiodic structures with high coherence are *model sets* [23], which are a natural object arising from so-called *cut-and-project schemes* (CPS).

We are interested in a special subclass of model sets known as *fully Euclidean* model sets. A fully Euclidean model set $\Lambda \subseteq \mathbb{R}^d$ is obtained by starting with a lattice \mathcal{L} in some higher dimensional space \mathbb{R}^{d+m} , which sits at an irrational angle with respect to \mathbb{R}^d , cutting a sufficiently nice strip within a bounded distance of \mathbb{R}^d , and projecting the lattice points inside this strip onto \mathbb{R}^d ; see Definition 3.1.1 below for a formal definition. As these model sets form the basis of our project, a brief review of their history is warranted.

Model sets were initially introduced by Meyer [24] and independently rediscovered by de Bruijn [6] when studying the Penrose tilings, by Kramer [13], Kramer–Neri [14], by Kalugin, Kitaev and Levitov [12], and by Duneau–Katz [8]. Their use in aperiodic order was popularised by both Moody [23, 24] and Lagarias [15]. For a general review on the subject we refer the reader to [3, 23, 24].

Studies regarding the behaviour of model sets were initially restricted to the fully Euclidean case; the setting where everything lives in some real space. Today the theory has advanced to the more abstract case of locally compact Abelian groups, see [2, 5, 26, 27, 35, 36] for some examples. It is for simplicity that we restrict ourselves to the fully Euclidean case.

The diffraction formula for fully Euclidean model sets was first proven for some particular cases by Hof [9, 10] and later proven in full generality by

Schlotman [30]. Alternative proofs via almost periodicity were also provided by [4, 22, 32] and more recently in [17, 18]. Moreover, a proof via the Poisson summation formula (PSF) was given in [15], generalising the earlier results in this direction [9, 10, 19, 20].

The goal of this project is to provide an elementary proof, using only tempered distributions and the PSF for lattices in Euclidean space, that fully Euclidean regular model sets produce a pure-point diffraction measure. Our approach is based off of the work of [26]. This result is well known in greater generality and more elegant proofs exist, see [4, 9, 17, 26].

The project is structured as follows. We first provide a simple overview of basic properties of functions and distributions, define pure point tempered measures, and prove the classic PSF for lattices (Theorem 2.3.10). In Chapter 3 we introduce cut-and-project schemes and extend the PSF for both fully Euclidean CPS and $PK(\mathbb{R}^d)$, the class of compactly supported continuous functions with a positive Fourier transform (Theorem 3.3.2). We also prove the density formula for regular model sets (Theorem 3.4.7) and use it to show the existence of the autocorrelation measure for fully Euclidean model sets and derive its formula (Theorem 3.5.4). Combining the results of this chapter, we prove that the diffraction measure of a regular model set exists and is a positive pure point tempered measure and we derive the formula for the intensity of each Bragg peak (Theorem 3.6.4). We conclude by providing in Chapter 4 a simple worked example of the diffraction measure for the well-known silver mean substitution.

Chapter 2

Functions and Distributions

2.1 Functions

In this chapter we review basic definitions and properties of functions on \mathbb{R}^d . We will denote the standard Euclidean vector norm by $\|\cdot\|$. For a bounded function $f : \mathbb{R}^d \rightarrow \mathbb{C}$ we denote by $\|\cdot\|_\infty$ the sup-norm. We say a function f has compact support in \mathbb{R}^d if there exists some $R > 0$ such that $f(x) = 0$ whenever $\|x\| \geq R$. Let $C_u(\mathbb{R}^d)$, $C_c(\mathbb{R}^d)$, C^∞ , and $C_c^\infty(\mathbb{R}^d)$ respectively denote the space of uniformly continuous and bounded functions, continuous functions with compact support, infinitely differentiable functions, and those functions which are compactly supported and infinitely differentiable.

As is standard, we define $L^1(\mathbb{R}^d)$ to be the set of complex valued Lebesgue integrable functions, that is $|f(x)|$ is integrable and

$$\int_{\mathbb{R}^d} |f(x)| dx < \infty.$$

We also take the norm on $L^1(\mathbb{R}^d)$ to be

$$\|f\|_1 = \int_{\mathbb{R}^d} |f(x)| dx.$$

In this project, we will primarily be interested in those functions contained in $L^1(\mathbb{R}^d) \cap C_u(\mathbb{R}^d)$. As usual, for $f \in L^1(\mathbb{R}^d)$, we define its *Fourier transform* by

$$\hat{f}(y) := \int_{\mathbb{R}^d} e^{-2\pi i x \cdot y} f(x) dx$$

and its *inverse Fourier transform* by

$$\check{f}(y) := \int_{\mathbb{R}^d} e^{2\pi i x \cdot y} f(x) dx.$$

For a function $f : \mathbb{R}^d \rightarrow \mathbb{C}$ we define $\tilde{f} : \mathbb{R}^d \rightarrow \mathbb{C}$ by $\tilde{f}(x) := \overline{f(-x)}$. Throughout we will also use the following notations.

$$T_t f(x) = f(x-t) \quad f_\alpha(x) = f(\alpha x) \quad \|f\|_2 = \left(\int_{\mathbb{R}^d} |f(x)|^2 dx \right)^{\frac{1}{2}}$$

The convolution of two functions $f * g$ is defined as

$$(f * g)(x) = \int_{\mathbb{R}^d} f(x-t)g(t)dt$$

if the integral makes sense for all x . Note that the convolution exists whenever $f \in L^1(\mathbb{R}^d)$ and $g \in C_u(\mathbb{R}^d)$ or $f \in C_u(\mathbb{R}^d)$ and $g \in L^1(\mathbb{R}^d)$. In particular, it exists whenever one function is in $C_c(\mathbb{R}^d)$ and the other in $C_u(\mathbb{R}^d)$.

Next, for $f : \mathbb{R}^d \rightarrow \mathbb{C}$ and $g : \mathbb{R}^m \rightarrow \mathbb{C}$ we define the tensor product $f \otimes g : \mathbb{R}^{d+m} \rightarrow \mathbb{C}$ as

$$(f \otimes g)(x, y) = f(x)g(y).$$

We now provide an example of class of functions which will be used repeatedly.

Example 2.1.1. [7, Example 1.4] There exists some non-trivial $f \in C_c^\infty(\mathbb{R}^d)$ such that $f(x) \geq 0$ and $\text{supp}(f) \subseteq B_1(0)$.

Proof. Define $f : \mathbb{R}^d \rightarrow \mathbb{C}$ and $g : \mathbb{R} \rightarrow \mathbb{C}$ by

$$f(x) := \begin{cases} e^{\frac{-1}{1-\|x\|^2}} & 1 > \|x\| \\ 0 & 1 \leq \|x\| \end{cases}$$

and

$$g(x) := \begin{cases} e^{\frac{-1}{x}} & x > 0 \\ 0 & x \leq 0. \end{cases}$$

Then $g \in C^\infty(\mathbb{R})$ and $f(x) = g(1-\|x\|^2) = g(1-x_1^2 - \dots - x_d^2)$ is the composition of g with a polynomial, thus $f \in C_c^\infty(\mathbb{R}^d)$. \square

This example motivates us to introduce the following definition.

Definition 2.1.2. A function $f_n \in C_c^\infty(\mathbb{R}^d)$ is called an *approximate identity* if it satisfies the following.

- (a) $\text{supp}(f_n) \subset B_{\frac{1}{n}}(0)$.
- (b) $f_n(x) \geq 0$ for all n, x .
- (c) $\int_{\mathbb{R}^d} f_n(t)dt = 1$ for all n .

Note that if f is the function from Example 2.1.1, taking $C_n := \int_{\mathbb{R}^d} f(nx)dx$ gives

$$f_n(x) := \frac{1}{C_n} f(nx)$$

is an approximate identity.

Lemma 2.1.3. *For $f \in C_u(\mathbb{R}^d)$ and f_n an approximate identity, we have*

$$\lim_n \|f * f_n - f\|_\infty = 0.$$

Proof. Let $\epsilon > 0$. By uniform continuity there exists N such that, whenever $x - y \in B_{\frac{1}{N}}(0)$, we have $|f(x) - f(y)| < \epsilon$. It follows, that for all $n \geq N$ and all $x \in \mathbb{R}^d$ we have,

$$\begin{aligned} |f * f_n(x) - f(x)| &= \left| \int_{\mathbb{R}^d} f(x-t)f_n(t)dt - f(x) \right| \\ &= \left| \int_{\mathbb{R}^d} f(x-t)f_n(t) - f_n(t)f(x)dt \right| \\ &\leq \int_{\mathbb{R}^d} |f(x-t) - f(x)|f_n(t)dt \\ &= \int_{B_{\frac{1}{N}}(0)} |f(x-t) - f(x)|f_n(t)dt < \epsilon. \end{aligned}$$

Taking the supremum over all $x \in \mathbb{R}^d$ we get, for all $n \geq N$

$$\|f * f_n - f\|_\infty \leq \epsilon,$$

which proves the claim. □

2.2 Distributions

In this section we briefly review the notions of distributions, tempered distributions, and their associated Fourier transforms. For a general review of these concepts, we refer the reader to [7]. Note that the author in [7] uses a different convention for the Fourier transform, however the theory is unchanged up to a constant multiple.

Definition 2.2.1. A *distribution* on \mathbb{R}^d is a complex-valued linear functional μ on $C_c^\infty(\mathbb{R}^d)$, such that for every $[-A, A]^d \in \mathbb{R}^d$, there exists constants C and k such that

$$|\mu(\phi)| \leq C \sum_{|\alpha| \leq k} \|D^\alpha \phi\|_\infty,$$

for all $\phi \in C_c^\infty(\mathbb{R}^d)$ with support in $[-A, A]^d$. If the same smallest k can be used for all $[-A, A]^d$, we say μ has order k . In the case of a distribution of order 0, we refer to it as a *measure*.

We will denote the set of distributions on \mathbb{R}^d by $\mathcal{D}(\mathbb{R}^d)$. Next we recall the space of smooth functions with rapidly decaying derivatives.

Definition 2.2.2. The Schwartz class of functions on \mathbb{R}^d , denoted $\mathcal{S}(\mathbb{R}^d)$, is the set of infinitely differentiable functions that are rapidly decreasing. That is, for all k, α ,

$$\sup_{x \in \mathbb{R}^d} (1 + |x|^2)^k |D^\alpha \phi(x)| < \infty.$$

Moreover, we say $f_n \rightarrow 0 \in \mathcal{S}(\mathbb{R}^d)$ if, for all k and α

$$\sup_{x \in \mathbb{R}^d} (1 + |x|^2)^k |D^\alpha f_n(x)| \rightarrow 0.$$

Note that $C_c^\infty(\mathbb{R}^d) \subset \mathcal{S}(\mathbb{R}^d)$. Moreover, if $f \in \mathcal{S}(\mathbb{R}^d)$ and $g \in \mathcal{S}(\mathbb{R}^m)$ then $f \otimes g \in \mathcal{S}(\mathbb{R}^{d+m})$. We also have the following properties for Schwartz functions, whose proofs are standard and are thus omitted.

Proposition 2.2.3. For $f, g \in \mathcal{S}(\mathbb{R}^d)$ we have the following.

(a)

$$\widehat{x^\alpha f} = \left(\frac{i}{2\pi}\right)^\alpha D^\alpha \widehat{f}.$$

(b)

$$\widehat{(D^\alpha f)}(y) = (2\pi i y)^\alpha \widehat{f}(y).$$

(c)

$$\widehat{T_t f}(y) = e^{-2\pi i t \cdot y} \widehat{f}(y).$$

(d)

$$\widehat{e^{2\pi i x \cdot t} f}(y) = T_t \widehat{f}(y) = \widehat{f}(t - y).$$

(e) If $a \neq 0$ then

$$\widehat{f_a}(y) = \frac{1}{|a|^d} \widehat{f}\left(\frac{y}{a}\right).$$

(f)

$$\widehat{f}(y) = \overline{\widehat{f}(-y)}.$$

(g)

$$\int_{\mathbb{R}^d} f(y) \widehat{g}(y) dy = \int_{\mathbb{R}^d} \widehat{f}(y) g(y) dy.$$

(h)

$$\widehat{f * g} = \widehat{f} \widehat{g}.$$

(i)

$$\widehat{f} \in \mathcal{S}(\mathbb{R}^d).$$

$$(j) \quad \|\widehat{f}\|_\infty \leq \|f\|_1.$$

$$(k) \quad \widehat{f \otimes g} = \widehat{f} \otimes \widehat{g}.$$

□

Next we review Plancherel's theorem, a fundamental result which says that the Fourier transform is an isometry on $(\mathcal{S}(\mathbb{R}^d), \|\cdot\|_2)$.

Theorem 2.2.4 (Plancherel). *For $f, g \in \mathcal{S}(\mathbb{R}^d)$ we have*

$$\int_{\mathbb{R}^d} f(t)\overline{g(t)}dt = \int_{\mathbb{R}^d} \widehat{f}(t)\overline{\widehat{g}(t)}dt.$$

In particular,

$$\|f\|_2 = \|\widehat{f}\|_2.$$

Proof. Let $h := \check{g} = \overline{\widehat{g}}$. Then, by Proposition 2.2.3 we have

$$\int_{\mathbb{R}^d} f(t)\widehat{h}(t)dt = \int_{\mathbb{R}^d} \widehat{f}(t)h(t)dt.$$

Thus

$$\int_{\mathbb{R}^d} f(t)\overline{g(t)}dt = \int_{\mathbb{R}^d} \widehat{f}(t)\overline{\widehat{g}(t)}dt.$$

The final claim is achieved by setting $g(t) := f(t)$. □

We are now able to introduce a class of functions acting on $\mathcal{S}(\mathbb{R}^d)$.

Definition 2.2.5. A *tempered distribution* is a linear functional μ on $\mathcal{S}(\mathbb{R}^d)$ such that $\mu(f_n) \rightarrow 0$ whenever $f_n \rightarrow 0$. We denote the space of tempered distributions by $\mathcal{S}'(\mathbb{R}^d)$.

Next, we show that each function $h \in C_u(\mathbb{R}^d)$ defines a tempered distribution θ_h . Note that while it is common to also denote this tempered distribution by h , to avoid confusion we will use θ_h to denote the corresponding distribution.

Lemma 2.2.6. *Let h be continuous and bounded. For each $f \in \mathcal{S}(\mathbb{R}^d)$ define*

$$\theta_h(f) := \int_{\mathbb{R}^d} h(t)f(t)dt.$$

Then θ_h is a tempered distribution.

Proof. Clearly θ_h is linear and well defined, so we show continuity. As h is bounded we have $|h(x)| \leq C$ for some $C > 0$. Thus, whenever $f_n \rightarrow 0 \in \mathcal{S}(\mathbb{R}^d)$,

$$\begin{aligned} \left\| \int_{\mathbb{R}^d} h(x)f_n(x)dx \right\|_\infty &\leq C \left(\int_{\mathbb{R}^d} \frac{1}{x_1^2+1} \cdots \frac{1}{x_d^2+1} dx \right) \|(x_1^2+1) \cdots (x_d^2+1)f_n\|_\infty \\ &\leq CC_1 \|(x_1^2+1) \cdots (x_d^2+1)f_n\|_\infty \rightarrow 0. \end{aligned}$$

Where $C_1 := \int_{\mathbb{R}^d} \frac{1}{x_1^2+1} \cdots \frac{1}{x_d^2+1} dx < \infty$ is a constant independent of n . □

The tempered distribution θ_h defined above is known as the regular distribution associated to h . Note that, in measure theory, this is known as the absolutely continuous measure with density function h ; however this is beyond our interest for this project.

For approximate identities we have the following convergence.

Lemma 2.2.7. *Let $h : \mathbb{R}^d \rightarrow \mathbb{C}$ be continuous and bounded. Then, for f_n an approximate identity,*

$$\theta_h(f_n) \rightarrow h(0).$$

Proof. Let $\epsilon > 0$. By continuity of h , there exists N such that whenever $\|t\| \leq \frac{1}{N}$ we have $|h(t) - h(0)| < \epsilon$. It follows, for $n \geq N$

$$\begin{aligned} |\theta_h(f_n)(t) - h(0)| &= \left| \int_{\mathbb{R}^d} f_n(t)h(t)dt - \int_{\mathbb{R}^d} f_n(t)h(0)dt \right| \\ &\leq \int_{B_{\frac{1}{n}}(0)} f_n(t) |h(t) - h(0)| dt < \epsilon. \end{aligned}$$

□

We immediately get the following equivalence of tempered distributions.

Corollary 2.2.8. *For $g, h : \mathbb{R}^d \rightarrow \mathbb{C}$, both continuous and bounded, we have $\theta_g = \theta_h \iff g = h$.* □

2.3 Pure Point Tempered Measures

The goal of this section is to prove a few basic results on the behaviour of pure point tempered measures, such as the Poisson summation formula, which will be used later.

Definition 2.3.1. By a *pure point tempered measure* we understand a sum of the form

$$\mu = \sum_{x \in \Lambda} c(x)\delta_x$$

where $\Lambda \subseteq \mathbb{R}^d$ and $c : \Lambda \rightarrow \mathbb{C} \setminus \{0\}$ with the property that, for all $f \in \mathcal{S}(\mathbb{R}^d)$, the sum

$$\sum_{x \in \Lambda} |c(x)f(x)| < \infty$$

and $\mu(f) = \sum_{x \in \Lambda} c(x)f(x)$ is a tempered measure. If $c(x) \geq 0$ for all $x \in \Lambda$ then we say μ is *positive*.

The set Λ is often called the measurable support of μ . We start by proving the following results, which show that any pure point tempered measure is a so-called *Radon measure*. See [28] for definitions and properties.

Lemma 2.3.2. *If $\mu = \sum_{x \in \Lambda} c(x)\delta_x$ is a pure point tempered measure then, for all $n \in \mathbb{N}$,*

$$\sum_{x \in \Lambda \cap B_n(0)} |c(x)| < \infty.$$

Proof. Pick arbitrary non-zero $n \in \mathbb{N}$ and $f \in C_c^\infty(\mathbb{R}^d)$ such that $f \geq 1_{B_n(0)}$. It follows

$$\sum_{x \in \Lambda \cap B_n(0)} |c(x)| \leq \sum_{x \in \Lambda \cap B_n(0)} |c(x)f(x)| \leq \sum_{x \in \Lambda} |c(x)f(x)| < \infty.$$

□

An interesting consequence of this result is that the support of any pure point tempered measure is at most countable.

Lemma 2.3.3. *If $\mu = \sum_{x \in \Lambda} c(x)\delta_x$ is a pure point measure then Λ is at most countable.*

Proof. Define $\Lambda_{n,m} := \{x \in \Lambda \cap B_n(0) : |c(x)| > 1/m\}$, which is finite by Lemma 2.3.2. Then

$$\Lambda = \bigcup_{n \geq 1} \bigcup_{m \geq 1} \Lambda_{n,m}$$

is also countable. □

Next we provide sufficient conditions on the coefficients $c(x)$ for $\mu = \sum_{x \in \Lambda} c(x)\delta_x$ to be a pure point tempered measure.

Lemma 2.3.4. *If there exists some $k \geq 0$ such that*

$$\sum_{x \in \Lambda} \frac{|c(x)|}{1 + \|x\|^k} < \infty$$

then $\mu = \sum_{x \in \Lambda} c(x)\delta_x$ is a pure point tempered measure.

Proof. Let $C = \sum_{x \in \Lambda} \frac{|c(x)|}{1 + \|x\|^k}$. It follows

$$\sum_{x \in \Lambda} |c(x)f(x)| \leq \sum_{x \in \Lambda} \frac{|c(x)|}{1 + \|x\|^k} \|1 + \|x\|^k f\|_\infty = C \|1 + \|x\|^k f\|_\infty < \infty.$$

Moreover, when $f_n \rightarrow 0$, we have $|\mu(f_n)| \rightarrow 0$. □

Note that by [11], the above is actually both a necessary and sufficient condition. As the proof is technical and we do not use the full equivalence, we skip it.

Now, as we are working with pure point measures, there is a natural extension to considering the measure of a set. For a given bounded set B and pure point measure $\mu = \sum_{x \in \Lambda} c(x)\delta_x$, define

$$\mu(B) = \sum_{x \in B \cap \Lambda} c(x).$$

Picking $1_\Lambda \leq f \in C_c^\infty(\mathbb{R}^d)$, necessary as $1_\Lambda \notin C_c(\mathbb{R}^d)$, gives

$$|\mu(B)| \leq |\mu(f)| < \infty,$$

and is indeed well defined. Note that this implies for a singleton set $\{x\}$

$$\mu(\{x\}) = \begin{cases} c(x) & x \in \Lambda \\ 0 & x \notin \Lambda. \end{cases}$$

The above definition turns out to be not very useful for computations. We will use instead the following equivalent characterisation.

Lemma 2.3.5. *Let μ be a pure point tempered measure. Let $a \in \mathbb{R}^d$ be arbitrary, and take $f_n \in C_c(\mathbb{R}^d)$ such that $0 \leq f_n \leq 1$, with $\text{supp}(f_n) \subseteq B_{\frac{1}{n}}(0)$ and $f_n(a) = 1$. Then*

$$\lim_n \mu(f_n) = \mu(\{a\}).$$

Proof. Let $\epsilon > 0$. We first deal with the case of $a \in \Lambda$. Let $\mu = \sum_{x \in \Lambda} c(x) \delta_x$. By Lemma 2.3.3, we have that Λ is countable. Let $x_1 = a, x_2, x_3, \dots$ be an enumeration of $\Lambda \cap B_1(a)$. Note that $B_1(a) \subseteq B_n(0)$ for some n . By Lemma 2.3.2,

$$\sum_{x \in \Lambda \cap B_1(a)} |c(x)| < \infty$$

or equivalently $\sum_n |c(x_n)| < \infty$. Thus, there exists some N such that, for all $n > N$,

$$\sum_{n > N} |c(x_n)| < \epsilon.$$

Take $M > 0$ such that

$$\frac{1}{M} < \min\{d(x_i, a) : 2 \leq i \leq N\}.$$

It follows, for $n > M$, $f_n(x_2) = \dots = f_n(x_N) = 0$ and

$$\begin{aligned} |\mu(f_n) - c(a)| &= \left| \left(\sum_{x \in \Lambda} c(x) f_n(x) \right) - c(a) \right| = \left| \left(\sum_{x \in \Lambda \cap B_1(a)} c(x) f_n(x) \right) - c(a) \right| \\ &= \left| \left(\sum_m c(x_m) f_n(x_m) \right) - c(a) \right| \\ &\leq \left| \left(\sum_{m=1}^N c(x_m) f_n(x_m) \right) - c(a) \right| + \left| \left(\sum_{m > N} c(x_m) f_n(x_m) \right) \right| \\ &= |c(a) - c(a)| + \left| \sum_{m > N} c(x_m) f_n(x_m) \right| \leq \sum_{m > N} |c(x_m)| < \epsilon. \end{aligned}$$

Now if $\mu(\{a\}) = 0$, define $v := \mu + \delta_a$. Then $v(f_n) \rightarrow v(\{a\}) = 1$ by the above. It follows

$$\mu(f_n) = v(f_n) - \delta_a(f_n) \rightarrow 0 = \mu(\{a\})$$

which proves the claim. \square

Let us next recall a special class of point sets defining tempered distributions.

Definition 2.3.6. A point set $\mathcal{L} \subseteq \mathbb{R}^d$ is called a *lattice* in \mathbb{R}^d if there exists an \mathbb{R} -basis $\{v_1, \dots, v_d\}$ such that

$$\mathcal{L} = \mathbb{Z}v_1 \oplus \dots \oplus \mathbb{Z}v_d.$$

Given a lattice $\mathcal{L} \in \mathbb{R}^d$, we also define its *dual* \mathcal{L}° , given by

$$\mathcal{L}^\circ := \{y \in \mathbb{R}^d \mid x \cdot y \in \mathbb{Z} \text{ for all } x \in \mathcal{L}\},$$

where \cdot denotes the standard scalar product. However, we can give a simpler description of the dual lattice.

Lemma 2.3.7. *Let $\mathcal{L} \subset \mathbb{R}^d$ be a lattice with basis $\{v_1, \dots, v_d\}$ and let A be the matrix whose columns are precisely v_1, \dots, v_d . Denote the rows of A^{-1} by w_1, \dots, w_d . Then with \mathcal{L}° the dual lattice defined above,*

$$\mathcal{L}^\circ = \mathbb{Z}w_1 \oplus \dots \oplus \mathbb{Z}w_d.$$

Proof. Note that, as w_1, \dots, w_d are the rows of an invertible matrix, they are an \mathbb{R} -basis for \mathbb{R}^d . Now, for arbitrary $w \in \mathcal{L}^\circ$, as $w \cdot v_j \in \mathbb{Z}$, we have

$$w \cdot v_j = \sum_1^d c_i w_i \cdot v_j = c_j \in \mathbb{Z}$$

thus $w \in \mathbb{Z}w_1 \oplus \dots \oplus \mathbb{Z}w_d$. Conversely, for $w = \sum_1^d c_i w_i \in \mathbb{Z}w_1 \oplus \dots \oplus \mathbb{Z}w_d$ and arbitrary $v = \sum_1^d b_i v_i \in \mathcal{L}$ we have

$$w \cdot v = \sum_1^d c_i w_i \cdot \sum_1^d b_i v_i = \sum_i c_i b_i \in \mathbb{Z}$$

thus $w \in \mathcal{L}^\circ$, which proves the statement. \square

Proposition 2.3.8. *Let $\mathcal{L} \subset \mathbb{R}^d$ be a lattice. Then $\delta_{\mathcal{L}}(f) = \sum_{x \in \mathcal{L}} \delta_x(f)$ is a pure point tempered measure.*

Proof. We first prove the claim for $\mathcal{L} = \mathbb{Z}^d$, from which the general claim will follow. As $\delta_{\mathbb{Z}^d} = \sum_{x \in \mathbb{Z}^d} \delta_x$ we have

$$\sum_{x \in \mathbb{Z}^d} \frac{1}{1 + \|x\|^{2d}} < \infty,$$

thus $\delta_{\mathbb{Z}^d}$ is indeed a pure point tempered measure. Let $\mathcal{L} = \mathbb{Z}v_1 \oplus \cdots \oplus \mathbb{Z}v_d$ and let A be the matrix consisting of the lattice basis vectors. Now for all $f \in \mathcal{S}(\mathbb{R}^d)$ we have

$$\sum_{x \in \mathcal{L}} |f(x)| = \sum_{y \in \mathbb{Z}^d} |f(Ay)| < \infty$$

as $f \circ A \in \mathcal{S}(\mathbb{R}^d)$. Moreover, as $f \rightarrow f \circ A$ is continuous with respect to the topology of $\mathcal{S}(\mathbb{R}^d)$ we have,

$$\delta_{\mathcal{L}}(f) = \delta_{\mathbb{Z}^d}(f \circ A)$$

is a tempered distribution. \square

Now we briefly recall an important theorem whose proof is standard, we follow that of [2, Section 9.2.1].

Theorem 2.3.9 (Poisson Summation Formula). *For all $f \in \mathcal{S}(\mathbb{R}^d)$ we have,*

$$\sum_{m \in \mathbb{Z}^d} f(m) = \sum_{k \in \mathbb{Z}^d} \hat{f}(k).$$

Proof. Consider $F(x) = \sum_{n \in \mathbb{Z}^d} f(x+n)$. Then the sum is uniformly convergent by Proposition 2.3.8 and F is a \mathbb{Z}^d -periodic function, so we may write its Fourier coefficients

$$\begin{aligned} c_k &= \int_0^1 F(x) e^{-2\pi i k x} dx = \int_0^1 \sum_{n \in \mathbb{Z}^d} f(x+n) e^{-2\pi i k x} dx \\ &= \sum_{n \in \mathbb{Z}^d} \int_0^1 f(x+n) e^{-2\pi i k x} dx = \sum_{n \in \mathbb{Z}^d} \int_n^{n+1} f(x) e^{-2\pi i k x} dx \\ &= \int_{\mathbb{R}^d} f(x) e^{-2\pi i k x} dx = \hat{f}(k). \end{aligned}$$

By definition of Fourier series, $F(x) = \sum_{k \in \mathbb{Z}^d} c_k e^{-2\pi i k x}$, and picking $x = 0$ gives

$$\sum_{n \in \mathbb{Z}^d} f(n) = \sum_{k \in \mathbb{Z}^d} \hat{f}(k).$$

\square

We conclude the section by extending the PSF to arbitrary lattices in \mathbb{R}^d .

Theorem 2.3.10 (PSF for lattices). *Let $\mathcal{L} \subset \mathbb{R}^d$ be a lattice and $f \in \mathcal{S}(\mathbb{R}^d)$. Then, with $\det(\mathcal{L}) := \det(A)$ where A consists of the lattice basis vectors,*

$$\sum_{x \in \mathcal{L}} f(x) = \frac{1}{|\det(\mathcal{L})|} \sum_{y \in \mathcal{L}^\circ} \hat{f}(y).$$

Proof. By Theorem 2.3.9,

$$\begin{aligned}\sum_{x \in \mathcal{L}} f(x) &= \sum_{l \in \mathbb{Z}} (f \circ A)(l) = \sum_{l \in \mathbb{Z}} \widehat{(f \circ A)}(l) = |\det(\mathcal{L})|^{-1} \sum_{l \in \mathbb{Z}} \widehat{f}((A^{-1})^T)(l) \\ &= |\det(\mathcal{L})|^{-1} \sum_{y \in \mathcal{L}^\circ} \widehat{f}(y).\end{aligned}$$

□

Note that a more general result, for a closed topological subgroup of an arbitrary locally compact Abelian group, is well known; see [1, Prop 6.2]. Our result is simply a particular instance by taking the closed subgroup to be a lattice in \mathbb{R}^d .

Chapter 3

Model Sets

3.1 Cut-and-Project Schemes

First we review some basic definitions and preliminary lemmas, following the notations used in the monograph [2]. We also recommend [21, 23, 24] for further reading.

Definition 3.1.1. Let $\Lambda \subseteq \mathbb{R}^d$. We say Λ is

- *relatively dense* if there exists some $R > 0$ such that for all $x \in \mathbb{R}^d$, the intersection $\Lambda \cap B_R(x)$ is nonempty.
- *uniformly discrete* if there exists some $r > 0$ such that for all $x \in \mathbb{R}^d$, the intersection $\Lambda \cap B_r(x)$ contains at most a single point.
- *Delone* if it is both relatively dense and uniformly discrete.

Now we review the notion of cut-and-project schemes and model sets.

Definition 3.1.2. By a fully Euclidean *cut-and-project scheme* (CPS), we understand a triple $(\mathbb{R}^d, \mathbb{R}^m, \mathcal{L})$ with lattice $\mathcal{L} \subset \mathbb{R}^d \times \mathbb{R}^m$ with the following properties:

- The restriction $\pi_1|_{\mathcal{L}}$ of the first canonical projection π_1 onto \mathbb{R}^d is injective.
- The image of \mathcal{L} under the second canonical projection π_2 onto \mathbb{R}^m is dense.

Note that this definition can be generalised beyond Euclidean space to locally compact Abelian groups, see [2, 23] for a thorough treatment of the topic. For a given CPS, we define $L := \pi_1(\mathcal{L})$. As the canonical projection π_1 is a bijection between L and \mathcal{L} , we can define the \star -mapping as $\star : L \rightarrow \mathbb{R}^m$ by

$$\star = \pi_2 \circ (\pi_1|_{\mathcal{L}})^{-1}.$$

Note that for any $x \in \mathcal{L}$, x^\star is the unique $y \in \mathbb{R}^m$ such that $(x, y) \in \mathcal{L}$. We summarize a CPS in the following diagram.

$$\begin{array}{ccccc}
\mathbb{R}^d & \xleftarrow{\pi_1} & \mathbb{R}^d \times \mathbb{R}^m & \xrightarrow{\pi_2} & \mathbb{R}^m \\
\cup & & \cup & & \parallel \\
\pi_1(\mathcal{L}) & \xleftarrow[1-1]{} & \mathcal{L} & \xrightarrow{\text{dense}} & \mathbb{R}^m \\
\parallel & & & & \cup \\
L & \xrightarrow{\quad \star \quad} & & & L^\star
\end{array}$$

Equipped with the dual lattice \mathcal{L}° we have that $(\mathbb{R}^d, \mathbb{R}^m, \mathcal{L}^\circ)$ is also a CPS, referred to as the *dual cut-and-project scheme* [29, 34]. With the \star -mapping we can now construct the following set.

Definition 3.1.3. Given a CPS $(\mathbb{R}^d, \mathbb{R}^m, \mathcal{L})$ and some bounded set $W \subset \mathbb{R}^m$ with non-empty interior, denote by $\wedge(W)$ its pre-image under the \star -mapping

$$\wedge(W) := \{x \in L : x^\star \in W\}.$$

Then $\wedge(W)$ is referred to as a model set with window of W . Moreover, W is called a *regular window* if, for all $\epsilon > 0$, there exists non-negative $f, g \in C_c^\infty(\mathbb{R}^d)$ such that

$$f \leq 1_W \leq g \quad \text{and} \quad \int_{\mathbb{R}^d} g(x) - f(x) dx < \epsilon.$$

In this case, $\wedge(W)$ is then called a regular model set.

Note that by regularity of Lebesgue measure and Urysohn's lemma, this is equivalent to the boundary of W having Haar measure zero, i.e $\lambda(\partial(W)) = 0$.

Next we show that the translate of a regular window and the intersection of two regular windows is regular.

Lemma 3.1.4. *If W, W' are regular then, for all $t \in \mathbb{R}^d$,*

- (a) $t + W$ is regular.
- (b) $W \cap W'$ is regular.

Proof. The first statement is trivial as the integral is invariant under translation.

Let $\epsilon > 0$ be given. As W, W' are regular, there exists $f, g, f_1, g_1 \in C_c^\infty(\mathbb{R}^d)$ such that $f \leq 1_W \leq g$ and $f_1 \leq 1_{W'} \leq g_1$. In particular, we may take

$$\int_{\mathbb{R}^d} g(x) - f(x) dx < \frac{\epsilon}{2(\|f_1\|_\infty + 1)}$$

and

$$\int_{\mathbb{R}^d} g_1(x) - f_1(x) dx < \frac{\epsilon}{2(\|g\|_\infty + 1)}.$$

Then clearly $f f_1 \leq 1_{W \cap W'} \leq g g_1$ and

$$\begin{aligned}
& \int_{\mathbb{R}^d} g(x)g_1(x) - f(x)f_1(x)dx \\
&= \int_{\mathbb{R}^d} g(x)g_1(x) - g(x)f_1(x) + g(x)f_1(x) - f(x)f_1(x)dx \\
&\leq \|g\|_\infty \int_{\mathbb{R}^d} g_1(x) - f_1(x)dx + \|f_1\|_\infty \int_{\mathbb{R}^d} g(x) - f(x)dx \\
&< \|g\|_\infty \frac{\epsilon}{2(\|g\|_\infty + 1)} + \|f_1\|_\infty \frac{\epsilon}{2(\|f_1\|_\infty + 1)} < \epsilon.
\end{aligned}$$

Which proves the statement. \square

The following result, which is needed to prove the regularity of a bounded interval, is standard; we omit the proof.

Lemma 3.1.5. [7] *If $c < a < b < d \in \mathbb{R}$, there exists $f \in C_c^\infty(\mathbb{R})$ such that*

$$1_{[a,b]} \leq f \leq 1_{[c,d]}.$$

\square

Note that in Euclidean space, any bounded interval is indeed regular.

Lemma 3.1.6. *If $I \subset \mathbb{R}$ is a bounded interval, then I is regular.*

Proof. As I is bounded, there exists $a < b$ such that

$$(a, b) \leq I \leq [a, b].$$

Thus for arbitrarily fixed n , there exists $f, g \in C_c^\infty(\mathbb{R})$ such that

$$1_{(a+\frac{1}{n}, b-\frac{1}{n})} \leq f \leq 1_{(a,b)} \leq 1_I \leq 1_{[a,b]} \leq g \leq 1_{[a-\frac{1}{n}, b+\frac{1}{n}]}$$

It follows, for sufficiently large n ,

$$\int_{\mathbb{R}^d} g(x) - f(x)dx \leq \int_{\mathbb{R}^d} 1_{[a-\frac{1}{n}, b+\frac{1}{n}]}(x) - 1_{(a+\frac{1}{n}, b-\frac{1}{n})}(x)dx \leq \frac{4}{n} < \epsilon.$$

\square

We will now outline the silver mean model set as a motivating example; it will be revisited in Chapter 4.

Example 3.1.7 (Silver mean model set). Consider the following CPS:

$$\begin{array}{ccccc}
\mathbb{R} & \xleftarrow{\pi_1} & \mathbb{R} \times \mathbb{R} & \xrightarrow{\pi_2} & \mathbb{R} \\
\uparrow & & \uparrow & & \uparrow \text{dense} \\
L & \xleftarrow{1-1} & \mathcal{L} := \mathbb{Z}(1, 1) \oplus \mathbb{Z}(\sqrt{2}, -\sqrt{2}) & \xrightarrow{\pi_2} & L^\star \\
\parallel & & & & \parallel \\
\mathbb{Z}[\sqrt{2}] & \xrightarrow{\quad \star \quad} & & & \mathbb{Z}[\sqrt{2}]
\end{array}$$

With the \star -mapping given by the Galois conjugation

$$(m + n\sqrt{2})^\star = m - n\sqrt{2}, \quad \forall m, n \in \mathbb{Z}.$$

Then, with window $W := [-\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}]$, we obtain the silver mean model set,

$$\wedge(W) := \{x \in L : x^\star \in W\}$$

Essentially, after picking a lattice and cutting the strip corresponding to the sought for window, the model set then consists of the projections of lattice points laying in the strip. This is illustrated later in Figure 4.1.

3.2 PSF for CPS

Throughout this section we will fix a CPS $(\mathbb{R}^d, \mathbb{R}^m, \mathcal{L})$ with dual $(\mathbb{R}^d, \mathbb{R}^m, \mathcal{L}^\circ)$. Recall that for two functions $f \in \mathcal{S}(\mathbb{R}^d)$ and $g \in \mathcal{S}(\mathbb{R}^m)$ we define the tensor $(f \otimes g)(x, y) \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^m)$ as

$$(f \otimes g)(x, y) := f(x)g(y).$$

Definition 3.2.1. For some $g : \mathbb{R}^m \rightarrow \mathbb{C}$ define the weighted comb of \mathcal{L} as

$$\omega_g := \sum_{(x, x^\star) \in \mathcal{L}} g(x^\star) \delta_x$$

with the weighted comb of the dual lattice

$$\omega_g^\star := \sum_{(y, y^\star) \in \mathcal{L}^\circ} g(y^\star) \delta_y.$$

If $f : \mathbb{R}^d \rightarrow \mathbb{C}$ is such that $\sum_{(x, x^\star) \in \mathcal{L}} |g(x^\star)f(x)|$ is convergent, then we define

$$\omega_g(f) := \sum_{(x, x^\star) \in \mathcal{L}} g(x^\star)f(x)$$

with $w_g^\star(f)$ defined similarly.

Note that the above definition is regarded only as a formal sum. We are interested in cases where ω_g is a positive measure or tempered distribution, in which case it is referred to as a weighted Dirac comb.

Lemma 3.2.2. *If $g \in \mathcal{S}(\mathbb{R}^m)$, then ω_g is a tempered distribution and for all $f \in \mathcal{S}(\mathbb{R}^d)$,*

$$\omega_g(f) = \delta_{\mathcal{L}}(f \otimes g).$$

Proof. Follows immediately from Proposition 2.3.8, as $f \otimes g \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^m)$,

$$\delta_{\mathcal{L}}(f \otimes g) = \sum_{(x, x^\star) \in \mathcal{L}} f(x)g(x^\star) = \omega_g(f)$$

is indeed a tempered distribution. \square

The above lemma holds for any g that is bounded and with compact support, the proof being identical after picking $h \in \mathcal{S}(\mathbb{R}^m)$ such that $|g| \leq h$. Note that, if $g = 1_W$ with W a given window, then $\omega_g = \delta_{\wedge(W)}$ is the Dirac comb of the model set $\wedge(W)$.

We conclude this section by showing that the PSF also holds for a CPS, compare [26] for more details.

Theorem 3.2.3 (PSF for CPS). *For all $g \in \mathcal{S}(\mathbb{R}^m)$ we have*

$$\widehat{\omega}_g = \frac{1}{\det(\mathcal{L})} \omega_g^*.$$

Proof. Let $f \in \mathcal{S}(\mathbb{R}^d)$. Then by definition,

$$\widehat{\omega}_g(f) = \omega_g(\widehat{f}) = \delta_{\mathcal{L}}(\widehat{f} \otimes g).$$

Now Theorem 2.3.10 implies, for all $f \in \mathcal{S}(\mathbb{R}^d)$,

$$\begin{aligned} \delta_{\mathcal{L}}(\widehat{f} \otimes g) &= |\det(\mathcal{L})|^{-1} \delta_{\mathcal{L} \circ}(\widehat{f \otimes g}) = |\det(\mathcal{L})|^{-1} \delta_{\mathcal{L} \circ}(f \otimes \check{g}) \\ &= |\det(\mathcal{L})|^{-1} \omega_g^*(f). \end{aligned}$$

□

3.3 PSF for PK

Let us recall [27] the set of compactly supported continuous functions with positive Fourier transform, that is

$$PK(\mathbb{R}^d) = \{f \in C_c(\mathbb{R}^d) : \widehat{f} \geq 0\}.$$

Note that for any $f \in PK(\mathbb{R}^d)$, we have $\widehat{f} \in L^1(\mathbb{R}^d)$ [26, Lemma 3.6]. We first prove a proposition needed for the $PK(\mathbb{R}^d)$ version of the PSF.

Proposition 3.3.1. *If $\phi \in PK(\mathbb{R}^d)$, then*

$$\sum_{m \in \mathbb{Z}^d} \widehat{\phi}(m) < \infty.$$

Proof. Let $\phi \in PK(\mathbb{R}^d)$ be given. Then $F(x) := \delta_{\mathbb{Z}^d} * \phi$ is uniformly continuous and bounded so let μ be the regular distribution associated with it; that is

$$\mu(g) := \int_{\mathbb{R}^d} F(x)g(t)dt.$$

Then

$$\widehat{\mu} = \widehat{\delta_{\mathbb{Z}^d} * \phi} = \widehat{\phi} \widehat{\delta_{\mathbb{Z}^d}} = \widehat{\phi} \delta_{\mathbb{Z}^d}$$

is clearly a positive measure; we show that it is finite. Let f_n be an approximate identity, then by Lemma 2.2.7, $\widehat{\mu}(\check{f}_n)$ converges to $F(0)$.

Now for fixed $m \in \mathbb{N}$, pick n such that $\frac{1}{n} \leq \frac{1}{4\pi m}$. It follows, for $x \in B_m(0)$

$$\left| \int_{\mathbb{R}^d} e^{2\pi ixy} f_n(y) dy - 1 \right| \leq \int_{B_{\frac{1}{n}}} f_n(y) dy |e^{2\pi ixy} - 1| \leq 2\pi |xy| \leq 2\pi m \frac{1}{n} \leq \frac{1}{2}$$

as $|e^{2\pi ixy} - 1| = 2 |\sin(\pi xy)| \leq 2\pi |xy|$. This gives

$$\check{f}_n(x) = \int_{\mathbb{R}^d} e^{2\pi ixy} f_n(y) dy \geq \frac{1}{2}.$$

Now $\widehat{\mu}(\check{f}_n)$ is convergent, thus bounded by some C , which implies for fixed m

$$C \geq \widehat{\mu}(\check{f}_n) = \int_{\mathbb{R}^d} \delta_{\mathbb{Z}^d} \widehat{\phi}(t) \check{f}_n(t) dt = \sum_{j \in \mathbb{Z}^d} \widehat{\phi}(j) \check{f}_n(j) \geq \sum_{j \in \mathbb{Z}^d \cap B_m(0)} \widehat{\phi}(j) \frac{1}{2}.$$

As C does not depend on m , letting $m \rightarrow \infty$ gives

$$\sum_{j \in \mathbb{Z}^d} \widehat{\phi}(j) \leq 2C < \infty.$$

□

We can prove an extended version of PSF for the class of $PK(\mathbb{R}^d)$. Note that while the intersection of $PK(\mathbb{R}^d)$ and $\mathcal{S}(\mathbb{R}^d)$ is non-empty, neither set sits completely in the other.

Theorem 3.3.2 (Extended PSF). *Let $\mathcal{L} \subset \mathbb{R}^d$ be a lattice and $\phi \in PK(\mathbb{R}^d)$. Then*

$$\sum_{x \in \mathcal{L}} \phi(x) = \frac{1}{|\det(\mathcal{L})|} \sum_{y \in \mathcal{L}^\circ} \widehat{\phi}(y).$$

Proof. Let μ be the regular distribution associated with $\delta_{\mathbb{Z}^d} * \phi$ as in the above proposition and define $\eta := \delta_{\mathbb{Z}^d} \widehat{\phi}$, which is a finite measure by the above proposition. Define $g(y) := \sum_{x \in \mathbb{Z}^d} e^{2\pi ixy} \widehat{\phi}(x)$ as a function in $C_u(\mathbb{R}^d)$.

As $\eta = \sum_{x \in \mathbb{Z}^d} e^{2\pi ixy} \widehat{\phi}$ is simply the regular distribution associated to g , and

$$\widehat{\eta} = \eta = \widehat{\mu} \iff \check{\eta} = \mu$$

then Corollary 2.2.8 gives $g(x) = \delta_{\mathbb{Z}^d} * \phi(x)$ as functions. Finally we have

$$\sum_{x \in \mathbb{Z}^d} \widehat{\phi}(x) = g(0) = \delta_{\mathbb{Z}^d} * \phi(0) = \sum_{n \in \mathbb{Z}^d} \phi(n).$$

Then, exactly as in Theorem 2.3.10, we get

$$\sum_{x \in \mathcal{L}} \phi(x) = |\det(\mathcal{L})|^{-1} \sum_{y \in \mathcal{L}^\circ} \widehat{\phi}(y).$$

□

The next natural question is whether we can define weighted Dirac combs for functions in $PK(\mathbb{R}^d)$. To do so, we need to bound the Schwartz functions.

Proposition 3.3.3. *For all $g \in \mathcal{S}(\mathbb{R}^d)$, there exists $f \in PK(\mathbb{R}^d)$ such that*

$$|\check{g}| \leq \check{f}.$$

Proof. First we will construct our $f \in PK(\mathbb{R})$. Define

$$f(x) := \frac{e^{-|x|}}{8} \cdot 1_{[-1,1]} * \tilde{1}_{[-1,1]}(x).$$

Now fix $a > 0$ such that $|\text{sinc}(2\pi x) - 1| \leq \frac{1}{2}$ on $[-a, a]$. This gives, on this interval,

$$\text{sinc}^2(2\pi x) \geq \frac{1}{2}.$$

By [2, Example 8.3] it follows, for $y \geq a$,

$$\begin{aligned} \hat{f}(y) &= \frac{\widehat{e^{-|y|}}}{8} * \widehat{1_{[-1,1]} * \tilde{1}_{[-1,1]}}(y) \\ &= \frac{1}{4(4\pi^2 y^2 + 1)} * 4 \text{sinc}^2(2\pi y) = \frac{1}{4\pi^2 y^2 + 1} * \text{sinc}^2(2\pi y) \\ &= \int_{\mathbb{R}^d} \frac{1}{4\pi^2(y-t)^2 + 1} \text{sinc}^2(2\pi t) dt \geq \int_{-a}^a \frac{1}{4\pi^2(y-t)^2 + 1} \text{sinc}^2(2\pi t) dt \\ &\geq \frac{1}{4} \int_{-a}^a \frac{1}{4\pi^2(y-t)^2 + 1} dt \geq \frac{1}{4} \int_{-a}^a \frac{1}{4\pi^2 4y^2 + 1} dt = \frac{a}{2} \frac{1}{16\pi^2 y^2 + 1} > 0. \end{aligned}$$

As a can be made arbitrarily small, this shows $\hat{f}(y) > 0$ when $y > 0$, thus $f \in PK(\mathbb{R})$. In an identical calculation we get the same lower bound for $\check{f}(y)$; in particular, there exists some $C_1, r_1 > 0$ such that for all $y > r_1$,

$$\check{f}(y) \geq C_1 \frac{1}{16\pi^2 y^2 + 1}.$$

Now for $g \in \mathcal{S}(\mathbb{R}^d)$ we have, with $x := (x_1, \dots, x_d) \in \mathbb{R}^d$

$$\check{g}(x)(16\pi^2 x_1^2 + 1) \dots (16\pi^2 x_d^2 + 1) \rightarrow 0$$

which implies there exists $r_2 > 0$, such that for $\|x\| \geq r_2$

$$|\check{g}(x)| \leq \frac{1}{(16\pi^2 x_1^2 + 1) \dots (16\pi^2 x_d^2 + 1)}.$$

Thus, for $\|x\| \geq \max\{r_1, r_2\}$ this gives

$$C_1 |\check{g}(x)| \leq \check{f}(x_1) \otimes \dots \otimes \check{f}(x_d).$$

By continuity, \check{g} is bounded for all $\|x\| < \max\{r_1, r_2\}$, thus there exists some C_2 such that

$$|\check{g}| \leq C_2 \leq C_2 C_1 |\check{g}(x)| \leq \check{f}(x_1) \otimes \cdots \otimes \check{f}(x_d)$$

which gives, for all $x \in \mathbb{R}^d$

$$|\check{g}| \leq \max\{C_1, C_2\} (\check{f}(x_1) \otimes \cdots \otimes \check{f}(x_d)) \in PK(\mathbb{R}^d).$$

□

Combining these results gives us the following, which concludes the section.

Theorem 3.3.4. *For $g \in PK(\mathbb{R}^m)$ we have*

$$\hat{\omega}_g = \frac{1}{|\det(\mathcal{L})|} \omega_g^*.$$

Moreover, ω_g^* is a tempered distribution for all $g \in PK(\mathbb{R}^m)$.

Proof. The first claim is immediate. For $f \in PK(\mathbb{R}^d)$, as $f \otimes g \in PK(\mathbb{R}^{d+m})$ by Theorem 3.3.2 we have

$$\hat{\omega}_g(\check{f}) = \omega_g(f) = \delta_{\mathcal{L}}(f \otimes g) = \frac{1}{|\det(\mathcal{L})|} \delta_{\mathcal{L}^\circ}(\check{f} \otimes \check{g}) = \omega_g^*(\check{f}). \quad (3.1)$$

Note that Equation 3.1 holds for all f in the span of $PK(\mathbb{R}^d) \cap \mathcal{S}(\mathbb{R}^d)$, which is dense in $\mathcal{S}(\mathbb{R}^d)$. What remains is to show is that ω_g^* is indeed a tempered distribution.

Let $\phi \in \mathcal{S}(\mathbb{R}^d)$ be given and define $h := \hat{\phi}$. Then by Proposition 3.3.3, there exists $f \in PK(\mathbb{R}^d)$ such that

$$|\phi| = |\check{h}| \leq \check{f}.$$

It follows

$$\omega_g^*(\phi) = \sum_{(x,y) \in \mathcal{L}^\circ} \phi(x) \check{g}(y) \leq \sum_{(x,y) \in \mathcal{L}^\circ} |\phi(x)| \check{g}(y) \leq \sum_{(x,y) \in \mathcal{L}^\circ} \check{f}(x) \check{g}(y) = \delta_{\mathcal{L}^\circ}(\check{f} \otimes \check{g}) < \infty$$

which implies ω_g^* is a tempered distribution. □

3.4 Density Formula for Model Sets

In this section we derive the density formula for regular model sets. Throughout we fix a a model set $\wedge(W)$ in some Euclidean CPS $(\mathbb{R}^d, \mathbb{R}^m, \mathcal{L})$. First let us define our notion of density of a set and mean of a measure.

Definition 3.4.1. For a model set $\wedge(W)$, we define its *density* as

$$\text{dens}(\wedge(W)) = \lim_n \frac{\text{card}(\wedge(W) \cap [-n, n]^d)}{(2n)^d},$$

if such a limit exists.

Definition 3.4.2. For a pure point measure $\mu = \sum_{x \in \Lambda} c(x)\delta_x$, we define the *mean* of μ as

$$M(\mu) = \lim_n \frac{1}{(2n)^d} \sum_{x \in \Lambda \cap [-n, n]^d} c(x),$$

if the limit exists.

Note that the above limit will not always exist, as in the following example.

Example 3.4.3. Take the set

$$\Lambda := \{1, 4, 5, 6, 7, 16, 17, 18, \dots, 31, 64, 65, \dots\} = \bigcup_{n \in \mathbb{N}} \{2^{2n}, 2^{2n} + 1, \dots, 2^{2n+1} - 1\}.$$

Equivalently,

$$\Lambda = \{m \in \mathbb{N} : \exists n \text{ such that } 2^{2n} \leq m < 2^{2n+1}\}.$$

Intuitively, we list the first natural number, skip the next two, list the next four, skip the next eight, list the next 16, skip the next 32 and so on. Define

$$a_n := \frac{1}{2n} \text{card}(\Lambda \cap [-n, n])$$

and note that $\text{dens}(\Lambda) = \lim_n a_n$. We will show that this limit does not exist. Now consider

$$a_{2^{2n}} = \frac{1}{2 \cdot 2^{2n}} \text{card}(\Lambda \cap [-2^{2n}, 2^{2n}]) = \frac{1}{2^{2n+1}} \text{card}(\Lambda \cap [0, 2^{2n}])$$

and

$$a_{2^{2n+1}} = \frac{1}{2 \cdot 2^{2n+1}} \text{card}(\Lambda \cap [-2^{2n+1}, 2^{2n+1}]) = \frac{1}{2^{2n+2}} \text{card}(\Lambda \cap [0, 2^{2n+1}]).$$

Through a recursive argument, we get that

$$\text{card}(\Lambda \cap [0, 2^{2n}]) = 1 + \sum_{k=0}^n 2^{2k}$$

and

$$\text{card}(\Lambda \cap [0, 2^{2n+1}]) = \sum_{k=0}^n 2^{2k}.$$

Which implies

$$\begin{aligned} \lim_n a_{2^{2n}} &= \lim_n \frac{1}{2^{2n+1}} \text{card}(\Lambda \cap [0, 2^{2n}]) = \lim_n \frac{1}{2^{2n+1}} \left(1 + \sum_{k=0}^n 2^{2k} \right) \\ &= \lim_n \frac{1}{2^{2n+1}} \frac{4^{n+1} + 2}{3} = \frac{2}{3} \end{aligned}$$

and

$$\begin{aligned}\lim_n a_{2^{2n+1}} &= \lim_n \frac{1}{2^{2n+2}} \text{card}(\Lambda \cap [0, 2^{2n+1}]) = \lim_n \frac{1}{2^{2n+2}} \sum_{k=0}^n 2^{2k} \\ &= \lim_n \frac{1}{2^{2n+2}} \frac{4^{n+1} - 1}{3} = \frac{1}{3}.\end{aligned}$$

Thus $\lim_n a_{2^{2n+1}} \neq \lim_n a_{2^{2n}}$, and $\text{dens}(\Lambda) = \lim_n a_n$ does not exist. Now set $\mu := \sum_{x \in \Lambda} 1\delta_x$ a measure on \mathbb{R} . Then

$$M(\mu) = \lim_n \frac{1}{2n} \sum_{x \in \Lambda \cap [-n, n]} \delta_x = \lim_n a_n$$

does not exist by the above, which implies that μ is a measure without mean.

Next we show that if the Fourier transform of a measure is pure point, then the mean exists. This result was first proven in \mathbb{R}^d by Hof [9, 10], with a general proof via dynamical systems given by [16]. More recently, this was also proven via almost periodicity in [25]. Our proof does not require knowledge of any such theory.

Theorem 3.4.4. *If $\mu = \sum_{x \in \Lambda} c(x)\delta_x \in \mathcal{S}'(\mathbb{R}^d)$ with $\hat{\mu}$ a pure point measure, then $M(\mu)$ exists and*

$$M(\mu) = \hat{\mu}(\{0\}).$$

Proof. We prove first the claim for \mathbb{R} . Pick $g \in C_c^\infty(\mathbb{R})$ with $\text{supp}(g) \subseteq [-1, 1]$, both $g, \hat{g} \geq 0$, and $\int_{\mathbb{R}} g(x)dx = 1$. Such a function always exists in the following way. Trivially, by Example 2.1.1, there exists $f_1 \in C_c^\infty(\mathbb{R})$ such that $f_1 \geq 0$ and $f_1 \neq 0$, $\text{supp}(f_1) \subseteq [-\frac{1}{2}, \frac{1}{2}]$, potentially after a scaling argument. Defining

$$f(x) := \frac{1}{\int_{\mathbb{R}} f_1(x)dx} f_1(x)$$

gives $\int_{\mathbb{R}} f(x)dx = 1$, as $\int_{\mathbb{R}} f_1(x)dx > 0$. Then $g(x) := f * \tilde{f}(x)$ satisfies the above requirements. Indeed, we have $\hat{g} = \hat{f} \cdot \hat{\tilde{f}} = |\hat{f}|^2$, and

$$\text{supp}(g) \subseteq \text{supp}(f * \tilde{f}) \subseteq \left[-\frac{1}{2}, \frac{1}{2} \right] + \left[-\frac{1}{2}, \frac{1}{2} \right] = [-1, 1]$$

moreover, by Fubini's theorem,

$$\int_{\mathbb{R}} g(t)dt = \int_{\mathbb{R}} f * \tilde{f}(t)dt = \int_{\mathbb{R}} \int_{\mathbb{R}} f(s)\tilde{f}(t-s)dsdt = \int_{\mathbb{R}} f(s) \overline{\int_{\mathbb{R}} f(s-t)dt} ds = 1.$$

Now we may define

$$f_n(x) = \frac{1}{2n} 1_{[-n, n]} * g(x).$$

It follows $\text{supp}(f_n(x)) \subseteq [-(n+1), n+1]$ and

$$f_n(x) = \frac{1}{2n} \int_{\mathbb{R}} 1_{[-n, n]}(x-y)g(y)dy = \begin{cases} \frac{1}{2n} & |x| \leq n-1 \\ 0 \leq f_n(x) \leq \frac{1}{2n} & n-1 < |x| < n+1 \\ 0 & n+1 \leq |x|. \end{cases}$$

Thus $f_{n-1} \leq \frac{1}{2n} 1_{[-n, n]} \leq f_{n+1}$, which implies

$$\mu(f_{n-1}) \leq \frac{1}{2n} \mu([-n, n]) \leq \mu(f_{n+1}).$$

Thus it is sufficient to show $\mu(f_n)$ converges to $\hat{\mu}(\{0\})$, with the desired result following via the squeeze theorem.

By Fourier inversion, we have $\mu(f_n) = \hat{\mu}(\check{f}_n)$, with

$$\check{f}_n(x) = \frac{1}{2n} \check{1}_{[-n, n]}(x) \cdot \check{g}(x) = \frac{2n}{2n} \text{sinc}(2n\pi x) \cdot \check{g}(x) = \text{sinc}(2n\pi x) \cdot \check{g}(x),$$

by [2, Example 8.3] and the fact that sinc is even.

As $\hat{\mu}$ is pure point, we may write $\check{\mu} = \sum_{x \in \Lambda} c(x) \delta_x$. Moreover, as $\check{g} \in \mathcal{S}(\mathbb{R})$ we have

$$C := \sum_{x \in \Lambda} |\check{g}(x)| |c(x)| < \infty.$$

Let $\epsilon > 0$. Now, as $|\text{sinc}(x)| \leq \frac{1}{|x|}$, there exists some A such that, for all x such that $|x| > A$ we have

$$|\text{sinc}(x)| < \frac{\epsilon}{2C+1}.$$

Take $h \in C_c^\infty(\mathbb{R})$ such that $\text{supp}(h) \subseteq [-A-1, A+1]$, $0 \leq h(x) \leq 1$, and $h(x) = 1$ for all $x \in [-A, A]$. We can now define

$$h_1 := h \text{sinc}(x).$$

and

$$h_2 := (1-h) \text{sinc}(x).$$

Note that $h_1 \in C_c^\infty(\mathbb{R}^d)$ and $h_2 \in \mathcal{S}(\mathbb{R})$ with, for all $x \in \mathbb{R}$,

$$|h_2(x)| \leq \frac{\epsilon}{2C+1}.$$

Moreover,

$$\check{f}_n(x) = (h_1(2\pi n x) \check{g}(x)) + (h_2(2\pi n x) \check{g}(x)).$$

Now as $\text{supp}(h_1) \subseteq [-A-1, A+1]$ we have

$$\text{supp}(h_1(2\pi n x) \check{g}(x)) \subseteq \left[\frac{-A}{2n\pi}, \frac{A}{2n\pi} \right]$$

and Lemma 2.3.5 gives

$$\lim_n \widehat{\mu}(h_1(2\pi n x) \check{g}(x)) = \widehat{\mu}(\{0\}).$$

It follows that there exists some N_1 such that for all $n > N_1$

$$|\widehat{\mu}(h_1(2\pi n x)) - \widehat{\mu}(\{0\})| < \frac{\epsilon}{2}.$$

Now as $\check{g}, h_2 \in \mathcal{S}(\mathbb{R})$, meaning the following sums are absolutely convergent, we have,

$$\begin{aligned} |\widehat{\mu}(h_1(2\pi n x) \check{g}(x))| &= \left| \sum_{x \in \Lambda} \check{g}(x) c(x) (h_2(2\pi n x)) \right| \leq \sum_{x \in \Lambda} |\check{g}(x)| |c(x)| |h_2(2\pi n x)| \\ &\leq \frac{\epsilon}{2C+1} \sum_{x \in \Lambda} |\check{g}(x)| |c(x)| = \frac{\epsilon}{2C+1} C \end{aligned}$$

with the second inequality coming from the fact that $|h_2| \leq \frac{\epsilon}{2C+1}$. It follows,

$$\begin{aligned} \left| \widehat{\mu}(\widetilde{f}_n) - \widehat{\mu}(\{0\}) \right| &= |\widehat{\mu}(h_1(2\pi n x) \check{g}(x)) + \widehat{\mu}(h_1(2\pi n x) \check{g}(x)) - \widehat{\mu}(\{0\})| \\ &\leq |\widehat{\mu}(h_1(2\pi n x) \check{g}(x)) - \widehat{\mu}(\{0\})| + |\widehat{\mu}(h_1(2\pi n x) \check{g}(x))| \\ &< \frac{\epsilon}{2} + \frac{\epsilon}{2}. \end{aligned}$$

Thus $\mu(f_n) = \widehat{\mu}(\widetilde{f}_n)$ converges to $\widehat{\mu}(\{0\})$ as required. The higher dimensional argument is analogous, taking instead

$$\underbrace{f_n \otimes f_n \otimes \cdots \otimes f_n}_{d\text{-times}}.$$

□

The above equation is known as the formula for the intensity of the Bragg peak at the origin. We can also easily calculate the Bragg peak at any other position as follows.

Corollary 3.4.5. *If $\mu = \sum_{x \in \Lambda} c(x) \delta_x \in \mathcal{S}'(\mathbb{R}^d)$ with $\widehat{\mu}$ a pure point measure, then, for all $k \in \mathbb{R}^d$ we have*

$$\widehat{\mu}(\{k\}) = \lim_n \frac{1}{(2n)^d} \sum_{x \in \Lambda \cap [-n, n]^d} e^{-2\pi i k x} c(x).$$

Proof. Follows from Theorem 3.4.4, and recalling that, where $T_t f(y) := f(y-t)$,

$$\widehat{\mu}(\{k\}) = (T_k \widehat{\mu})(\{0\}) = \widehat{(e^{-2\pi i x \cdot k} \mu)}(\{0\}) = \lim_n \frac{1}{(2n)^d} \sum_{x \in \Lambda \cap [-n, n]^d} e^{-2\pi i k x} c(x).$$

□

We now show a nice result for the mean of a Dirac comb, which will be needed for the density formula for model sets.

Lemma 3.4.6 (Density formula for weighted combs). *For $g \in \mathcal{S}(\mathbb{R}^d)$,*

$$M(\omega_g) = \lim_n \frac{1}{(2n)^d} \sum_{x \in [-n, n]^d} \omega_g(x) = \frac{1}{|\det(\mathcal{L})|} \int_{\mathbb{R}^d} g(x) dx.$$

Proof. By Theorem 3.2.3,

$$M(\omega_g) = \widehat{\omega_g}(\{0\}) = \frac{1}{|\det(\mathcal{L})|} \omega_{\check{g}}^*(\{0\}) = \frac{1}{|\det(\mathcal{L})|} \check{g}(0) = \frac{1}{|\det(\mathcal{L})|} \int_{\mathbb{R}^d} g(x) dx.$$

With the last two equalities following from

$$\omega_g^*(\{0\}) = \sum_{(x, x^*) \in \mathcal{L}^\circ} \check{g}(x^*) \delta_x(\{0\}) = \check{g}(0) = \int_{\mathbb{R}^d} e^{2\pi i x \cdot 0} g(x) dx.$$

with the third equality following from injectivity of the \star -mapping. \square

Combining these results allows to prove the main result of this section.

Theorem 3.4.7 (Density formula for model sets). *If $W \subset \mathbb{R}^m$ is pre-compact and regular then,*

$$\text{dens}(\wedge(W)) = \frac{1}{|\det(\mathcal{L})|} \lambda(W).$$

Proof. Let $\epsilon > 0$ and pick $f, g \in C_c^\infty(\mathbb{R}^d)$ such that $f \leq 1_W \leq g$ and

$$\int_{\mathbb{R}^d} (g - f)(x) dx < \epsilon.$$

Such f, g exist by the regularity of W . It follows that $\omega_f \leq \omega_{1_W} \leq \omega_g$ and

$$\frac{1}{(2n)^d} \omega_f([-n, n]^d) \leq \frac{1}{(2n)^d} \text{card}(\wedge(W) \cap [-n, n]^d) \leq \frac{1}{(2n)^d} \omega_g([-n, n]^d),$$

where we write $\omega_f([-n, n]^d) := \sum_{x \in [-n, n]^d} \omega_f(\{x\})$ for brevity. By Lemma 3.4.6 we have

$$\frac{1}{|\det(\mathcal{L})|} \int_{\mathbb{R}^d} f(x) dx = \lim_n \frac{1}{(2n)^d} \omega_f([-n, n]^d)$$

and

$$\frac{1}{|\det(\mathcal{L})|} \int_{\mathbb{R}^d} g(x) dx = \lim_n \frac{1}{(2n)^d} \omega_g([-n, n]^d).$$

In particular, taking N large enough, for $n > N$ we have both

$$\frac{1}{(2n)^d} \omega_g([-n, n]^d) < \frac{1}{|\det(\mathcal{L})|} \int_{\mathbb{R}^d} g(x) dx + \epsilon$$

and

$$\frac{1}{(2n)^d} \omega_f([-n, n]^d) > \frac{1}{|\det(\mathcal{L})|} \int_{\mathbb{R}^d} f(x) dx - \epsilon.$$

Which implies,

$$\begin{aligned} \frac{\lambda(W)}{|\det(\mathcal{L})|} - 2\epsilon &< \frac{1}{|\det(\mathcal{L})|} \int_{\mathbb{R}^d} g(x) dx - 2\epsilon \\ &< \frac{1}{|\det(\mathcal{L})|} \int_{\mathbb{R}^d} f(x) dx - \epsilon < \frac{1}{(2n)^d} \omega_f([-n, n]^d) \end{aligned}$$

and

$$\begin{aligned} \frac{1}{(2n)^d} \omega_g([-n, n]^d) &< \frac{1}{|\det(\mathcal{L})|} \int_{\mathbb{R}^d} g(x) dx + \epsilon \\ &< \frac{1}{|\det(\mathcal{L})|} \int_{\mathbb{R}^d} f(x) dx + 2\epsilon < \frac{\lambda(W)}{|\det(\mathcal{L})|} + 2\epsilon. \end{aligned}$$

Combining these inequalities we obtain, for all $n > N$,

$$\frac{\lambda(W)}{|\det(\mathcal{L})|} - 2\epsilon \leq \frac{\text{card}(\wedge(W) \cap [-n, n]^d)}{(2n)^d} \leq \frac{\lambda(W)}{|\det(\mathcal{L})|} + 2\epsilon.$$

Thus the claim follows. \square

For a generalization of the above result, see [3, Lemma 4.10.7].

3.5 Autocorrelation of Model Sets

In this section we derive the formula for the autocorrelation measure of regular model sets. We first show that for a bounded set W , the corresponding model set is uniformly discrete. This result is well-known and holds in greater generality, see [23, Prop. 2.6].

Lemma 3.5.1. *If $\wedge(W) \subset \mathbb{R}^d$ is a fully Euclidean model set then $\wedge(W)$ is uniformly discrete.*

Proof. By definition of \mathcal{L} , there exists a linear transformation $T : \mathbb{R}^{d+m} \rightarrow \mathbb{R}^{d+m}$ such that its restriction to \mathcal{L} gives an isomorphism between \mathcal{L} and \mathbb{Z}^{d+m} . Now as T is uniformly continuous and \mathbb{Z}^{d+m} is uniformly discrete, so is \mathcal{L} .

Thus, as $[-1, 1]^d \times (W - W)$ is bounded and \mathcal{L} is uniformly discrete,

$$\text{card}(\mathcal{L} \cap ([-1, 1]^d \times (W - W))) < \infty$$

which implies $\pi_1(\mathcal{L} \cap ([-1, 1]^d \times (W - W)))$ is also finite. Moreover, as

$$0 \in \pi_1(\mathcal{L} \cap ([-1, 1]^d \times (W - W))),$$

there exists some $r > 0$ such that

$$B_r(0) \cap \pi_1(\mathcal{L} \cap ([-1, 1]^d \times (W - W))) = \{0\}.$$

As π_1 is injective, this gives

$$\mathcal{L} \cap (B_r(0) \times (W - W)) = \{(0, 0)\}.$$

We show this r is the needed minimal radius. Let $x, y \in \wedge(W)$ be such that $d(x, y) < r$. Then $x^*, y^* \in W$ and

$$((x - y), (x - y)^*) \in \mathcal{L} \cap (B_r(0) \times (W - W)) = \{(0, 0)\}.$$

Hence $x = y$, which completes the proof. \square

An immediate consequence of this result is that every fully Euclidean model set satisfies the so-called Meyer property.

Corollary 3.5.2 (Meyer property). $\wedge(W) - \wedge(W)$ is uniformly discrete.

Proof. By Lemma 3.5.1 it is sufficient to show $\wedge(W) - \wedge(W) \subseteq \wedge(W - W)$.

Let $x \in \wedge(W) - \wedge(W)$. Then $x = y - z \in \wedge(W) - \wedge(W)$, which by definition gives $(y - z)^* \in W - W$, thus $x \in \wedge(W - W)$. \square

For several equivalent definitions of Meyer sets, we refer the reader to [15, 21, 23, 24, 35]. We now define the concept of autocorrelation for model sets where we follow the approach of [4]. Note that by [2, Example 9.2] and Corollary 3.5.2, this definition coincides with the usual definition of autocorrelation, see [2, Chpt. 9] for details.

Definition 3.5.3. We say $\wedge(W)$ has a well defined autocorrelation if, for all $z \in \wedge(W) - \wedge(W)$, the following limit exists:

$$\eta(z) := \lim_n \frac{\text{card}\{x \in (\wedge(W) \cap [-n, n]^d) : x + z \in \wedge(W)\}}{(2n)^d}.$$

The autocorrelation is then given by

$$\gamma(z) := \sum_{z \in \wedge(W) - \wedge(W)} \eta(z) \delta_z.$$

Note that $\eta(z)$ is simply counting how often, on average, the vector z appears between two points of $\wedge(W)$; for this reason the autocorrelation is also known as the 2-point correlation.

Theorem 3.5.4. If $\wedge(W)$ is regular then $\eta(z)$ exists and

$$\eta(z) = \begin{cases} \frac{1}{|\det(\mathcal{L})|} \lambda(W \cap (-z^* + W)) & z \in L \\ 0 & z \notin L. \end{cases}$$

Proof. In the case of $z \notin L$, then $x + z \notin \wedge(W)$ as $\wedge(W) \subseteq L$ and L is a subgroup of \mathbb{R}^d . Trivially it follows

$$\eta(z) = 0 = \text{dens}(W \cap (-z^* + W)).$$

Now let $z \in L$ and define $\Lambda_n := \{x \in \wedge(W) \cap [-n, n]^d : x + z \in \wedge(W)\}$. Then we have

$$\begin{aligned} x \in \Lambda_n &\Leftrightarrow x \in \wedge(W) \cap [-n, n]^d; x + z \in \wedge(W) \\ &\Leftrightarrow x \in L \cap [-n, n]^d; x^*, (x + z)^* \in W \\ &\Leftrightarrow x \in L \cap [-n, n]^d; x^* \in W \cap (-z^* + W) \\ &\Leftrightarrow x \in \wedge(W \cap (-z^* + W)) \cap [-n, n]^d. \end{aligned}$$

Therefore $\Lambda_n = (\wedge(W \cap (-z^* + W))) \cap [-n, n]^d$. As W is regular, by Lemma 3.1.4, so is $W \cap (-z^* + W)$. Therefore, by Theorem 3.4.7 we have

$$\eta(z) = \lim_n \frac{\Lambda_n}{(2n)^d} = \text{dens}(\wedge(W \cap (-z^* + W))) = \frac{1}{|\det(\mathcal{L})|} \lambda(W \cap (-z^* + W)).$$

This completes the proof. \square

Theorem 3.5.4 motivates us to introduce the following notation.

Definition 3.5.5. Denote the Lebesgue measure by λ and define $C_W : \mathbb{R}^m \rightarrow \mathbb{R}$ by

$$C_W(x) = \lambda(W \cap (-x + W)).$$

Then C_W is known as the covariogram function of W .

Note that Theorem 3.5.4 gives that for all $z \in L$ we have

$$C_W(z^*) = |\det(\mathcal{L})| \text{dens}(\wedge(W) \cap (-z^* + \wedge(W))),$$

meaning that the covariogram of the window measures the internal coherence of the solid. We now list the basic properties of C_W .

Proposition 3.5.6. *Let W be a regular window. The covariogram function has the following properties.*

- (a) $C_W \equiv 0$ outside $W - W$.
- (b) $C_W(-x) = C_W(x)$.
- (c) $C_W(x) = 1_W * \widetilde{1}_W(x)$.
- (d) $C_W(x)$ is continuous.

Proof. First if $C_W(x) \neq 0$ then $\lambda(W \cap (-x + W)) \neq 0$ which implies

$$W \cap (-x + W) \neq \emptyset.$$

Let $z \in W \cap (-x + W)$. Then there exists some $t \in W$ such that $z = -x + t$; thus $x = t - z \in W - W$ which proves (a). The second claim follows from the translational invariance of the Lebesgue measure.

Now by (b),

$$1_W * \tilde{1}_W(x) = \int_{\mathbb{R}^d} 1_W(t)1_W(t-x)dt = \int_{\mathbb{R}^d} 1_{W \cap (x+W)}dt = C_W(-x) = C_W(x),$$

which proves (c). Finally, we show continuity.

Let $\epsilon > 0$ and, by regularity of W , we may take $f, g \in C_c(\mathbb{R}^d)$ such that $f \leq 1_W \leq g$ and $\int_{\mathbb{R}^d} (g-f)(x)dx < \frac{\epsilon}{4}$. This gives

$$f * \tilde{f} \leq 1_W * \tilde{1}_W \leq g * \tilde{g}.$$

As f is uniformly continuous, there exists δ such that whenever $|x-y| < \delta$, then $|f(x) - f(y)| < \frac{\epsilon}{4\lambda(W)+1}$. It follows, for $|x-y| < \delta$,

$$\begin{aligned} & \left| 1_W * \tilde{1}_W(x) - 1_W * \tilde{1}_W(y) \right| = \left| \int_{\mathbb{R}^d} (1_W(x-t) - 1_W(y-t))\tilde{1}_W(t)dt \right| \\ & \leq \int_{\mathbb{R}^d} |1_W(x-t) - g(x-t)|\tilde{1}_W(t)dt + \int_{\mathbb{R}^d} |g(x-t) + f(x-t)|\tilde{1}_W(t)dt \\ & + \int_{\mathbb{R}^d} |f(x-t) - f(y-t)|\tilde{1}_W(t)dt + \int_{\mathbb{R}^d} |f(y-t) - 1_W(y-t)|\tilde{1}_W(t)dt \\ & \leq \int_{\mathbb{R}^d} |1_W(x-t) - g(x-t)|dt + \int_{\mathbb{R}^d} |g(x-t) + f(x-t)|dt \\ & + \int_{\mathbb{R}^d} \frac{\epsilon}{4\lambda(W)+1} \tilde{1}_W(t)dt + \int_{\mathbb{R}^d} |f(y-t) - 1_W(y-t)|dt \\ & < 3 \int_{\mathbb{R}^d} |g(x-t) - f(x-t)|dt + \frac{\epsilon}{4} < \frac{4\epsilon}{4}. \end{aligned}$$

□

The covariogram allows us to re-write the autocorrelation coefficients as

$$\eta(z) = \begin{cases} \frac{1}{|\det(\mathcal{L})|} C(z^*) & z \in L \\ 0 & z \notin L \end{cases}$$

which gives, noting that $C_W(x) \notin \mathcal{S}(\mathbb{R}^d)$,

$$\gamma(z) = \frac{1}{|\det(\mathcal{L})|} \sum_{z \in \wedge(W) - \wedge(W)} C(z^*) \delta_z = \frac{1}{|\det(\mathcal{L})|} \omega_{C_W}.$$

3.6 Diffraction by Regular Model Sets

Recall for finite set F the normalised diffraction intensity function, known as the Patterson function, is defined as

$$I_F(y) = \frac{1}{|F|} \left| \sum_{x \in F} e^{-2\pi i x y} \right|^2.$$

This function highlights the so called *phase problem* in crystallography: when making a physical measurement the intensity of the sample points are known, while the phase information is lost. For more details regarding diffraction theory, we refer the reader to [2, Chapter 9]. Now, as $\widehat{\delta}_x = e^{-2\pi i x y}$, we have

$$I_F(y) = \frac{1}{|F|} \left| \widehat{\delta}_F \right|^2 = \frac{1}{|F|} \widehat{\delta_F * \widetilde{\delta}_F}.$$

This observation leads to the following commutative diagram, known as the Wiener diagram.

$$\begin{array}{ccc} \delta_F & \xrightarrow{\widehat{}} & \widehat{\delta}_F \\ \downarrow & & \downarrow \\ \frac{1}{|F|} \delta_F * \widetilde{\delta}_F & \xrightarrow{\widehat{}} & \frac{1}{|F|} \left| \widehat{\delta}_F \right|^2 \end{array}$$

Figure 3.1: Wiener diagram for finite samples.

Note that in the case of an infinite set $\Lambda \subseteq \mathbb{R}^d$, the above diagram only works when considering $\widehat{\delta}_\Lambda$ as a distribution, and $|\widehat{\delta}_\Lambda|^2$ is thus meaningless. Therefore, for $\Lambda \subseteq \mathbb{R}^d$ we instead define $F_n := \Lambda \cap [-n, n]^d$ which gives the following commutative diagram, with δ_{F_n} a tempered distribution. Note that the diffraction is the limit of the bottom right term with respect to the topology of tempered distributions.

$$\begin{array}{ccc} \delta_{F_n} & \xrightarrow{\widehat{}} & \widehat{\delta}_{F_n} \\ \downarrow & & \downarrow \\ \frac{1}{|F_n|} \delta_{F_n} * \widetilde{\delta}_{F_n} & \xrightarrow{\widehat{}} & \frac{1}{|F_n|} \left| \widehat{\delta}_{F_n} \right|^2 \end{array}$$

Figure 3.2: Wiener diagram for infinite samples.

As is standard, we assume our solid to be homogeneous, thus for any sample we can replace F_n with the respective volume of $(2n)^d$. Now in a similar way as [9], we can define the autocorrelation of an arbitrary Delone set.

Definition 3.6.1. Let $\Lambda \subseteq \mathbb{R}^d$ be Delone. We say Λ has a well defined autocorrelation with respect to $[-n, n]^d$ if the sequence

$$\gamma_n := \frac{1}{(2n)^d} \delta_{F_n} * \tilde{\delta}_{F_n}$$

converges in the tempered distribution topology to some tempered measure γ , which is referred to as the autocorrelation measure. Moreover, the Fourier transform $\hat{\gamma}$ of γ , as a tempered distribution, is called the diffraction measure of Λ .

Remark. As γ_n converges to γ in the tempered distribution topology, and the Fourier transform is continuous in this topology, we have

$$\hat{\gamma} = \lim_n \widehat{\gamma_n}.$$

When working with measures in general, the continuity of the Fourier transform is subtle, see [33] for a discussion. However, we are able to claim that the diffraction measure is a positive distribution.

Corollary 3.6.2. $\hat{\gamma}$ is a positive distribution.

Proof. For all $f \in \mathcal{S}(\mathbb{R}^d)$ with $f \geq 0$ we have, by continuity of Fourier transform in this case,

$$\begin{aligned} \hat{\gamma}(f) &= \lim_n \widehat{\gamma_n}(f) = \lim_n \frac{1}{(2n)^d} \int_{\mathbb{R}^d} \left((\delta_{F_n} * \tilde{\delta}_{F_n}) \hat{f} \right) (t) dt \\ &= \lim_n \frac{1}{(2n)^d} \int_{\mathbb{R}^d} \left(|\hat{\delta}_{F_n}|^2 f \right) (t) dt \geq 0. \end{aligned}$$

□

Note that $\hat{\gamma}$ models the physical diffraction. Now, [9] gives that the limit in Definition 3.6.1 exists as a limit of measures, however does not claim the convergence in the sense of tempered distributions. Some work must be done to show that these convergences are in fact equivalent, which is a consequence of the uniform discreteness of the support. These equivalences are what we now prove.

Theorem 3.6.3. Let $\Lambda \subseteq \mathbb{R}^d$ be such that $\Lambda - \Lambda$ is uniformly discrete. Then the following are equivalent.

- (i) γ_n converges as a tempered distribution to some tempered distribution γ .
- (ii) γ_n converges as a measure to some measure γ_1 .
- (iii) For all $z \in \Lambda - \Lambda$, the following limit exists

$$\eta(z) := \lim_n \frac{\text{card}\{x \in \Lambda \cap [-n, n]^d : x + z \in \Lambda\}}{(2n)^d}.$$

Moreover, in this case we have,

$$\gamma = \gamma_1 = \sum_{z \in \Lambda - \Lambda} \eta(z) \delta_z.$$

Proof. Note first that

$$\begin{aligned} \gamma_n &= \frac{1}{(2n)^d} \delta_{\Lambda \cap [-n, n]^d} * \widetilde{\delta_{\Lambda \cap [-n, n]^d}} = \frac{1}{(2n)^d} \sum_{x \in \Lambda \cap [-n, n]^d} \delta_x * \sum_{y \in \Lambda \cap [-n, n]^d} \delta_{-y} \\ &= \sum_{x, y \in \Lambda \cap [-n, n]^d} \frac{\delta_{x-y}}{(2n)^d} = \sum_{z \in \Lambda - \Lambda} \left(\sum_{\substack{x, y \in \Lambda \cap [-n, n]^d \\ x-y=z}} \frac{\delta_z}{(2n)^d} \right) = \sum_{z \in \Lambda - \Lambda} \eta_n(z) \delta_z \end{aligned}$$

where

$$\eta_n(z) := \frac{1}{(2n)^d} \text{card}\{x, y \in \Lambda \cap [-n, n]^d : x - y = z\}.$$

Now the claim is essentially that of [33, Prop. 4.6]; we include it for completeness.

(i) \Rightarrow (iii) Fix $z \in \Lambda - \Lambda$, and pick $f \in C_c^\infty(\mathbb{R}^d)$ such that $f(z) = 1$ and $f(t) = 0$ for $t \in (\Lambda - \Lambda) \setminus \{z\}$. Such an f exists by the uniform discreteness of $\Lambda - \Lambda$. Since $C_c^\infty(\mathbb{R}^d) \subseteq C_c(\mathbb{R}^d)$, by (i) we have

$$\gamma_1(f) = \lim_n (\gamma_n)(f) = \lim_n \eta_n(z) = \lim_n \frac{\text{card}\{x, y \in \Lambda \cap [-n, n]^d : x - y = z\}}{(2n)^d}$$

exists. Note that

$$\begin{aligned} A &:= \{x \in \Lambda \cap [-n, n]^d : x + z \in \Lambda \cap [-n, n]^d\} \\ &= \{x \in \Lambda \cap [-n, n]^d : \exists y \in \Lambda \cap [-n, n]^d \text{ such that } x - y = z\}. \end{aligned}$$

We show that, after defining $B := \{x \in \Lambda \cap [-n, n]^d : x + z \in \Lambda\}$,

$$\lim_n \frac{\text{card}(B \setminus A)}{(2n)^d} = 0$$

which implies the desired limit exists. Indeed, as

$$B \setminus A = \{x \in \Lambda \cap [-n, n]^d : x + z \notin \Lambda \cap [-n, n]^d\}$$

this implies that $x + z \notin [-n, n]^d$, thus there exists some $1 \leq i \leq d$ such that $x_i + z_i \notin [-n, n]$. In particular,

$$x_i \geq n - z_i \geq n - \|z\| \quad \text{or} \quad x_i \leq -n - z_i \leq -n - \|z\|.$$

This gives,

$$B \setminus A \subseteq \Lambda \cap \left(\bigcup_{i=1}^d [-n, n]^{i-1} \times ([-n, -n + \|z\|] \cup [n - \|z\|, n] \times [-n, n]^{d-i}) \right).$$

Note that, as $\Lambda - \Lambda$ is uniformly discrete, say with radius r , then so is $\Lambda - a$ for any fixed $a \in \Lambda$. It follows that, for any distinct $x, y \in \Lambda$ we have

$$d(x, y) = d(x - a, y - a) \geq r$$

thus Λ is uniformly discrete. Hence, the above intersection is finite, which implies

$$\lim_n \frac{\text{card}(B \setminus A)}{(2n)^d} = 0$$

as required.

(iii) \Rightarrow (ii) Let $f \in C_c^\infty(\mathbb{R}^d)$ be arbitrary, then

$$\gamma_n(f) = \sum_{z \in \Lambda - \Lambda} \eta_n(z) f(z) = \sum_{\substack{z \in \Lambda - \Lambda \\ z \in \text{supp}(f)}} \eta_n(z) f(z).$$

Note that $(\Lambda - \Lambda) \cap \text{supp}(f)$ is finite for each z . Moreover, by the above argument,

$$\lim_n \eta_n(z) = \lim_n \frac{\text{card}\{x \in \Lambda \cap [-n, n]^d : x + z \in \Lambda\}}{(2n)^d} =: \eta(z).$$

Combining these facts gives,

$$\gamma_1(f) := \lim_n \gamma_n(f) = \lim_n \sum_{\substack{z \in \Lambda - \Lambda \\ z \in \text{supp}(f)}} \eta_n(z) f(z) = \sum_{\substack{z \in \Lambda - \Lambda \\ z \in \text{supp}(f)}} \eta(z) f(z) = \sum_{z \in \Lambda - \Lambda} \eta(z) \delta_z(f)$$

exists finitely.

(ii) \Rightarrow (i) Note that Λ is uniformly discrete by the same argument as above. In particular,

$$l := \limsup_n \frac{1}{(2n)^d} \text{card}(\Lambda \cap [-n, n]^d) < \infty.$$

Moreover, there exists some $l' \geq l$ such that for all n we have

$$\frac{1}{(2n)^d} \text{card}(\Lambda \cap [-n, n]^d) \leq l' < \infty.$$

It follows immediately that for all $z \in \Lambda - \Lambda$ we have

$$\eta_n(z), \eta(z) \leq l'.$$

As $\Lambda - \Lambda$ is uniformly discrete, it suffices to prove the claim for $f \in C_c^\infty(\mathbb{R}^d)$. But this follows from (ii).

This completes the proof. \square

By combining everything we have obtained thus far, we get that every regular model set has a well defined autocorrelation and diffraction. Moreover, the diffraction is a positive pure point tempered measure.

Let $\wedge(W)$ to be a regular model set in some fully Euclidean model set $(\mathbb{R}^d, \mathbb{R}^m, \mathcal{L})$.

Recall that by Theorem 3.6.3 and Proposition 3.5.6, the autocorrelation exists and equals

$$\gamma_{\wedge(W)} = \frac{1}{|\det(\mathcal{L})|} \omega_{C_W}.$$

As the covariogram is continuous by Proposition 3.5.6 and as

$$\widehat{C_W} = \widehat{1_W} \widehat{1_W} = |\widehat{1_W}|^2 \geq 0$$

we have that $C_W \in PK(\mathbb{R}^m)$. Thus, by Theorem 3.3.4, we get the following.

Theorem 3.6.4. *Let $(\mathbb{R}^d, \mathbb{R}^m, \mathcal{L})$ be a CPS and let $W \subseteq \mathbb{R}^m$ be a regular window. Then $\Lambda = \wedge(W)$ has a well defined autocorrelation*

$$\gamma_\Lambda = \frac{1}{|\det(\mathcal{L})|} \omega_{C_W} = \sum_{z \in \wedge(W-W)} C_W(z^*) \delta_z$$

and diffraction given by

$$\widehat{\gamma}_\Lambda = \frac{1}{|\det(\mathcal{L})|} \widehat{\omega_{C_W}} = \frac{1}{|\det(\mathcal{L})|^2} \omega_{\widehat{C_W}}^* = \frac{1}{|\det(\mathcal{L})|^2} \sum_{k \in L^\otimes} I(k) \delta_k$$

where $L^\otimes = \pi_1(\mathcal{L}^\circ)$ is the Fourier module and

$$I(k) = \left| \int_W e^{2\pi i k^* y} dy \right|^2 \geq 0 \quad \forall k \in L^\otimes.$$

In particular, $\widehat{\gamma}_\Lambda$ is a positive pure point tempered measure. □

Chapter 4

Diffraction of the Silver Mean Model Set

In this chapter we provide a short worked example of the diffraction measure of the silver mean model set.

4.1 Silver Mean Model Set

The silver mean substitution and corresponding substitution matrix are respectively given by

$$\begin{array}{l} a \rightarrow aba \\ b \rightarrow a \end{array} \quad M_{sm} := \begin{pmatrix} 2 & 1 \\ 1 & 0 \end{pmatrix}$$

with Perron-Frobenius eigenvalue $\lambda_{sm} = 1 + \sqrt{2}$. The left-hand endpoints of the geometric realisation of this substitution form the following CPS and model set. For further background and properties, we refer the reader to [2, Example 4.5].

Example 4.1.1. Consider the following CPS:

$$\begin{array}{ccccc} \mathbb{R} & \xleftarrow{\pi_1} & \mathbb{R} \times \mathbb{R} & \xrightarrow{\pi_2} & \mathbb{R} \\ \uparrow & & \uparrow & & \uparrow \text{dense} \\ L & \xleftarrow{1-1} & \mathcal{L} := \mathbb{Z}(1, 1) \oplus \mathbb{Z}(\sqrt{2}, -\sqrt{2}) & \xrightarrow{\pi_2} & L^* \\ \parallel & & & & \parallel \\ \mathbb{Z}[\sqrt{2}] & \xrightarrow{\quad \star \quad} & & & \mathbb{Z}[\sqrt{2}] \end{array}$$

With the \star -mapping given by the Galois conjugation

$$(m + n\sqrt{2})^* = m - n\sqrt{2}, \quad \forall m, n \in \mathbb{Z}.$$

Then, with window $W := [-\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}]$, we obtain the silver mean model set,

$$\wedge(W) := \{x \in L : x^* \in W\}$$

illustrated below in Figure 4.1. Moreover, by Lemma 2.3.7, the dual lattice is given by

$$\mathcal{L}^\circ = \mathbb{Z} \left(\frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4} \right) \oplus \mathbb{Z} \left(\frac{1}{2}, \frac{1}{2} \right)$$

which gives the dual CPS $(\mathbb{R}, \mathbb{R}, \mathcal{L}^\circ)$.

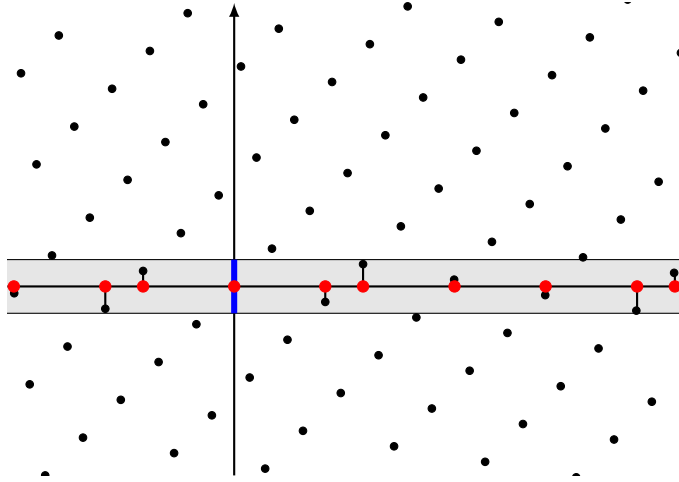


Figure 4.1: Silver mean model set. The window is in blue and the model set in red.

Note that this is called the *silver mean* CPS as the corresponding substitution matrix has Perron-Frobenius eigenvalue of $1 + \sqrt{2}$, which is indeed the silver mean. Moreover, the choice of window is a consequence of Hutchinson's contraction principle on an iterated function system for the point sets of the substitution; see [2, Chapter 7.1] for details. Next, we calculate the diffraction for the silver mean model set.

Lemma 4.1.2. *With $\wedge(W)$ the model set from Example 4.1.1, the diffraction measure is given by*

$$\hat{\gamma} = \frac{1}{4} \sum_{k \in \frac{\sqrt{2}}{4}\mathbb{Z}[\sqrt{2}]} \left| \text{sinc}(\sqrt{2}\pi k^*) \right|^2 \delta_k.$$

Proof. Note that $L^\circ = \pi_1(\mathcal{L}^\circ) = \frac{\sqrt{2}}{4}\mathbb{Z}[\sqrt{2}]$. Then by Theorem 3.6.4, as $\wedge(W)$ is a regular model set, its diffraction $\hat{\gamma}$ is given by

$$\hat{\gamma} = \frac{1}{|\det(\mathcal{L})|^2} \sum_{k \in L^\circ} I(k) \delta_k$$

where, recalling that $\sin(x)$ is odd and the interval is symmetric,

$$\begin{aligned} I(k) &= \left| \int_W e^{2\pi i k^* y} dy \right|^2 = \left| \int_{-\sqrt{2}}^{\sqrt{2}} \cos(2\pi k^* y) + i \sin(2\pi k^* y) dy \right|^2 \\ &= \left| \frac{\sin(2\pi k^* y) + -i \cos(2\pi k^* y)}{2\pi k^*} \Big|_{-\sqrt{2}}^{\sqrt{2}} \right|^2 \\ &= \left| \frac{\sin(2\pi k^* \sqrt{2})}{\pi k^*} \right|^2 = \left| \sqrt{2} \operatorname{sinc}(\sqrt{2}\pi k^*) \right|^2. \end{aligned}$$

Thus,

$$\hat{\gamma} = \frac{1}{4} \sum_{k \in L^{\circledast}} |\operatorname{sinc}(\sqrt{2}\pi k^*)|^2 \delta_k.$$

□

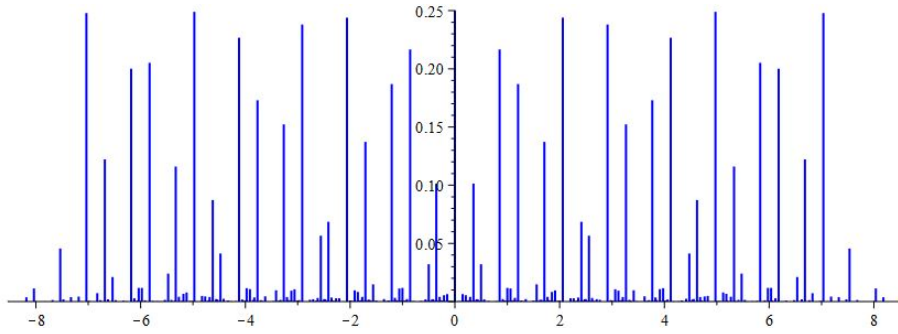


Figure 4.2: Sketch of the diffraction measure of the silver mean chain. Note that the intensity is bounded by $\frac{1}{4}$. Moreover, when the entire dual lattice \mathcal{L}° is included, the diffraction pattern is symmetric in k .

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