Diffraction of point sets with structural disorder

Kai Miguel Matzutt

To all my mathematical teachers

Diffraction of point sets with structural disorder

Dissertation zur Erlangung des akademischen Grades eines

Doktors der Mathematik

der
Fakultät für Mathematik
Universität Bielefeld

Vorgelegt von

Kai Miguel Matzutt

Fakultät für Mathematik
Universität Bielefeld

Juli 2010

1. Berichterstatter: Prof. Dr. Michael Baake
2. Berichterstatter: Juniorprof. Dr. Matthias Birkner

Datum der mündlichen Prüfung: 21. September 2010

Gedruckt auf alterungsbeständigem Papier ♾ ISO 9706.

Contents

List of Figures

Introduction

The structural analysis of crystals by X-ray diffraction experiments has a long history. As of today, it is broadly treated and theoretically well understood, see e.g. [**30, 48**]. W. L. and W. H. Bragg were awarded the Nobel price in physics in 1915 for their experiments and explanations in that context. The so called *Bragg peaks*, i.e. sharp point-like components in the diffraction image of a solid or other material, are a strong indicator for some sort of long-range order of the structure of given material. Although the term 'long-range order' has still no uniformly accepted sharp definition, the appearance of Bragg peaks in the diffraction image of a structure or even a diffraction image consisting only of Bragg peaks is a widely accepted hint at long-range order in the structure for any such definition; compare the discussion in [**95**]. In this sense, long-range order is not restricted to periodic structures, i.e. structures that have a translational symmetry of some sort, like crystals. The discoveries of metallic alloys with Bragg peaks in their diffraction images but without any translation symmetry [**90**], later subsumed under the term *quasicrystals*, and similar theoretical objects, namely *aperiodic tilings* [**79, 22, 61, 62**], triggered the question of what kind of (matter) distributions share those point-like parts in their diffraction spectra [**26**]. The question has been studied intensively since then, experimentally and mathematically, and lead to mathematical answers such as those presented in [**41, 50**].

Also the other parts of the diffraction image of aperiodic structures, i.e. the absolutely continuous (e.g. [**50, 51**]) and singular continuous parts (e.g. [**45**]), were investigated. In particular, random components in the structures lead to absolutely continuous parts in diffraction, respectively to diffuse scattering (for a broad picture of diffraction of random structures see [**6**]). Contributions by Gouéré [**46**] led to new insight into diffraction in the even more random situations of ergodic point processes.

The question whether one can (uniquely) determine the structure from the diffraction image is a very natural one. This question is referred to as the corresponding *inverse problem*. Unfortunately, the answer is not affirmative. If the diffraction spectrum has continuous parts, the inverse problem gets even more intricate. For instance, Höffe and Baake [**8**] came up with an example where some deterministic structure (the Rudin-Shapiro sequence) has the same diffraction as one with maximal entropy (a Bernoulli chain). It is therefore useful to enlarge the collection of worked out examples. This thesis is a contribution to that, with particular focus on continuous spectral components.

Mathematically, we follow Hof [**50**] in the modelling of kinematic diffraction. The diffraction of a given structure for us is the positive measure that

is the Fourier transform of the volume averaged autocorrelation measure. A good introduction to why this is an adequate way to model the physical experiments can for instance be found in [**52, 54, 97**].

The systems we consider have structural disorder that is described by stochastic elements. The first kind of structure is given by randomly weighted aperiodic point sets (i.e. the underlying structure has long-range order) and the disorder is introduced by a Gibbs measure that puts the random weights to the points, similar to lattice gases. The second kind of structure is strongly disordered by itself, being realisations of the Matérn hard-core point process, a local thinning of a Poisson point process.

Structure of the thesis

The thesis is organised as follows.

In *Chapter* 1, we briefly introduce the notation and elementary methods used in the later chapters. After the notation is fixed, the necessary objects and results about Fourier transforms of Radon measures are introduced. They are then put into context with mathematical diffraction theory as introduced by Hof [**49, 50, 51**]. At the end of Chapter 1, a few definitions concerning point processes are recalled.

In *Chapter* 2, we analyse diffraction properties of randomised sets of *finite local complexity* (FLC sets). Therefore, in Section 2.1, FLC sets and weighted FLC sets are introduced. Adapted topological spaces and dynamical systems are presented and their properties are discussed in that section, too. The next section is concerned with the involved random mechanism. A class of appropriate Gibbs measures is presented, starting with a recapitulation of general Gibbs measures, then going over to the construction of Gibbs measures that attach weights from a compact weight set to single FLC sets, where the weighting process is governed by a short-range pair interaction. A high temperature regime ensures uniqueness with the help of Dobrushin's criterion and gives an estimate for the covariances of one-point functions. The next step is to extend those Gibbs measures to dynamical systems of FLC sets. As a first result, we give conditions for this kind of Gibbs measure to be ergodic. With the ergodicity of this measure and the estimates of the covariances, we can then analyse the diffraction of its realisations in the next section by using theory on the spectrum of dynamical systems. We get the main result for this chapter:

Result. *If uniquely ergodic and pure point diffractive FLC sets are randomised by a short-ranged Gibbs measure at sufficiently high temperatures, no singular continuous part is present in their diffraction measure.*

Chapter 3 discusses the diffraction properties of the Matérn hard-core point process. Starting from observations and claims given in [**6**] the chapter provides a detailed treatment of the diffraction of this process.

The first section recapitulates the connection between second order properties of a stationary ergodic point process and the autocorrelation measure of its realisations. A connection between the Bartlett spectrum and the diffraction measure is also drawn.

Section 3.2 introduces the Matérn hard-core point process and some of its properties, its ergodicity in particular.

This ergodicity then allows us to use the connection between autocorrelation and Palm measure observed by Gouéré [**46**] and the second order product density of the Matérn hard-core point process as calculated by Stoyan and Stoyan [**94**] to analyse the diffraction of the process in Section 3.3. In the one-dimensional case the diffraction can be computed analytically. The observations in this case can be extended to higher dimensions. Although the explicit values of the absolutely continuous part of the diffraction measure can only be computed numerically, we can still rigorously describe the asymptotic behaviour of the density for large arguments.

Result. *The diffraction of the Matérn hard-core point process in dimension d is that of a refined Poisson point process plus an additional radially symmetric absolutely continuous part that is $\mathcal{O}\big(\|y\|^{-(d+1)/2}\big)$ as $\|y\| \to \infty$.*

Acknowledgements

It is a great pleasure to thank so many kind people who contributed to the creation of this thesis in manifold ways.

First and foremost, I would like to thank my advisor Michael Baake for sharing his brilliant intuition and great insights into the topic with me to make this thesis possible.

I am very much obliged to Natali Zint. We worked together on the diffraction of FLC sets and I profited a lot from our joint activities. Additionally, when the mathematical problems seemed too big for us, we gave confidence to each other.

Further, I wish to thank Matthias Birkner for helpful discussions.

I thank Justine Swierkot for reading parts of my thesis and giving several useful comments on the manuscript. Franz Gähler gave several helpful suggestions for the introduction. I want to thank Robin Hill for carefully reading my thesis and providing the English language and style skills I lack.

I also wish to thank Ellen Baake, for providing the great working environment at the institution that also gave the financial support for the biggest parts of this thesis, the Research Centre for Mathematical Modelling (FSPM) at Bielefeld University.

During the first months of my work at this thesis, I was employed at the Collaborative Research Centre 701 "Spectral Structures and Topological Methods in Mathematics". I want to thank the speaker Friedrich Götze as a representative, for financial support and the excellent mathematical environment provided by this centre – of that I also profited after the end of my employment there.

I want to thank the working group "Mathematik in den Naturwissenschaften" for the stimulating and friendly atmosphere and several fruitful disscussions, in particular (alphabetically ordered) Michael Baake, Nadine Eisner, Dirk Frettlöh, Franz Gähler, Svenja Glied, Manuela Heuer, Christian Huck, Manuel Loquias, Claudia Lütkehölter, Markus Moll, Natascha Neumärker, Johan Nilsson, Christoph Richard, Oliver Schmidt, Uwe Schwerdtfeger, Bernd Sing and Peter Zeiner.

Although my mathematical home was in the above mentioned group, the working group of Ellen Baake "Biomathematik" treated me as if I was part of them. It was a great pleasure. In particular, I wish to thank (again in alphabetical order) Ellen Baake, Anne-Katrin Hoffmann, Thiemo Hustedt, Sandra Kluth, Hayk Mashurian, Florian Lipsmeier, Ulrike Schlägel, Ute v. Wangenheim and Natali Zint.

Good parts of the above mentioned people also belong to the group of friends that gave the necessary comfort and advice to endure the sometimes stressful and demanding parts of writing a thesis. I do not want to make a list of them, because the list could never be exhaustive. The same is true for my family. They gave me the loving and stable background I needed so much.

Last but not least, I wish to thank Nadine Geppert. Solving problems in mathematics and real life is so much easier if you know there is someone at your side.

CHAPTER 1

Notation and preliminaries

1.1. Notation

Throughout this text, we try to use standard notation for the different mathematical objects. Still, we give some basic information for reasons of completeness.

1.1.1. Sets and numbers. The natural numbers $\{1, 2, 3, \ldots\}$ will be denoted by $\mathbb{N}$, $\mathbb{N} \cup \{0\}$ by $\mathbb{N}_0$, the integers by $\mathbb{Z}$, the reals by $\mathbb{R}$ and the complex numbers by $\mathbb{C}$. The positive reals are given by $\mathbb{R}^+$ and the non-negatives by $\mathbb{R}_0^+$. The absolute values of real or complex numbers z are written as $|z|$. The argument of a complex z as $\arg z$ and the complex conjugate as $\overline{z}$, imaginary and real part of z will be denoted by $\operatorname{Im}(z)$ and $\operatorname{Re}(z)$, respectively. The symbol ∞ shall be used for infinity on the positive real line (or complex infinity), while $-\infty$ will be used for the negative counterpart.

The standard d-dimensional Euclidean space will be denoted by $\mathbb{R}^d$ and the corresponding Euclidean norm of elements x by $\|x\|$. By $B_r(x)$ we denote the *closed* ball in $\mathbb{R}^d$ of radius r around x, the *open* version by $B_r^o(x)$. By B_r we abbreviate $B_r(0)$. We will write $\#A$ or $\#(A)$ for the cardinality of an arbitrary set A, including infinite ones. If Ω is any space and $A \subseteq \Omega$ is some subset then we denote its complement $\Omega \setminus A$ by $A^{\complement}$. The characteristic function of a set A is defined via

$$1_A(\omega) = \begin{cases} 1\,, & \text{if } \omega \in A\,, \\ 0\,, & \text{otherwise.} \end{cases}$$

For a set $A \subseteq \mathbb{R}^d$, $t \in \mathbb{R}^d$ let

$$A + t := \{x + t \,|\, x \in A\}$$

be the shifted set. For two subsets A, B of $\mathbb{R}^d$ we denote their Minkowski sum and difference by

$$A \pm B := \{x \pm y \,|\, x \in A,\, y \in B\}\,,$$

For a topological space X let further $\mathscr{K}(X)$ denote the set of compact subsets of X. The interior of a set A will be denoted by A^o, its boundary by ∂A.

1.1.2. Functions. The Landau symbols $\mathcal{O}$ and o, as well as the symbol $\sim$, to describe asymptotic behaviour of a real or complex valued function are used as defined in [**75**]. By log we denote the natural logarithm with base e. The restriction of a mapping $f : X \to Y$ to some $X' \subset X$ will be denoted by $f|_{X'}$.

Some *special functions* will also appear in our calculations. Since some have slightly different definitions in different books, we will give the ones we are going to use:

$$\operatorname{Si}(z) := \int_0^z \frac{\sin t}{t}\,\mathrm{d}t\,,$$
$$\operatorname{Ci}(z) := -\int_z^\infty \frac{\cos t}{t}\,\mathrm{d}t$$

and

$$\operatorname{Ei}(z) := -\int_{-z}^\infty \frac{\exp(-t)}{t}\,\mathrm{d}t\,,$$

namely the integral sine and cosine and the exponential integral. While Si is an entire function, Ci and Ei have a branch cut discontinuity on the negative real axis and Ei is to be understood as the Cauchy principal value of the integral. For more details and properties see e.g. [**1, 75**]. ${}_1F_0$ and ${}_2F_1$ denote the respective (generalised) hypergeometric functions, compare [**70**]. The Bessel functions of the first kind are denoted by $J_\nu(z)$, see [**1**] for definitions and properties.

1.2. Radon measures, Fourier transforms and diffraction

Large parts of this thesis are concerned with measures and their Fourier transforms, because diffraction is modelled as the Fourier transform of the so-called autocorrelation measure, an object that can be deduced from the structure under consideration.

In this section we will clarify our point of view and recapitulate important results (for our context), without going into details and just giving references to the proofs.

1.2.1. Measures and spaces of measures. Our perspective on measures is the simultaneous view of measures as (complex) σ-additive set functions and as continuous linear functionals, which is justified by versions of the Riesz-Markov theorems (compare e.g. [**78**]). For probability measures and standard probability theory we would like to simply refer to standard literature such as [**20, 21, 25, 77**].

We will focus on the set $\mathcal{M}(X)$ of complex (Radon) measures, i.e. duals of elements in $C_c(X)$, the set of continuous complex valued functions with compact support in X, where X is some locally compact metrizable space. Thus measures are (complex) linear functionals μ on $C_c(X)$ such that for any compact $K \subset X$ there exists some constant a_K with

$$|\mu(f)| \leqslant a_K \|f\|_\infty$$

for any $f \in C_c(X)$ with support in K. Here $\|\cdot\|_\infty$ is the usual sup-norm. The support $\operatorname{supp}\mu$ of a measure μ is then defined as the smallest closed set F such that $\mu(f) = 0$ for all $f \in C_c(X)$ with support outside of F. For further details, we would like to refer to [**10**],[**23**],[**2**] and [**35**].

We are going to flip between several ways to denote the evaluation of a function f by a measure μ, just to stress certain properties or for ease of

notation:

$$\mu(f) = \int_X f(x)\,\mathrm{d}\mu(x) = \mathbb{E}_\mu(f)\,,$$

where we use $\mathbb{E}_\mu(f)$ only if μ is a probability measure. Note that in the interpretation of μ as a set function on the corresponding Borel sets and with the interpretation of $\mu(f)$ as an integral, the function f only needs to be integrable, not necessarily continuous, e.g. $\mu(A) = \mu(1_A)$ for a Borel set A. We equip $\mathcal{M}(X)$ with the vague topology, i.e. a sequence $(\mu_n)_{n\in\mathbb{N}}$ in $\mathcal{M}(X)$ converges if and only if $(\mu_n(f))_{n\in\mathbb{N}}$ converges for every test-function $f \in C_c(X)$. The restriction of a measure μ to some Borel set A is given by the measure defined by $\mu_A(f) := \mu(1_A f)$. The complex conjugate of a measure is given by $\overline{\mu}(f) := \overline{\mu(\overline{f})}$ and also defines a measure.

Let us now turn to a special case, let $X = \mathbb{R}^d$. There are several subspaces of $\mathcal{M}(\mathbb{R}^d)$ of interest for our investigations. Let $C_c^{\mathbb{R}}(\mathbb{R}^d)$ be the set of *real valued* continuous functions on $\mathbb{R}^d$ with compact support and $C_c^+(\mathbb{R}^d)$ the functions $f \in C_c^{\mathbb{R}}(\mathbb{R}^d)$ with $f \geqslant 0$. A measure $\mu \in \mathcal{M}(\mathbb{R}^d)$ is called *positive* if for all $f \in C_c^+(\mathbb{R}^d)$ also $\mu(f) \geqslant 0$. The set of positive Radon measures will be denoted by $\mathcal{M}^+(\mathbb{R}^d)$. Each $\mu \in \mathcal{M}(\mathbb{R}^d)$ can be linked to a unique positive measure $|\mu|$, called the *total variation* or *absolute value* of μ and defined as

$$|\mu|(f) := \sup\left\{|\mu(g)| \,\middle|\, g \in C_c^{\mathbb{R}}(\mathbb{R}^d)\,,\ |g| \leqslant f\right\},$$

where $f \in C_c^+(\mathbb{R}^d)$. A measure in $\mathcal{M}(\mathbb{R}^d)$ is called *bounded* if $|\mu|(\mathbb{R}^d) < \infty$, and *unbounded* otherwise. We are going to extensively make use of the Dirac measures δ_x, where $\delta_x(f) := f(x)$, because sums of Dirac measures can be identified with point sets in $\mathbb{R}^d$.

We are especially interested in the following subsets of the Radon measures, because they have very nice topological properties:

Definition 1.1. Let $C > 0$ and also let V be a relatively compact open subset of $\mathbb{R}^d$. A measure $\mu \in \mathcal{M}(\mathbb{R}^d)$ is called (C, V)-*translation bounded* if for any $t \in \mathbb{R}^d$ we have

$$|\mu|(V + t) \leqslant C\,.$$

We denote the set of (C, V)-translation bounded measures by $\mathcal{M}_{C,V}(\mathbb{R}^d)$. A measure μ is called translation bounded, if any such C, V exist, which is equivalent to $\sup_{t\in\mathbb{R}^d} |\mu|(K + t) < \infty$ for any compact $K \subset \mathbb{R}^d$.

The set $\mathcal{M}_{C,V}(\mathbb{R}^d)$ is nice in the following sense:

Theorem 1.2. *Let C, V be as above. Then $\mathcal{M}_{C,V}(\mathbb{R}^d)$, equipped with the vague topology, is a compact metrizable Hausdorff space.*

Proof. A proof for arbitrary second countable locally compact Abelian groups can be found in [**10**]. □

Probably the most important measure in $\mathcal{M}(\mathbb{R}^d)$ is the Lebesgue measure λ^d. In Chapter 2, we also use $\mathrm{vol}(A)$ for $\lambda^d(A)$ for Borel sets A, because we do not want to confuse it with the Lebesgue measure λ on the complex weight set. Let $\mathscr{L}^1(\mathbb{R}^d)$ be the set of Lebesgue integrable functions on the Euclidean space $\mathbb{R}^d$.

As a consequence of the Lebesgue decomposition theorem (compare [**35**]), each measure $\mu \in \mathcal{M}(\mathbb{R}^d)$ can be uniquely decomposed with respect to the Lebesgue measure,

$$\mu = \mu_{\mathrm{ac}} + \mu_{\mathrm{pp}} + \mu_{\mathrm{sc}}\,,$$

where μ_{ac} is absolutely continuous with respect to λ^d, μ_{pp} is a pure point measure (concentrated on the countable set $\bigl\{x \in \mathbb{R}^d \,|\, \mu_{\mathrm{pp}}(\{x\}) > 0\bigr\}$) and μ_{sc} is singular continuous with respect to λ^d, i.e. μ_{sc} is a diffuse measure, concentrated on a Lebesgue 0-set. Not necessarily every part is present in such a decomposition. Indeed, one main goal of this thesis is to show the absence of the singular continuous part in a certain class of diffraction measures. If we use the terms absolutely/singular continuous without giving a reference measure we always mean this to be λ^d.

1.2.2. Fourier transform, diffraction and autocorrelation of Radon measures. A broad treatment of the Fourier transform on groups in general can be found in [**84**]. Further details with relevance to our point of view are given in [**23**] and in particular the Fourier transform of tempered distributions is considered in [**83**].

For functions $f \in \mathscr{L}^1(\mathbb{R}^d)$, we define the Fourier transform $\mathcal{F}(f) = \widehat{f}$ as the following uniformly continuous complex valued function (compare [**20**]): for $y \in \mathbb{R}^d$ let

$$\widehat{f}(y) := \int_{\mathbb{R}^d} f(x)\, \mathrm{e}^{-2\pi \mathrm{i}\, y\cdot x}\, \mathrm{d}\lambda^d(x)\,,$$

where $y \cdot x$ is the standard scalar product in $\mathbb{R}^d$. The inverse Fourier transform $\mathcal{F}^{-1}(f) = \check{f}$ of an integrable function f is given by

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

For *bounded* measures μ, the *Fourier-Stieltjes* transform $\widehat{\mu}$ is the analogously defined complex valued function

$$\widehat{\mu}(y) := \int_{\mathbb{R}^d} \mathrm{e}^{-2\pi \mathrm{i}\, y\cdot x}\, \mathrm{d}\mu(x)\,.$$

Let the inverse Fourier-Stieltjes transform of a measure be defined analogously and be denoted by $\check{\mu}$. The Fourier Stieltjes transform has the nice property that it is a uniformly continuous bounded function (see [**84**]).

For our considerations, it is necessary to extend the above definitions to certain *unbounded* measures and to interpret the Fourier transform of these again as a measure. In order to achieve that, we use the theory of tempered distributions. So let $\mathcal{S}(\mathbb{R}^d)$ be the set of rapidly decreasing or Schwartz-functions in $\mathbb{R}^d$ and $\mathcal{S}'(\mathbb{R}^d)$ be its dual, the set of tempered distributions (see e.g. [**83, 40**]). Since $\mathcal{S}(\mathbb{R}^d) \subseteq \mathscr{L}^1(\mathbb{R}^d)$ and the Fourier transform of a Schwartz-function is again in $\mathcal{S}(\mathbb{R}^d)$, the following definition for the Fourier transform $\mathcal{F}(T) = \widehat{T}$ of tempered distributions T is valid and defines again a distribution: for $\varphi \in \mathcal{S}(\mathbb{R}^d)$ let

$$\widehat{T}(\varphi) := T(\widehat{\varphi})\,.$$

The inverse Fourier transform $\mathcal{F}^{-1}(T) = \check{T}$ of a tempered distribution T again is defined and denoted similar to the $\mathscr{L}^1$-case, i.e.

$$\check{T}(\varphi) := T(\check{\varphi}) \, .$$

In case of function spaces where the Fourier transform defines a continuous bijection, e.g. $\mathcal{S}(\mathbb{R}^d)$ or $\mathrm{L}^2(\mathbb{R}^d)$, one has

$$\check{\hat{f}} = \hat{\check{f}} = f \, ,$$

see e.g. [**83**]. We then obviously also have for tempered distributions T

$$\hat{\check{T}} = \check{\hat{T}} = T \, .$$

Several unbounded measures in $\mathcal{M}(\mathbb{R}^d)$ also define tempered distributions and their Fourier transform is again a measure. We will call measures which are also tempered distributions *tempered measures*. Every translation bounded measure is tempered (see [**50**]). If the Fourier transform is again a measure, we refer to them as *Fourier transformable*. Prominent examples are given by the Lebesgue measure λ^d, with δ_0 as the Fourier transform, and δ_0 with λ^d as its Fourier transform (in this interpretation), compare [**85**].

If one identifies $\widehat{f}$ and $\widehat{\mu}$ as densities with respect to the Lebesgue measure, then the definitions coincide. In particular (by the obvious implication of the Radon-Nikodym Theorem [**21**, Satz 17.10]), in this respect the Fourier transform of a bounded measure or an integrable function is absolutely continuous with respect to the Lebesgue measure. We will later on need the following simple consequence:

Proposition 1.3. *Let $\Lambda \subset \mathbb{R}^d$ be countable, and let μ be the complex measure given by*

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

where $w(x) \in \mathbb{C}$ and $\sum_{x \in \Lambda} |w(x)| < \infty$. Then the Fourier transform of μ is absolutely continuous with respect to λ^d.

Proof. The condition $\sum_{x \in \Lambda} |w(x)| < \infty$ directly implies that μ is a bounded measure, so its Fourier transform is absolutely continuous. □

To model kinematic diffraction, we basically follow the mathematical formulation of Hof [**49, 50**]. The diffraction of a measure is thus given by the Fourier transform of its autocorrelation measure. For the definition of the latter we need some further well known concepts. If for two measures $\mu, \nu \in \mathcal{M}(\mathbb{R}^d)$ the object, given by

$$\mu * \nu(f) := \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} f(x+y) \, \mathrm{d}\mu(x) \, \mathrm{d}\nu(y) \, ,$$

where $f \in C_c(\mathbb{R}^d)$, is well defined[1] and again a measure, then this measure is called the *convolution* of μ and ν. This is for example the case if at least one of the measures is finite and the other one is translation bounded, compare [**23**, Prop. 1.13.]. Further, for $f \in C_c(\mathbb{R}^d)$ let $\widetilde{f}(z) := \overline{f(-z)}$ and for

[1] At least one of the integrals $\int_{\mathbb{R}^d} f(x+y) \, \mathrm{d}\mu(x)$ or $\int_{\mathbb{R}^d} f(x+y) \, \mathrm{d}\nu(y)$ needs to be integrable for all y or x, respectively

$\mu \in \mathcal{M}(\mathbb{R}^d)$ let $\widetilde{\mu}$ be the measure defined by $\widetilde{\mu}(f) := \overline{\mu\big(\widetilde{f}\big)}$. Let $\mu \in \mathcal{M}(\mathbb{R}^d)$ be an unbounded measure and μ_R be the (finite) restriction of μ to B_R. Consider the following well defined 'volume averages':

$$\gamma_R := \frac{\mu_R * \widetilde{\mu_R}}{\operatorname{vol}\big(B_R\big)} .$$

Every vague accumulation point of the family of measures $(\gamma_R)_{R\in\mathbb{R}}$ will be called an *autocorrelation measure* of μ. If there is only one accumulation point, we will call this vague limit $\gamma := \lim_{R\to\infty} \gamma_R$ the *natural autocorrelation* of μ. Note that the definition is only interesting for unbounded measures, because for finite measures the limit will always be the 0-measure. In the case of finite measures ρ, the convolution $\rho * \widetilde{\rho}$ plays the same role. It is known as the *Patterson function*. Other increasing families of averaging sets instead of centred balls may be chosen and are more appropriate for other models, e.g. cubes, compare [**50**]. In general, the limits depend on the form of those sets. For this reason other authors demand stronger forms of convergence for a *unique* autocorrelation, in particular for every van Hove sequence. In short, a *van Hove sequence* in $\mathbb{R}^d$ is an increasing family of relatively compact Borel sets in $\mathbb{R}^d$ which grows to $\mathbb{R}^d$ and has somehow a vanishing surface to volume ratio (for details see e.g. [**88**]). In Chapter 2, Section 2.3 we will give a condition for the existence and formulae for the calculation of the autocorrelation of certain weighted point sets.

Since, by construction (an easy application of the Bochner-Schwartz-Theorem, see [**40**]), each γ_R is a positive definite measure and the set of positive definite measures is a vaguely closed set (see [**23**, p. 18]), every possible natural autocorrelation γ is again positive definite. Thus it is Fourier transformable and its Fourier transform $\widehat{\gamma}$ is a positive measure. This measure is called the *diffraction (measure)* of μ. For details on why this measure is also physically a sensible description of diffraction experiments, we would like to refer the reader to [**49, 30**] or other books on diffraction physics. Constructs like the *first Born approximation*, *far-field approximation* of *kinematic diffraction* play important roles. Short and very readable descriptions can also be found in [**54, 97**].

1.3. Some notes on point processes

Concepts, definitions and most part of the notation is based on [**59**], so for further information and details we would like to refer the reader to this book or to [**31, 89**]. We just introduce the most important definitions, objects and results for point processes in $\mathbb{R}^d$.

Let E be a subset of $\mathbb{R}^d$ and $\mathcal{N}(E)$ be the set of counting measures in E, i.e. measures that only take non-negative integer values for all relatively compact sets. It is known that they have a representation

$$\mu = \sum_{x\in\operatorname{supp}\mu} n_x\, \delta_x ,$$

where $\operatorname{supp}\mu$ is a locally finite set in E and $n_x = \mu(\{x\}) \in \mathbb{N}$ for all $x \in \operatorname{supp}\mu$. If in addition $\mu(\{x\}) = 1$ for all $x \in \operatorname{supp}\mu$, the counting measures is called *simple*. We will denote the set of simple counting measures by $\mathcal{N}_1(E)$.

Let $\mathscr{B}_0(E)$ be the set of relatively compact Borel sets in E. We define $\mathscr{F}(E)$ to be the σ-algebra that is generated by the sets $\{\mu \in \mathcal{N}(E) \,|\, \mu(B) = n\}$, for all $B \in \mathscr{B}_0(E)$ and $n \in \mathbb{N}_0$, i.e. $\mathscr{F}(E)$ is the σ-algebra generated by the random variables $\zeta_B(\mu) := \mu(B)$. The set $\mathcal{N}(E)$ may also be viewed as a subset of the positive Radon measures $\mathcal{M}^+(E)$ in E. The vague topology on $\mathcal{M}^+(E)$ restricted to $\mathcal{N}(E)$ is known to also generate $\mathscr{F}(E)$ as corresponding Borel sets (see [**76, 55**]). Probability measures on $(\mathcal{N}(E), \mathscr{F}(E))$ are called *point processes* in E; in case they are concentrated on $\mathcal{N}_1(E)$ they are called *simple*.

In case P is a simple point process in $E = X \times M$, where $X \subseteq \mathbb{R}^n$ and $M \subseteq \mathbb{R}^m$, $n+m = d$, such that $\{x \in X \,|\, \exists m \in M : (x,m) \in \operatorname{supp} \mu\}$ is locally finite in X for P-almost all μ, we speak of *marked* point processes. They can be imagined as random point sets in X with marks in M, the realisations may again be written as

$$\mu = \sum_{(x,m) \in \operatorname{supp} \mu} \delta_{(x,m)} \,.$$

Because the support of μ is locally finite, the points of the support are countable and may be expressed as a sequence of random pairs of locations and marks $\big((x_i(\mu), m_i(\mu))\big)_{i \in \mathbb{N}}$, where the counting is done in a unique measurable way. We say the marked point process has *independent mark distribution*, if the random elements m_i are independent and identically distributed and independent of the random elements x_i. For details see [**89**].

A point process is said to have *independent increments*, if for disjoint $A_1, A_2 \in \mathscr{B}_0(E)$ the random variables ζ_{A_1} and ζ_{A_2} are independent. A point process P is called *stationary* or *translation invariant*, if for any $B \in \mathscr{B}_0(E)$ and any $t \in E$ the random variables ζ_B and ζ_{B+t} have the same distribution, i.e. if the image of P under the translation T_t is again P. The most prominent and best understood simple point process is the *stationary Poisson point process* P_κ in $\mathbb{R}^d$ with intensity $\kappa > 0$. It is characterised as being the only stationary point process with independent increments such that the random variables ζ_B, $B \in \mathscr{B}_0(\mathbb{R}^d)$, are distributed as follows:

$$P_\kappa\big(\{\zeta_B = n\}\big) = \frac{\big(\kappa \lambda^d(B)\big)^n}{n!} \exp\big(-\kappa \lambda^d(B)\big) \,,$$

for $n \in \mathbb{N}_0$, compare [**59**]. Here we abbreviated $\{\mu \in \mathcal{N}(\mathbb{R}^d) \,|\, \zeta_B(\mu) = n\}$ by $\{\zeta_B = n\}$ and use $\{\zeta_B \leqslant n\}$, etc. similarly.

Consider the following subclass of $\mathscr{F}(E)$:

$$\mathscr{I}(E) := \{F \in \mathscr{F}(E) \,|\, F + t = F \,\forall t \in E\} \,,$$

the set of translation invariant events, where $F + t := \{T_t(\mu) \,|\, \mu \in F\}$. The set $\mathscr{I}(E)$ is obviously again a σ-algebra. If for a stationary point process P either $P(F) = 0$ or $P(F) = 1$ for all $F \in \mathscr{I}(E)$, it is called *ergodic*. The Poisson point process is also an example for an ergodic point process [**89**].

Let us finally note that *random measures* in $\mathbb{R}^d$ are defined similarly to point processes. One has just to make one little modification: instead of the space $\mathcal{N}(E)$ one takes the set of locally finite measures in $\mathbb{R}^d$. The mappings ζ_B can be extended naturally to this space.

CHAPTER 2

Gibbs measures on weighted FLC sets and the absence of singular continuous diffraction

The diffraction properties of sets of finite local complexity (FLC sets), especially of regular model sets, have been widely explored [**12, 50, 69, 74, 87, 88, 93**]. There are also several results for randomly weighted lattices [**16, 17, 51**] or situations where a Gibbs measure or simpler random mechanisms are responsible for random displacements of the points [**11, 63, 64**]. A large class of the models for diffraction of structures close to crystals have an absolutely continuous part in the spectrum. This diffuse scattering is most of the time connected to random components. Those models nevertheless do only occasionally lead to diffraction spectra with singular continuous parts, which is also not too far from experimental experience in crystallography [**30, 48, 96**].

Our model puts random weights to the sites of an FLC set, which might be interpreted as different atoms/molecules, or as a variation of their effective scattering strength.

In case the weighting process is independently done, Baake and Zint [**17, 97**] show that, at least for finite complex weight-sets, the absence of the singular continuous part remains.

In case the weights are chosen dependently from a finite weight-set, according to some Gibbs measure at high temperatures, joint work with Zint shows that this property still holds.

The main goal of this chapter is to extend the result to a compact complex weight-set. On the way, we will also need to define a suitable class of Gibbs measures. The ergodicity of the latter, together with the known diffraction properties of dynamical systems with pure point dynamical spectrum (compare e.g. [**10, 11, 12, 69, 88**]) allow us to achieve our aim.

Several elementary topological concepts are used, all of which might be found in the standard literature, such as [**82, 27, 28**].

2.1. Weighted FLC sets and the corresponding dynamical system

In this section, we introduce the measurable spaces for the later theory. As mentioned above, the objects of interest are given by certain sets with attached complex weights out of a compact set.

Firstly, we need to clarify properties such as FLC and appropriate topological structures for point sets. For a more extensive and broader discussion with complete proofs, we would like to refer the reader to the articles of Solomyak [**93**], Schlottmann [**88**], Baake and Lenz [**10**] and Lenz [**69**]. These articles also introduce the necessary tools from the theory of dynamical systems, which we again only briefly introduce. Whereas the concepts remain

valid for much more general situations, we restrict ourselves to the case we need, where the point sets lie in Euclidean space $\mathbb{R}^d$.

Then, we need to adapt the concepts and structures to weighted sets.

2.1.1. Some concepts for discrete point sets. For completeness, we give short definitions of well-known concepts for point sets.

Definition 2.1. A subset D of $\mathbb{R}^d$ is called

(i) *locally finite*, if every compact set intersects D only in a finite subset,
(ii) *discrete*, if every point x from D has a neighbourhood U such that $U \cap D = \{x\}$,
(iii) *uniformly discrete*, if there exists some $r > 0$, such that any open ball of radius r contains at most one point from D,
(iv) *relatively dense*, if there exists some $R > 0$ such that every open ball of radius R contains at least one point from D,
(v) a *Delone set*, if it is uniformly discrete and relatively dense.

We will denote the set of closed discrete subsets of $\mathbb{R}^d$ by $\mathscr{D}(\mathbb{R}^d)$.

There are several equivalent definitions for the notion of finite local complexity, but the most intuitive one is given via patches. Let $D \in \mathscr{D}(\mathbb{R}^d)$. A *patch* P of size $S > 0$ around $x \in D$ is given by

$$P = (D - x) \cap B_S \,.$$

Proposition 2.2. *Let D be a Delone set. The following statements are equivalent:*

(i) *For any $S > 0$ we have*

$$\#\{(D - x) \cap B_S \,|\, x \in D\} < \infty \,,$$

i.e. there are only finitely many different patches of size S in D (up to translation).
(ii) *The set $D - D$ is discrete and closed.*
(iii) *The set $D - D$ is locally finite.*

For a proof see [**65**]. □

If a Delone set has one of the above properties we will call it a set of *finite local complexity* or an *FLC* set for short. FLC sets have one more important characterising property related to point dynamical systems. Before we discuss it, let us take a brief look at our basic class of examples for FLC sets, namely regular model sets:

Definition 2.3. Consider the following diagram of mappings:

$$\begin{array}{ccccc} \mathbb{R}^d & \xleftarrow{p_{\mathrm{phys}}} & \mathbb{R}^d \times G & \xrightarrow{p_{\mathrm{int}}} & G \\ \cup & & \cup & & \cup \\ p_{\mathrm{phys}}(L) & \xleftarrow{p_{\mathrm{phys}}|_L} & L & \xrightarrow{p_{\mathrm{int}}|_L} & p_{\mathrm{int}}(L) \end{array}$$

Here G is a locally compact Abelian group, p_{phys} and p_{int} are the canonical projections from the *embedding space* $\mathbb{R}^d \times G$ to the *physical space* $\mathbb{R}^d$, respectively to the *internal space* G. Also let L be a lattice in $\mathbb{R}^d \times G$, i.e. a discrete subgroup such that the quotient $(\mathbb{R}^d \times G)/L$ is compact. We assume

that $p_{\mathrm{phys}}|_L$ is injective and that $p_{\mathrm{int}}(L)$ is dense in G. Such a diagram is then called a *cut and project scheme*.

Now consider an arbitrary $W \subset G$ and define

$$\Lambda(W) := \{p_{\mathrm{phys}}(x) \,|\, x \in L,\, p_{\mathrm{int}}(x) \in W\} \subset \mathbb{R}^d\,.$$

The set is called a *model set* if W is non-empty, compact and $W = \overline{W^o}$. In this context, W is called the *window*. A model set is called *regular* if ∂W has Haar measure 0.

Model sets might be viewed as natural extensions of lattices. Indeed, there are similarities when it comes to their diffractive nature, at least for regular model sets.

Remark 2.4. Every regular model set is an FLC set [**74**].

For a broad treatment of model sets see [**74**]. There are some prominent examples for regular model sets:

Example 2.5. (i) A 1-dimensional model set: The silver mean chain (Figure 1 illustrates its construction) is a regular model set [**7, 11**].

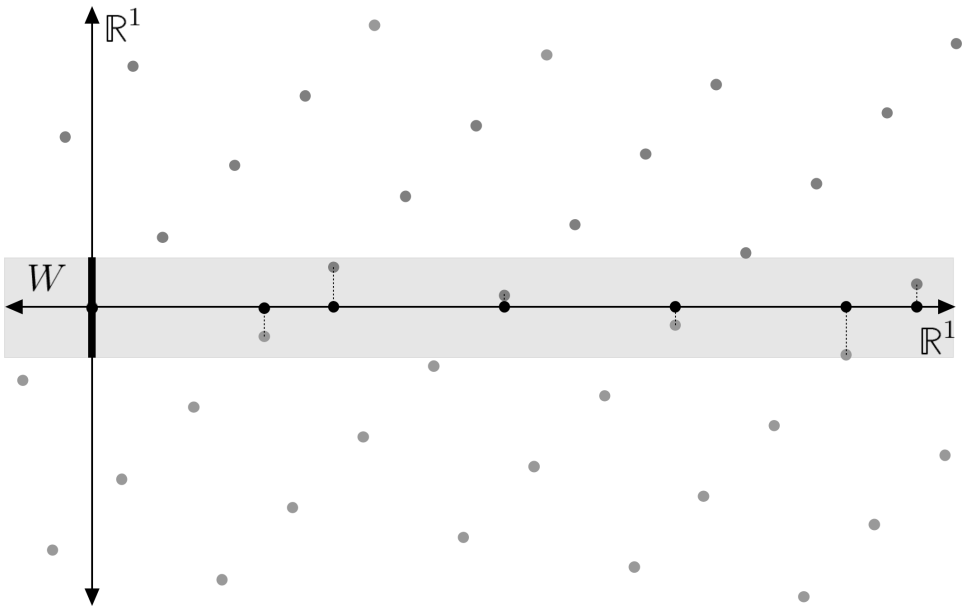


FIGURE 1. The silver mean chain is a model set in $\mathbb{R} \times \mathbb{R}$, where $L = \{(u+v\sqrt{2},\, u-v\sqrt{2}) \,|\, u, v \in \mathbb{Z}\}$ and $W = \left[\frac{-1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right]$

(ii) A 2-dimensional model set: The vertex-set of the Penrose rhombus tiling (Figure 2 and its diffraction in Figure 3) is known to be a regular model set, see e.g. [**33, 34, 9, 14**]. Since it is built from rotations and shifts from two different rhombuses, its Delone property is obvious. That it is an FLC set follows from the observation that there are only finitely many prototiles (up to translation) and, for any given patch size, only finitely many ways to put the rhombuses together.

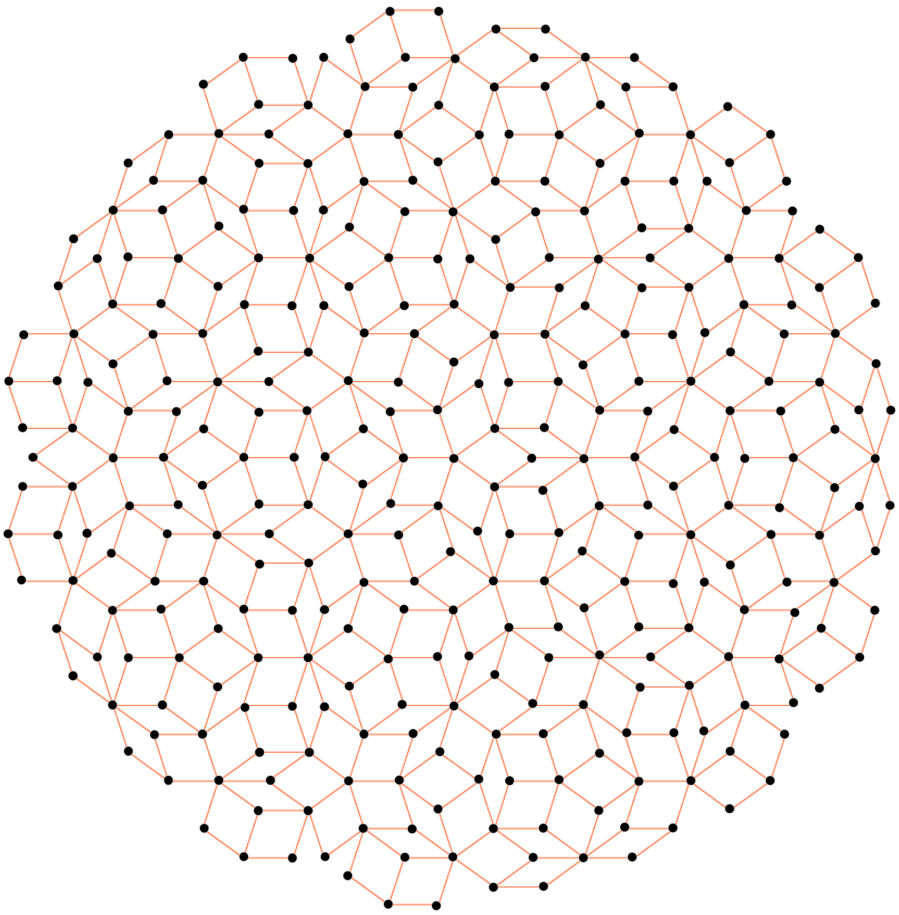


FIGURE 2. A regular model set: the vertex-set of the Penrose rhombus tiling, a central patch. This figure is a modified version of a picture in [**4**]

2.1.2. Two topologies on the closed discrete sets of $\mathbb{R}^d$. Both the so-called local topology (LT) and the local rubber topology (LRT) are topologies on the set $\mathscr{D}(\mathbb{R}^d)$ of closed and discrete subsets of $\mathbb{R}^d$. (They can also be considered as topologies on the closed sets of $\mathbb{R}^d$, see [**10**].) We will give bases of open neighbourhoods (derived from certain uniformities, for details see [**88**] and [**10**]) to define them. So for a compact $K \subset \mathbb{R}^d$, an open neighbourhood V of $0 \in \mathbb{R}^d$ and a closed discrete set D let

$$U_{K,V}(D) := \{D' \in \mathscr{D}(\mathbb{R}^d) \,|\, \exists\, t \in V : D \cap K = (D' + t) \cap K\}\,,$$

and

$$U^R_{K,V}(D) := \{D' \in \mathscr{D}(\mathbb{R}^d) \,|\, D \cap K \subset D' + V \text{ and } D' \cap K \subset D + V\}\,.$$

See [**88**] for a proof that those sets $U_{K,V}(D)$ form a valid base of neighbourhoods for a topology on $\mathscr{D}$, the *local topology*. The sets $U^R_{K,V}(D)$ form the neighbourhood base for the *local rubber topology*, see [**10**]. Both topologies make a complete Hausdorff space out of $\mathscr{D}$ (see [**10, 88**]). Because the corresponding uniformities have countable bases they are also metrizable

(compare [**88, 10**]) by [**57**, Metrization Theorem, p. 186]. For Delone sets, such a metric for the LT can be found e.g. in [**93**].

To make the two topologies transparent, one can picture two sets close in the local topology if, after a small shift, they agree in a large ball. In the local rubber topology they are close if, after a small shift, they *almost* agree in a large ball. We need the the LRT to describe the topology on the weighted point sets (viewed as subsets of $\mathbb{R}^d \times \mathbb{C}$), whereas we will use the local topology for the underlying structure. One can easily see that the LRT is coarser than the LT but there is an important connection that is given in [**10**, Prop. 5]:

Proposition 2.6. *Let Ω be a subset of $\mathscr{D}(\mathbb{R}^d)$. If Ω is compact in the LT then it is compact in LRT and the topologies agree on Ω.* □

2.1.3. Dynamical systems of FLC sets. Consider the translation $T_t : D \mapsto D + t$. It is easy to check that $T = (T_t)_{t\in\mathbb{R}^d}$ defines a continuous action of $\mathbb{R}^d$ on $\mathscr{D}(\mathbb{R}^d)$ in both LT and LRT.

We can now state the above mentioned characterisation of the FLC sets:

Proposition 2.7. *A set $\Gamma \in \mathscr{D}(\mathbb{R}^d)$ is FLC, if and only if the orbit $\{\Gamma + t \,|\, t \in \mathbb{R}^d\}$ is precompact in the local topology. See* [**88**, Prop. 2.2] *for a proof.* □

Thus the set

$$\mathbb{X} := \mathbb{X}(\Gamma) := \overline{\{\Gamma + t \,|\, t \in \mathbb{R}^d\}}^{\mathrm{LT}},$$

the closure of the orbit of the FLC set Γ in the LT, is a compact Hausdorff space, and due to Prop. 2.6 the topology on $\mathbb{X}$ is the same as given by the LRT. If $\mathscr{B} = \mathscr{B}(\Gamma)$ is the σ-algebra of the corresponding Borel sets, then $(\mathbb{X}, \mathscr{B}, T)$ is a topological dynamical system.

The sets in $\mathbb{X}$ may be interpreted as measures by the following map:

$$\begin{aligned} \delta : \quad \mathbb{X} &\longrightarrow \mathcal{M}(\mathbb{R}^d)\,, \\ \Lambda &\longmapsto \delta_\Lambda := \sum_{x\in\Lambda} \delta_x\,. \end{aligned}$$

If we consider the topological dynamical system given by the set

$$\mathbb{X}^\delta := \{\delta_\Lambda \,|\, \Lambda \in \mathbb{X}\}\,,$$

equipped with the vague topology and the translation T on $\mathcal{M}(\mathbb{R}^d)$, then the two dynamical systems $(\mathbb{X}, T)$ and $(\mathbb{X}^\delta, T)$ are topological conjugates by [**10**, Theorem 4]. Justified by this relation, we also interpret a probability measure on $\mathbb{X}$ as a point process.

Obviously, a sequence $(\Lambda_n)_{n\in\mathbb{N}}$ in $\mathbb{X}$ converges to some $\Lambda \in \mathbb{X}$ if and only if there exist sequences $(r_n)_{n\in\mathbb{N}}$ and $(t_n)_{n\in\mathbb{N}}$ with $r_n > 0$, $r_n \to \infty$ for $n \to \infty$ and $t_n \in \mathbb{R}^d$, $\|t_n\| \to 0$ for $n \to \infty$, such that $\Lambda_n - t_n \cap B_{r_n} = \Lambda \cap B_{r_n}$.

Remark 2.8. Because by the structure of the LT each element Λ in $\mathbb{X}(\Gamma)$ is 'built from patches of Γ', also the difference sets obey $\Lambda - \Lambda \subseteq \Gamma - \Gamma$. Thus, also every element of $\mathbb{X}$ is again an FLC set.

This kind of structure is of special interest to diffraction theory: if the dynamical system $(\mathbb{X}(\Gamma), \mathscr{B}(\Gamma), T)$ of an FLC set Γ is uniquely ergodic[1], the autocorrelation of the system $\mathbb{X}(\Gamma)$ is known to exist [**88**].

2.1.4. Weighted FLC sets. The idea to the next construction is that dynamical and diffractive properties of a system $\mathbb{X}(\Gamma)$ of FLC sets are basically preserved, or only slightly disturbed, if one (randomly) adds weights from a compact complex set to the points under certain rules. To stick to that idea, we start by attaching weights to the sets of $\mathbb{X}$ in a very natural way: let W be a compact subset of $\mathbb{C}$ and put

$$\mathbb{Y} := \mathbb{Y}(\Gamma, W) := \dot{\bigcup_{\Lambda \in \mathbb{X}(\Gamma)}} W^{\Lambda} .$$

Thus, elements of $\mathbb{Y}$ are of the form $\omega = (\omega_x)_{x\in\Lambda}$, where $\Lambda \in \mathbb{X}$ and $\omega_x \in W$ for all $x \in \Lambda$. If we identify $\mathbb{C}$ with $\mathbb{R}^2$ and $\omega \in \mathbb{Y}$ with $\{(x, \omega_x) \,|\, x \in \Lambda\} \subset \mathbb{R}^d \times \mathbb{C}$ then we can interpret $\mathbb{Y}$ as a subspace of $\mathscr{D}(\mathbb{R}^d \times \mathbb{R}^2)$ and we can apply the concept of the LRT to it, which makes it a metrizable space. For convenience we will use the same notation for the neighbourhoods in the subspace-topology.

Proposition 2.9. *Let $\omega \in \mathbb{Y}$. Then the sets*

$$U^R_{K\times W, V\times V'}[\omega] ,$$

where $K \in \mathscr{K}(\mathbb{R}^d)$, $V \subset \mathbb{R}^d$ is an open neighbourhood of $0 \in \mathbb{R}^d$, and V' an open neighbourhood of $0 \in \mathbb{R}^2$, form a neighbourhood base for ω.

Proof. Since the sets $U^R_{\widetilde{K},\widetilde{V}}[\omega]$ get smaller for growing $\widetilde{K} \in \mathscr{K}(\mathbb{R}^d \times \mathbb{R}^2)$ and shrinking $\widetilde{V} \subset \mathbb{R}^d \times \mathbb{R}^2$, the proof is trivial. □

Consider the natural surjection

$$\begin{array}{rccc} \mathrm{supp}: & \mathbb{Y} & \longrightarrow & \mathbb{X} \\ & \omega = (\omega_x)_{x\in\Lambda} & \longmapsto & \underline{\omega} = \Lambda . \end{array}$$

We will call $\underline{\omega}$ *the support of* ω.

Proposition 2.10. *The mapping* supp *is a continuous surjection from the set $(\mathbb{Y}, LRT)$ to the set $(\mathbb{X}, LT)$.*

Proof. Let $(\omega^n)_{n\in\mathbb{N}}$ be a sequence in $\mathbb{Y}$ such that $\omega^n \to \omega \in \mathbb{Y}$ for $n \to \infty$. We have to show that for any neighbourhood $U_{K,V}[\underline{\omega}]$ there exists $N \in \mathbb{N}$ such that for all $n > N$ we have $\underline{\omega^n} \in U_{K,V}[\underline{\omega}]$. Due to the convergence of the ω^n, we know that there exists $N \in \mathbb{N}$ such that $\omega^n \in U^R_{K\times W, V\times V'}[\omega]$ for $n > N$ and any open neighbourhood V' of $0 \in \mathbb{R}^2$. If $\omega^n \in U^R_{K\times W, V\times V'}[\omega]$ then also $\underline{\omega^n} \in U_{K,V}[\underline{\omega}]$. □

[1] A dynamical system $(\Omega, \mathscr{A}, T)$ is called *uniquely ergodic*, if there exists exactly one invariant probability measure μ on $(\Omega, \mathscr{A})$ which is trivial on the T-invariant elements in $\mathscr{A}$.

This continuity property implies that, for a converging sequence in $\mathbb{Y}$, also the sequence of the corresponding supports converges in the LT. In other words: if a sequence $(\omega^n)_{n\in\mathbb{N}}$ in $\mathbb{Y}$ converges to some element ω in $\mathbb{Y}$ then after a small shift in $\mathbb{X}$, the supports $\underline{\omega^n}$ agree in growing balls for growing n.

Proposition 2.11. *$\mathbb{Y}$ is compact in the LRT.*

Proof. We show that any sequence in $\mathbb{Y}$ contains a converging subsequence.

Let $(\omega^n)_{n\in\mathbb{N}}$ be such a sequence. Because $\mathbb{X}$ is compact, we know that $(\underline{\omega^n})_{n\in\mathbb{N}}$ contains a convergent subsequence. So without loss of generality let us assume that already $\underline{\omega^n} \to \Lambda \in \mathbb{X}$ for $n \to \infty$. Of course every FLC set is countable. So let $\Lambda = \{x_1, x_2, \ldots\}$ and $(t(n))_{n\in\mathbb{N}}$, $(r(n))_{n\in\mathbb{N}}$ some sequences in $\mathbb{R}^d$ and $\mathbb{R}^+$ respectively such that $\|t(n)\| \to 0$, $|r(n)| \to \infty$ and $(\underline{\omega^n} - t(n)) \cap B_{r(n)} = \Lambda \cap B_{r(n)}$. Now let $n \in \mathbb{N}$ be large enough, such that $x_1 \in B_{r(n)}$ and for all larger indices. Thus also $x_1 + t(n) \in \underline{\omega^n}$. So we have a sequence $\left(\omega^n_{x_1+t(n)}\right)_n$ in the compact set W, which thus contains a converging subsequence $\left(\omega^{n_{1,k}}_{x_1+t(n_{1,k})}\right)_k$. For x_2 the same arguments can be applied to the sequence of the weights $\left(\omega^{n_{1,k}}_{x_2+t(n_{1,k})}\right)_k$ to extract a converging subsequence $\left(\omega^{n_{2,k}}_{x_2+t(n_{2,k})}\right)_k$. Inductively, we get converging sequences $\left(\omega^{n_{j,k}}_{x_j+t(n_{j,k})}\right)_k$. The diagonal sequence $\left(\omega^{n_{k,k}}\right)_k$ then obviously converges in the LRT. □

On $\mathbb{Y}$ we chose the $\mathbb{R}^d$ action induced by the one on $\mathbb{X}$: For $t \in \mathbb{R}^d$ let $T_t(\omega) = \omega + t$ be the weighted set obtained by shifting the support and keeping the weights, i.e. $(\omega + t)_x := \omega_{x-t}$. We will also denote this action by T. This action again makes $(\mathbb{Y}, T)$ a topological dynamical system. The next sections deal with the task of providing $(\mathbb{Y}, T)$ with an ergodic measure that is adapted to some potential ruling the weights.

2.2. Construction of appropriate Gibbs measures

The concept to describe equilibrium states of interacting particles in statistical mechanics by objects arising from conditional expectations was introduced in the late 1960's by Dobrushin, Lanford and Ruelle [**36, 37, 38, 39, 67, 86**]). Those objects are the so-called *Gibbs measures*.

Our point of view on Gibbs measures is mainly based on the books of Preston [**81**] and Georgii [**44**]. While we use the tools provided in [**44**] to examine the properties of the Gibbs measures on one FLC set, we need the more abstract definitions and results given in [**81**] to extend the results to the complete dynamical system generated by an FLC set.

2.2.1. Basic definitions. The definitions given here follow [**81**]. They are very general and are not restricted to situations where the state space is a lattice or countable. Let $(\Omega, \mathscr{A})$ be a measurable space and $\mathscr{P}(\Omega)$ the set of probability measures on $(\Omega, \mathscr{A})$. We further need a partially ordered index set. Although the theory allows much more general partially ordered sets, we directly choose this to be $\mathscr{K}$, the set of compact subsets of $\mathbb{R}^d$. The index can than later be identified with information about a structure inside or outside those sets.

We further need a family of sub-σ-algebras $(\mathscr{A}_K)_{K\in\mathscr{K}}$ such that $\mathscr{A}_{K_2} \subseteq \mathscr{A}_{K_1} \subseteq \mathscr{A}$, whenever $K_1 \subseteq K_2$. They represent the events "happening outside" of the compact sets.

The next objects give the probabilities of all events, constrained to have a fixed configuration outside its index:

Definition 2.12. A family of mappings $\pi = (\pi_K)_{K\in\mathscr{K}}$,

$$\begin{aligned} \pi_K : \quad \mathscr{A} \times \Omega \quad &\longrightarrow \quad \mathbb{R}_0^+ , \\ (A,\omega) \quad &\longmapsto \quad \pi_K(A \,|\, \omega) , \end{aligned}$$

is called a *specification*, if it has the following properties:

- (S_1) $\pi_K(\,\cdot\,|\,\omega) \in \mathscr{P}(\Omega)$ for all $\omega \in \Omega$;
- (S_2) $\pi_K(A \,|\,\cdot\,)$ is $\mathscr{A}_K$ measurable for all $K \in \mathscr{K}$, $A \in \mathscr{A}$;
- (S_3) $\pi_K(A \,|\,\cdot\,) = 1_A(\,\cdot\,)$ for all $K \in \mathscr{K}$, $A \in \mathscr{A}_K$ and
- (S_4) if $K_2 \subseteq K_1$ then $\pi_{K_1} = \pi_{K_1} \circ \pi_{K_2}$, where $\pi_{K_1} \circ \pi_{K_2}$ denotes the composition of the two kernels π_{K_1} and π_{K_2}, defined as

$$\pi_{K_1} \circ \pi_{K_2}(A \,|\, \omega) := \int_\Omega \pi_{K_2}(A \,|\, \widetilde{\omega}) \, \mathrm{d}\pi_{K_1}(\,\cdot\,|\,\omega)(\widetilde{\omega}) .$$

This property can be interpreted as a consistency check if the kernels for larger indices extend the information given by kernels for smaller indices in the right way.

In this sense the specification π *specifies* what a particle configuration may look like inside of K, if the outside looks like ω. This information might be enough to describe the whole behaviour of the system, but in general it is not. The concept is stated precisely by the following definition.

Definition 2.13. A *Gibbs measure* μ is a measure that can locally be described by the specifications, that is, given a set A from $\mathscr{A}_K$, then one representative of the conditional expectation of μ of 1_A given $\mathscr{A}_K$ is $\pi_K(\,\cdot\,, A)$. The set of Gibbs measures with respect to π is thus given by

$$\mathscr{G}(\pi) := \Big\{ \mu \in \mathscr{P}(\Omega) \,\Big|\, \mathbb{E}_\mu(1_A|\mathscr{A}_K) = \pi_K(A \,|\,\cdot\,) , \\ \mu\text{-almost surely for all } A \in \mathscr{A} \text{ and } K \in \mathscr{K} \Big\}$$

The set $\mathscr{G}(\pi)$ is a convex subset of $\mathscr{P}(\Omega)$ and its extremal points are referred to as pure phases. A well known example is the *2-dimensional Ising model*, a model where a nearest neighbourhood potential on $\mathbb{Z}^2$ describes the probabilities of having a negatively or positively charged particle at the positions on the lattice. In case of low temperatures, the set of Gibbs measures for this model is known to be spanned by 2 pure phases (compare e.g. [**44**]).

A definition equivalent to Def. 2.13, which is more practical for our calculations, is given by the so called DLR-equations (in honour of Dobrushin, Lanford and Ruelle): A probability μ on $(\Omega, \mathscr{A})$ is a Gibbs measure specified by π, if and only if, for all $A \in \mathscr{A}$ and $K \in \mathscr{K}$,

$$\mu(A) = \int_\Omega \pi_K(A \,|\, \omega) \, \mathrm{d}\mu(\omega) . \tag{DLR}$$

A proof for this equivalence can be found in [**81**]. The equation might be interpreted as follows: The Gibbs measures are the only measures which predict themselves even if only information outside a compact region is given.

In case a group of bijections is acting on Ω, one can also be interested in those Gibbs measures which are invariant under the group action. If the group is fixed in this context, we simply denote the set of invariant Gibbs measures by $\mathscr{G}_0(\pi)$.

We will concentrate on situations where $\mathscr{G}(\pi)$ or $\mathscr{G}_0(\pi)$ consists of only one element, because then this one element has special properties. Let us state the most important one for our later observations (see [**81**, Theorem 4.1]):

Theorem 2.14. *Let G be a separable group that acts on Ω via $(T_\alpha)_{\alpha\in G}$. If there exists a sequence $(\mathscr{F}_n)_{n\in\mathbb{N}}$ of sub-σ-algebras of $\mathscr{A}$ such that $\mathscr{A}$ is the smallest σ-algebra containing $\bigcup_{n\in\mathbb{N}}\mathscr{F}_n$, and such that for any $n\in\mathbb{N}$, $K\in\mathscr{K}$ there exists some $\alpha\in G$ such that $T_\alpha(\mathscr{F}_n)\subseteq\mathscr{A}_K$. Then for $\mu\in\mathscr{G}_0(\pi)$*

$$\mu \text{ is extremal} \iff \mu \text{ is ergodic.}$$

□

2.2.2. Gibbs measures on single FLC sets. A wide branch of statistical mechanics deals with interacting particles on a lattice. Thus, some of the first, maybe even the original ways to construct specifications are adapted to this model. Georgii [**44**] extends this model from a lattice to countable sets, such as one of our FLC sets.

In this section we will prepare a situation where the corresponding Gibbs measure is unique. Thus we need to introduce some restrictions to the potentials defining the interaction. On the one hand, the uniqueness ensures that we may interpret the Gibbs measure as a thermodynamic limit of the specifications with free boundary conditions. This will give the opportunity to compute certain diffraction properties. On the other hand, the uniqueness also prepares the ground to construct a unique translation invariant Gibbs measure on the dynamical system $\mathbb{Y}$ in the next section.

We are going to stick to the ideas presented in [**44**] for definitions and paths to uniqueness results.

Our longer term strategy is to construct unique measures on each of the disjoint components of $\mathbb{Y}$, namely W^Λ, $\Lambda\in\mathbb{X}$. But for now let Λ be some arbitrary FLC set in $\mathbb{R}^d$. We fix the state-space to be W^Λ. For a proper definition of a σ-algebra on that space we start with one on W. Let us equip W with the trace $\mathscr{W}$ of the standard Borel σ-algebra in $\mathbb{C}$. Any finite dimensional product of W has the usual product σ-algebra. Now we can use the canonical projections $p_{\Lambda\cap K}: W^\Lambda\to W^{\Lambda\cap K}$ to define all the σ-algebras needed.

Let $\mathscr{F}(\Lambda)$ be the σ-algebra that is generated by all the projections $p_{K\cap\Lambda}$, $K\in\mathscr{K}$. The projections also give a justification to the previously mentioned perspective on the needed σ-algebras as the events happening inside or outside a compact K: Let $\mathscr{F}_K(\Lambda)$ be the σ-algebra which is generated only by the projections $p_{\Lambda\cap K'}$, where $K'\subset K$. They present the events happening inside of K. The σ-algebra for the events outside of K, $\mathscr{T}_K(\Lambda)$ is thus given by the projections to compact sets that do not intersect with

K, i.e. $\mathscr{T}_K(\Lambda) = \mathscr{F}_{K^\complement}(\Lambda)$. The latter ones are the indexed family that we need to construct the specifications. We will make use of the abbreviation $p_{\Lambda\cap K}(\omega) =: \omega_K$ (even if K is not compact). In that notation, we have $\omega_{\{x\}} = \omega_x$.

Let $\mathcal{S}(\Lambda)$ be the set of finite subsets of Λ, thus a subset of $\mathscr{K}$. For us, a *potential* on W^Λ is a family $\Phi = (\Phi_S)_{S\in\mathcal{S}(\Lambda)}$ of mappings from W^Λ into $\mathbb{R}$. We interpret $\Phi_S(\omega)$ to be the interaction energy of the particles in S. Not every such family of mappings leads to a specification. The next steps take care to stay on the path given in [**44**].

We restrict ourselves to *pair interactions of short range*: let

$$\Phi_S(\omega) := \begin{cases} \beta\,\phi(\omega_x,\omega_y)\,J(x-y), & \text{if } S=\{x,y\}\,;\\ 0, & \text{otherwise}\,; \end{cases}$$

where $\beta > 0$, $\phi : W \times W \to \mathbb{R}$ and $J : \mathbb{R}^d \to \mathbb{R}$ are measurable mappings and symmetric under the exchange of x and y, i.e. $\phi(c_1,c_2) = \phi(c_2,c_1)$ for all $c_1, c_2 \in W$ and $J(z) = J(-z)$ for all $z \in \mathbb{R}^d$. We also assume ϕ to be continuous, so that $\phi(W \times W)$ is bounded and $|\phi(\omega_x,\omega_y)|$ takes a maximal value m_ϕ in $W \times W$. In this context, the parameter β is called the *inverse temperature*. We will later on adjust the temperature to apply a uniqueness theorem. With this definition, we chose to set $\phi_{\{x\}}(\omega) = 0$, for all $x \in \Lambda$ and $\omega \in W^\Lambda$, because such a self-interaction can be interpreted as an external potential, which we want to exclude. Therefore, we can assume $J(0) = 0$. The notion 'short range' comes in via the behaviour of J, which decays quickly enough for large distances $\|x - y\|$, i.e. we assume J to be either *algebraically* or *exponentially decaying*, that is, there exist some positive constants p, t such that $|J(z)| = \mathcal{O}(\|z\|^{-p})$ respectively $|J(z)| = \mathcal{O}\big(\exp(-t\|z\|)\big)$ for $\|z\| \to \infty$. The constants t and p are called the *order* of the respective decay. Exponential decay implies algebraic decay of any order and we shall concentrate on the latter. We note that this definition of the potential can and will be extended from $\omega \in W^\Lambda$ to $\omega \in \mathbb{Y}$ and arbitrary $x, y \in \mathbb{R}^d$ if we set $\Phi_{\{x,y\}} = 0$ for $\{x,y\} \nsubseteq \underline{\omega}$.

By means of the potential, we can now define the *local energy* of a configuration $\omega \in W^\Lambda$ in the compact set $K \subset \mathbb{R}^d$:

$$\mathcal{H}_K(\omega) := \sum_{\{x,y\}\subset\Lambda:\,\{x,y\}\cap K\neq\varnothing} \Phi_{\{x,y\}}(\omega) = \sum_{x\in\Lambda\cap K,\,y\in\Lambda} \beta\,\phi(\omega_x,\omega_y)\,J(x-y)\,.$$

For the intended definition of the specifications, we need all local energies to be finite. A first step in that direction is the following proposition.

Proposition 2.15. *Let Γ be an FLC set in $\mathbb{R}^d$. Suppose $|J(z)| = \mathcal{O}(\|z\|^{-p})$ for $\|z\| \to \infty$, where $p > d+1$. Then for $1 < \tilde{p} \leqslant p-d$ we have for all $x \in \Gamma$*

$$\sum_{y\in\Lambda} \|x-y\|^{\tilde{p}}\,|J(x-y)| < \infty\,.$$

More specifically, there exists some $c_\Gamma > 0$ such that for all $\Lambda \in \mathbb{X}(\Gamma)$ and $x \in \Lambda$

$$\sum_{y\in\Lambda} \|x-y\|^{\tilde{p}}\,|J(x-y)| < c_\Gamma\,. \tag{2.1}$$

PROOF. For this proof, we use the uniform discreteness of Γ in conjunction with avoiding the divergence of the harmonic series. Let us spell out the details.

By definition of the Landau symbol, there exist some $c, R > 0$ such that $|J(z)| < c \cdot \|z\|^{-p}$ for all z with $\|z\| > R$. Without loss of generality we may assume $R \geqslant 1$. Let $\Lambda \in \mathbb{X}(\Gamma)$ and $x \in \Lambda$. Consider

$$\sum_{y\in\Lambda} \|x-y\|^{\tilde{p}} \, |J(x-y)| \\ = \sum_{\substack{x-y\in\Lambda \\ \|x-y\|\leqslant R}} \|x-y\|^{\tilde{p}} \, |J(x-y)| + \sum_{\substack{y\in\Lambda \\ \|x-y\|>R}} \|x-y\|^{\tilde{p}} \, |J(x-y)| \, .$$

The first sum on the righthand side of this equation can be estimated as follows:

$$\sum_{\substack{x-y\in\Lambda \\ \|x-y\|\leqslant R}} \|x-y\|^{\tilde{p}} \, |J(x-y)| \leqslant \sum_{\substack{z\in\Lambda-\Lambda \\ \|z\|\leqslant R}} \|z\|^{\tilde{p}} \, |J(z)| \leqslant \sum_{\substack{z\in\Gamma-\Gamma \\ \|z\|\leqslant R}} R^{\tilde{p}} \, |J(z)| =: c_{\Gamma}^{-}(R) \, ,$$

where $c_{\Gamma}^{-}(R)$ is finite because $\Gamma - \Gamma$ is locally finite by the FLC property. Since $\tilde{p} - p < 1$, we have

$$\sum_{\substack{y\in\Lambda \\ \|x-y\|>R}} \|x-y\|^{\tilde{p}} \, |J(x-y)| \leqslant \sum_{k\geqslant\lfloor R\rfloor} \sum_{\substack{y\in\Lambda \\ k\leqslant\|x-y\|<k+1}} \|x-y\|^{\tilde{p}} \, |J(x-y)| \\ \leqslant \sum_{k\geqslant\lfloor R\rfloor} \sum_{\substack{y\in\Lambda \\ k\leqslant\|x-y\|<k+1}} c \, \|x-y\|^{\tilde{p}-p} \leqslant c \sum_{k\geqslant\lfloor R\rfloor} \sum_{\substack{y\in\Lambda \\ k\leqslant\|x-y\|<k+1}} k^{\tilde{p}-p} \\ = c \sum_{k\geqslant\lfloor R\rfloor} \#\{y\in\Lambda \mid k\leqslant\|x-y\|<k+1\} \, k^{\tilde{p}-p} \, .$$

Here, $\lfloor R\rfloor$ denotes the maximal integer lower or equal to R.

Every FLC set is by definition a Delone set and thus uniformly discrete. Hence, there exists some ρ_Λ such that

$$\#\{y\in\Lambda \mid k\leqslant\|x-y\|<k+1\} \\ \leqslant \rho_\Lambda \, \mathrm{vol}(B_{k+1}(0) \smallsetminus B_k(0)) = \rho_\Lambda \, b_{d,1} \left[(k+1)^d - k^d\right] \\ \leqslant \rho_\Lambda \, b_{d,1} \, d \, (k+1)^{d-1} \, ,$$

where $b_{d,1}$ is the volume of the unit-ball in $\mathbb{R}^d$. Since we only regard summands where $k \geqslant R \geqslant 1$, we have

$$(k+1)^{d-1} = \left(\frac{k+1}{k}\right)^{d-1} k^{d-1} \leqslant 2^{d-1} \, k^{d-1} \, .$$

Because the density constant ρ_Λ only depends on patches from Γ, we might also replace it by some ρ_Γ that keeps the inequality above valid for all

$\Lambda \in \mathbb{X}(\Gamma)$. Thus, we have

$$\sum_{\substack{y\in\Lambda \\ \|x-y\|>R}} \|x-y\|^{\tilde{p}}\,|J(x-y)| \leqslant c \sum_{k\geqslant\lfloor R\rfloor} \rho_\Gamma\, b_{d,1}\; d\, 2^{d-1}\, k^{d-1}\, k^{\tilde{p}-p}$$

$$= c\,\rho_\Gamma\, b_{d,1}\; d\, 2^{d-1} \sum_{k\geqslant\lfloor R\rfloor} k^{\tilde{p}-(p-d)-1} =: c_\Gamma^+(R)\,. \quad (2.2)$$

Because the exponent $\tilde{p}-(p-d)-1$ is smaller than -1 by assumption, the series converges. Both constants $c_\Gamma^-(R)$ and $c_\Gamma^+(R)$ only depend on Γ and J. If we set $c_\Gamma := c_\Gamma^-(R) + c_\Gamma^+(R)$ Equation (2.1) is true. □

Let us note that we may interpret the left-hand as well as the right-hand side of Inequality (2.2) as functions in R. The inequality in this interpretation remains true for all $\widetilde{R}$, where $\widetilde{R} > 1$ and the estimate for J induced by the Landau symbol holds for all arguments of absolute value $> \widetilde{R}$. In particular, $c_\Gamma^+(\widetilde{R})$ vanishes for $\widetilde{R} \to \infty$, because it is the tail of a converging series. We will use this estimate later on. For later calculations, we can extract the following conclusion from the proof of Prop. 2.15:

Corollary 2.16. *Let $J : \mathbb{R}^d \to \mathbb{R}$, as in the definition of the pair potential and such that $|J(z)| = \mathcal{O}(\|z\|^{-p})$ for some $p > d+1$. Then for all $\Lambda \in \mathbb{X}(\Gamma)$ and all $x \in \Lambda$*

$$\sum_{y\in\Lambda} |J(x-y)| < c_\Gamma\,, \quad (2.3)$$

where c_Γ is the same constant as in Prop. 2.15*.*

Proof. Let us define $R, c > 0$ as in the proof of Prop. 2.15. We may safely assume that $R > 1$. Then

$$\sum_{y\in\Lambda} |J(x-y)| = \sum_{\substack{y\in\Lambda \\ \|x-y\|\leqslant R}} |J(x-y)| + \sum_{\substack{y\in\Lambda \\ \|x-y\|>R}} |J(x-y)|\,.$$

Let $1 < \tilde{p} \leqslant p-d$. Now certainly $1 < R^{\tilde{p}}$, and thus the first sum in the above equation is smaller than $c_\Gamma^-(R)$. In addition, for $\|x-y\| > R$ we also have $1 < \|x-y\|^{\tilde{p}}$ which implies that the second sum is smaller than $c_\Gamma^+(R)$. Adding up these results we get the stated inequality. □

Remark 2.17. Easy calculations similar to those of Prop. 2.15 show that one has a similar property for exponential decay: Let $t > 0$ and $0 < \tilde{t} < t$. If $|J(z)| = \mathcal{O}(\exp(-t\|z\|))$ for $\|z\| \to \infty$ then there exists some $c'_\Gamma > 0$ such that for all $\Lambda \in \mathbb{X}(\Gamma)$ and $x \in \Lambda$ one has

$$\sum_{y\in\Lambda} \exp(\tilde{t}\,\|x-y\|)\,|J(x-y)| < c'_\Gamma\,.$$

Corollary 2.16 has the desired consequences for the local energies:

Corollary 2.18. *Let Λ be a FLC-set in $\mathbb{R}^d$. If $(\Phi_S)_{S\in\mathcal{S}(\Lambda)}$ is a pair potential, either exponentially or algebraically decaying of order $p > d+1$, then it has the property that all local energies are finite.*

PROOF. Because, as mentioned above, exponential decay is stronger than algebraic decay of any order, we need only check the latter case.

Let as above $m_\phi = |\max_{c,\tilde{c}\in W} \phi(c,\tilde{c})|$. Let $\omega \in W^\Lambda$ and $K \in \mathscr{K}$. We have

$$|\mathcal{H}_K(\omega)| = \Big| \sum_{x\in\Lambda\cap K} \sum_{y\in\Lambda} \beta\phi(\omega_x,\omega_y)\, J(x-y) \Big|$$
$$\leqslant \beta\, m_\phi \sum_{x\in\Lambda\cap K} \Big| \sum_{y\in\Lambda} J(x-y) \Big| \leqslant \beta\, m_\phi\, c_\Gamma\, \#(\Lambda\cap K) < \infty\,,$$

by Cor. 2.16. □

This corollary gives the first restriction for our construction:

Restriction 1. From now on, we assume the potential to be a pair interaction of short range, at least algebraically decaying of order $p > d+1$.

For the next definition we need some notation. Let S_1, S_2 be two disjoint subsets of Λ. For $\eta_1 = (\eta_{1,x})_{x\in S_1} \in W^{S_1}$ and $\eta_2 = (\eta_{2,x})_{x\in S_2} \in W^{S_2}$ we define the combined configuration $\eta_1 \otimes \eta_2 := \eta = (\eta_x)_{x\in S_1\cup S_2} \in W^{S_1\cup S_2}$ by $\eta_x = \eta_{1,x}$ if $x \in S_1$ and $\eta_x = \eta_{2,x}$ if $x \in S_2$. Further let λ be the common Lebesgue measure on W as a subspace of $\mathbb{C}$ and for $S \in \mathcal{S}(\Lambda)$ let λ^S be the standard finite-dimensional product measure on W^S.

Now we can define proper specifications on $(W^\Lambda, \mathscr{F}(\Lambda))$: For $K \in \mathscr{K}$ let

$$\begin{array}{rccc} \pi_K: & \mathscr{F}(\Lambda)\times W^\Lambda & \longrightarrow & \mathbb{R}_0^+\,, \\ & (A,\omega) & \longmapsto & \pi_K(A\,|\,\omega)\,, \end{array}$$

where

$$\pi_K(A\,|\,\omega) = \frac{1}{Z_K(\omega)} \int_{W^{\Lambda\cap K}} 1_A(\eta\otimes\omega_{K^\complement})\, \exp\left(-\mathcal{H}_K(\eta\otimes\omega_{K^\complement})\right)\, \mathrm{d}\lambda^{\Lambda\cap K}(\eta)$$

and the normalisation constant $Z_K(\omega)$, called the *partition function*, is given by

$$Z_K(\omega) = \int_{W^{\Lambda\cap K}} \exp\left(-\mathcal{H}_K(\eta\otimes\omega_{K^\complement})\right)\, \mathrm{d}\lambda^{\Lambda\cap K}(\eta)\,.$$

In statistical physics and finite state spaces, the partition function is also referred to as the *partition sum*. If the local energies are finite, it is easy to check that this makes $\pi := (\pi_K)_{K\in\mathscr{K}}$ a family of well-defined probability kernels and also a specification (for details see [**44**]). Therefore, it makes sense to examine the set of Gibbs measures $\mathscr{G}(\Lambda,\pi)$ on W^Λ specified by π. We will use the same notation π for all specifications on $(W^\Lambda, \mathscr{F}(\Lambda))$, $\Lambda \in \mathbb{X}(\Gamma)$, since they can be distinguished by the argument ω.

The next proposition is a consequence of the finite local energies and will help us to make several estimates:

Proposition 2.19. *Let $K \in \mathscr{K}$ and $\varepsilon > 0$. There exists some $R = R(K,\varepsilon) > 0$ such that for all $\omega \in \mathbb{Y}$*

$$\Delta_{\mathcal{H}}(K,R,\omega) := \Big| \sum_{x\in\underline{\omega}\cap K, y\in\underline{\omega}\cap B_R{}^\complement} \beta\phi(\omega_x,\omega_y) J(x-y) \Big| < \varepsilon\,, \tag{2.4}$$

where $B_R = B_R(0)$ is the closed ball of radius R around $0 \in \mathbb{R}^d$.

PROOF. Let m_ϕ again be the maximal absolute value of ϕ and $s(K) = \max_{\Lambda \in \mathbb{X}} \#(\Lambda \cap K)$. Note that $s(K)$ is finite because, up to translation, only patches of Γ appear inside K and Γ is an FLC set. We may assume that R is large enough to ensure $\|x-y\| > 1$ for all $x \in K$ and $y \in {B_R}^{\complement}$ as well as that the estimate $|J(x-y)| < c\,\|x-y\|^{-p}$ holds. Let $\tilde{R}$ be the minimal distance between points in K and ${B_R}^{\complement}$. Then

$$\begin{aligned}\Bigg| \sum_{x \in \underline{\omega} \cap K, y \in \underline{\omega} \cap {B_R}^{\complement}} \beta\phi(\omega_x, \omega_y) J(x-y) \Bigg| & \\ \leqslant \beta\, m_\phi \sum_{x \in \underline{\omega} \cap K} \sum_{y \in \underline{\omega} \cap {B_R}^{\complement}} & |J(x-y)| \\ \leqslant \beta\, m_\phi \sum_{x \in \underline{\omega} \cap K} \sum_{y \in \underline{\omega} \cap {B_R}^{\complement}} & \|x-y\|^{\tilde{p}}\, |J(x-y)| \\ & \leqslant \beta\, m_\phi\, s(K)\, c_\Gamma^+(\tilde{R})\,,\end{aligned}$$

where we again chose $1 < \tilde{p} < p - d$ and used $c_\Gamma^+(\tilde{R})$ as in the proof of Prop. 2.15. As previously noted, $c_\Gamma^+(\tilde{R})$ depends only on Γ and J and vanishes for growing $\tilde{R}$, thus also for growing R. □

In certain cases, short range potentials ensure existence and uniqueness of a Gibbs measure. In this situation, we have more information about the random variables called *one-point functions*, $H_x : W^\Lambda \to W$, $\omega \mapsto \omega_x$, where $x \in \Lambda$. Especially their covariances $\mathrm{cov}_{\mu_\Lambda}(H_x, H_y)$ with respect to a Gibbs measure μ_Λ can be controlled. This will be essential for the calculation of diffraction properties later on. The basic ingredient for the uniqueness results is Dobrushin's uniqueness condition:

Definition 2.20. A quasilocal[2] specification π on W^Λ is said to satisfy *Dobrushin's uniqueness condition* if

$$c(\Lambda, \pi) := \sup_{x \in \Lambda} \sum_{y \in \Lambda} C_{xy}(\Lambda, \pi) < 1\,,$$

where $(C_{xy}(\Lambda,\pi))_{x,y\in\Lambda}$ is the *Dobrushin interdependence matrix*, defined by

$$\begin{aligned}C_{xy}(\Lambda,\pi) = \sup \Big\{ \max_{A \in \mathscr{W}} \big| \pi_{\{y\}}(\{H_y \in A\} \,|\, \omega) - \pi_{\{y\}}(\{H_y \in A\} \,|\, \widetilde{\omega}) \big| & \\ \Big| \, \omega, \widetilde{\omega} \in W^\Lambda\,,\, \omega_{\Lambda \smallsetminus \{x\}} = \widetilde{\omega}_{\Lambda \smallsetminus \{x\}} \Big\}\,. &\end{aligned}$$

We note that our specification π is quasilocal due to Prop. 2.15 and [**44**, (2.12)]. The interdependence matrix is an indicator of how much the one-point functions at specific points depend on the values of the boundary condition at other points. If those dependencies are small (or even summable as in the condition), the specification is closer to an independent specification

[2] A real valued function on W^Λ is called *local* if it is $\mathscr{F}_K(\Lambda)$-measurable for some $K \in \mathscr{K}$. A limit (with respect to the sup-norm) of local functions is called *quasilocal*. A specification π on W^Λ is called *quasilocal* if, for any bounded quasilocal function f and any $K \in \mathscr{K}$, also $\pi_K(f\,|\,\cdot\,)$ is a bounded and quasilocal function.

(no interaction between the sites) which is known to lead to a single Gibbs measure.

Furthermore, the name of the uniqueness condition is well chosen:

Theorem 2.21. *Suppose a specification π on W^Λ satisfies Dobrushin's uniqueness condition. Then $\#\mathscr{G}(\Lambda,\pi)=1$.*

Proof. Because $(W,\mathscr{W})$ is a standard Borel space, i.e. isomorphic to a complete separable metric space, and thus also its countable products, we may apply [**44**, Theorem (8.7)]. □

Proposition 2.22. *If Φ is an exponentially or algebraically ($p > d+1$) decaying pair potential and at sufficiently high temperature (small β), there exists a uniquely determined Gibbs measure μ_Λ on W^Λ specified by π. Moreover, there exists some constant $c_b > 0$ such that for all $\Lambda \in \mathbb{X}$ and $x \in \Lambda$*

$$\sum_{y\in\Lambda} |\operatorname{cov}_{\mu_\Lambda}(H_x, \overline{H_y})| < c_b\,. \tag{2.5}$$

Proof. The proof is based on Dobrushin's uniqueness condition, and several other calculations in Chapter 8 of [**44**]. Firstly, let us note that

$$\begin{aligned} c(\Lambda,\pi) &\leqslant \frac{1}{2}\sup_{x\in\Lambda}\sum_{S\subset\Lambda:\,x\in S}(\#S-1)\sup_{\omega,\widetilde{\omega}\in W^\Lambda}|\Phi_S(\omega)-\Phi_S(\widetilde{\omega})| \\ &= \frac{1}{2}\sup_{x\in\Lambda}\sum_{y\in\Lambda}\beta\,|J(x-y)|\sup_{\omega,\widetilde{\omega}\in W^\Lambda}|\phi(\omega_x,\omega_y)-\phi(\omega_x,\omega_y)|\,, \end{aligned}$$

by [**44**, Prop. 8.8]. Now in terms of Cor. 2.16 we have

$$\frac{1}{2}\sup_{x\in\Lambda}\sum_{y\in\Lambda}\beta\,|J(x-y)|\sup_{\omega,\widetilde{\omega}\in W^\Lambda}|\phi(\omega_x,\omega_y)-\phi(\omega_x,\omega_y)| \leqslant \beta\, m_\phi\, c_\Gamma\,.$$

If we choose β such that $\beta < \frac{1}{m_\phi\, c_\Gamma}$ we are within the regime of the Dobrushin uniqueness condition. By Thm. 2.21 we then have $\#\mathscr{G}(\Lambda,\pi)=1$. Let us denote this unique Gibbs measure by μ_Λ.

For the examination of the covariances of the one-point functions, we need another object, which is closely related to Dobrushin's interdependence matrix $C = C(\Lambda,\pi)$:

$$D(\Lambda,\pi) := \sum_{n\in\mathbb{N}} C^n\,.$$

According to [**44**, Prop. 8.34] in case Dobrushin's uniqueness condition holds, one has the following estimate for covariances involving $D = D(\Lambda,\pi)$: let f, g be quasilocal functions on W^Λ, then

$$|\operatorname{cov}_{\mu_\Lambda}(f,g)| = |\mu_\Lambda(f\,g)-\mu_\Lambda(f)\mu_\Lambda(g)| \leqslant \frac{1}{4}\sum_{\tilde{x},\tilde{y}\in\Lambda}\Delta_{\tilde{x}}(f)\,D_{\tilde{x}\tilde{y}}\,\Delta_{\tilde{y}}(g)\,, \tag{2.6}$$

where for $x \in \Lambda$ and a quasilocal f

$$\Delta_x(f) := \sup\left\{|f(\omega)-f(\widetilde{\omega})|\,\middle|\,\omega,\widetilde{\omega}\in W^\Lambda, \omega_{\Lambda\setminus\{x\}} = \widetilde{\omega}_{\Lambda\setminus\{x\}}\right\}.$$

It is easy to check that the one-point functions and their conjugates are quasilocal[3]. If one sets

$$m_W := \sup_{c_1,c_2\in W} |c_1 - c_2|$$

then for $f = H_x$ and $g = \overline{H_y}$ Eq. (2.6) reduces to

$$|\operatorname{cov}_{\mu_\Lambda}(H_x, \overline{H_y})| \leqslant \frac{{m_W}^2}{4} D_{xy}\,,$$

because

$$\Delta_{\tilde{x}}(H_x) = \begin{cases} m_W\,, & \text{if } \tilde{x} = x\,, \\ 0 & \text{otherwise} \end{cases}$$

and

$$\Delta_{\tilde{y}}(\overline{H_y}) = \begin{cases} m_W\,, & \text{if } \tilde{y} = y\,, \\ 0 & \text{otherwise}\,. \end{cases}$$

Thus we have for any $x \in \Lambda$

$$\sum_{y\in\Lambda} |\operatorname{cov}_{\mu_\Lambda}(H_x, \overline{H_y})| \leqslant {m_W}^2 \sum_{y\in\Lambda} D_{xy}\,.$$

Consider

$$\sum_{y\in\Lambda} (C^2)_{xy} = \sum_{y\in\Lambda}\sum_{z\in\Lambda} C_{xz}C_{zy} = \sum_{z\in\Lambda} C_{xz} \sum_{y\in\Lambda} C_{zy} \leqslant c(\Lambda,\pi)^2\,,$$

by Dobrushin's uniqueness condition. Inductively we get

$$\sum_{y\in\Lambda} (C^n)_{xy} \leqslant c(\Lambda,\pi)^n\,,$$

for all $n \in \mathbb{N}$ and all $x \in \Lambda$. Thus

$$\sum_{y\in\Lambda} D_{xy} = \sum_{y\in\Lambda}\sum_{n\in\mathbb{N}} (C^n)_{xy} = \sum_{n\in\mathbb{N}}\sum_{y\in\Lambda} (C^n)_{xy} \leqslant \frac{1}{1 - c(\Lambda,\pi)} \leqslant \frac{1}{1 - \beta\, m_\phi\, c_\Gamma}\,, \tag{2.7}$$

by an application of the geometric series. Finally, we get

$$\sum_{y\in\Lambda} |\operatorname{cov}_{\mu_\Lambda}(H_x, \overline{H_y})| \leqslant \frac{{m_W}^2}{4(1 - \beta\, m_\phi\, c_\Gamma)}\,.$$

□

This proposition gives the next restriction.

Restriction 2. From now on, we assume the temperature to be high enough to ensure

$$\beta < \frac{1}{m_\phi\, c_\Gamma\, c_\beta} \tag{2.8}$$

for some $c_\beta > 1$.

[3]Our previous definition for quasilocal functions is the one given by [**44**, Def. 2.20]. This definition only handles real valued functions, but the extension to complex valued ones is trivial by separately treating real and imaginary parts. It does not interfere with the proofs of the results we use.

Here we added the constant c_β to refine β even more than needed for the proof of Prop. 2.22. Later on, this will become necessary.

In general, existence does not necessarily help to calculate things. Especially if the desired object is only given as a solution to some integral equation. Uniqueness, on the other hand, results in the following theorem:

Theorem 2.23. *Let μ_Λ be the unique Gibbs measure on W^Λ to the potential Φ. Further, for $m \in \mathbb{N}$, let B_m be the closed ball of radius m centred in the origin. Then for all bounded measurable functions f*

$$\mu_\Lambda(f) = \lim_{m\to\infty} \pi_{B_m}(f \,|\, \omega) \quad \textit{for } \mu_\Lambda\textit{-almost all } \omega \in W^\Lambda .$$

In our case we even have

$$\pi_{B_m}(f \,|\, \omega) \overset{m\to\infty}{\longrightarrow} \mu_\Lambda(f)$$

uniformly in $\omega \in W^\Lambda$.

Proof. This is a direct consequence of Proposition (7.11) and Theorem (7.12) in [**44**]. □

Another important note is the following: Because Φ only measures relative location of the interacting points, it is translation invariant, i.e. $\Phi_{S+t}(\omega + t) = \Phi_S(\omega)$. This leads to $\pi_{K+t}(A + t \,|\, \omega + t) = \pi_K(A \,|\, \omega)$ and thus to $\mu_{\Lambda+t}(A + t) = \mu_\Lambda(A)$ which gives the basic idea for the construction of the next paragraph.

2.2.3. Gibbs measures on the dynamical system $\mathbb{Y}$. The topologies on $\mathbb{X}$ and $\mathbb{Y}$ define Borel sets $\mathscr{B}$ and $\mathscr{F}$, respectively. For the existence of the natural autocorrelation on both systems we will later on need to restrict ourselves to the case that $(\mathbb{X}, T)$ is uniquely ergodic. Let us denote the corresponding ergodic probability measure by ν. The goal of the next lines is to construct a natural extension of ν to $\mathbb{Y}$ that is compatible with a chosen short range potential Φ. The theory presented here will give an extremal translation invariant Gibbs measure, which is known to be ergodic. That allows us to make sensible statements about the diffraction of the randomly generated weighted FLC sets in the next section.

Since we need the results from the previous sections, Restriction 1 and 2 still apply to Φ.

First, we need to construct proper families of σ-algebras and define valid specifications. So for $K \in \mathscr{K}$ let

$$\widetilde{\mathscr{T}_K} := \left\{ \dot{\bigcup_{\Lambda\in\mathbb{X}}} A_\Lambda \,\middle|\, A_\Lambda \in \mathscr{T}_K(\Lambda) \right\} .$$

It is easy to check that these are σ-algebras. Since those σ-algebra need not be contained in the Borel σ-algebra $\mathscr{F}$ on $\mathbb{Y}$ we need to reduce to the traces, so let

$$\mathscr{T}_K := \widetilde{\mathscr{T}_K} \cap \mathscr{F} .$$

As an intersection of σ-algebras, they are again σ-algebras. They are decreasing because the $\mathscr{T}_K(\Lambda)$ are decreasing. Let $\mathscr{F}_K$ be defined in the same manner.

The specification is defined as follows: For $K \in \mathscr{K}$ let

$$\begin{array}{rccl} \chi_K : & \mathscr{F} \times Y & \longrightarrow & \mathbb{R}_0^+ \\ & (A, \omega) & \longmapsto & \chi_K(A \,|\, \omega) := \pi_K(A \cap W^{\underline{\omega}} \,|\, \omega)\,. \end{array}$$

Before we can check the needed properties of a specification, we have to verify that χ_K is well-defined. Because $\omega \in W^{\underline{\omega}}$ by definition, we only need $A \cap W^\Lambda$ to be in $\mathscr{F}(\Lambda)$ for every $A \in \mathscr{F}$. So in analogy to the $\widetilde{\mathscr{T}_K}$ let $\widetilde{\mathscr{F}} := \left\{\dot{\bigcup}_{\Lambda\in\mathbb{X}} A_\Lambda \,\middle|\, A_\Lambda \in \mathscr{F}(\Lambda)\right\}$, which again is a σ-algebra. It is easy to show that $\mathscr{F}$ is contained in $\widetilde{\mathscr{F}}$, because each $U^R_{K\times W, V\times V'}[\omega]$ (in the sense of Prop. 2.9) is contained in $\widetilde{\mathscr{F}}$: (we may safely assume that V' is a ball around the origin)

$$\begin{aligned} &U^R_{K\times W,V\times V'}[\omega] \\ &= \left\{\tilde\omega \in \mathbb{Y} \,|\, \omega \cap K \times W \subseteq \tilde\omega + \left(V \times V'\right),\, \tilde\omega \cap K \times W \subset \omega + \left(V \times V'\right)\right\} \\ &\qquad = \left\{\tilde\omega \in \mathbb{Y} \,|\, \omega \cap K \times W \subset \tilde\omega + \left(V \times V'\right)\right\} \\ &\qquad\qquad \cap \left\{\tilde\omega \in \mathbb{Y} \,|\, \tilde\omega \cap K \times W \subseteq \omega + \left(V \times V'\right)\right\} \\ &\qquad\qquad\qquad \overbrace{\qquad\qquad\qquad\qquad}^{\in\mathscr{F}(\Lambda) \text{ as finite intersection of countable unions of measurable sets}} \\ &= \dot{\bigcup_{\substack{\Lambda\in\mathbb{X} \\ (\underline{\omega}\cap K)\subseteq(\Lambda+V)}}} \overbrace{\bigcap_{x\in\underline{\omega}\cap K} \bigcup_{\substack{y\in\Lambda \\ (x-y)\in V}} \left\{\tilde\omega \in W^\Lambda \,\middle|\, p_{\{y\}}(\tilde\omega) \in \omega_x + V'\right\}} \\ &\cap \dot{\bigcup_{\substack{\Lambda\in\mathbb{X} \\ (\Lambda\cap K)\subseteq(\underline{\omega}+V)}}} \underbrace{\bigcap_{y\in\Lambda\cap K} \bigcup_{\substack{x\in\underline{\omega} \\ (y-x)\in V}} \left\{\tilde\omega \in W^\Lambda \,\middle|\, p_{\{y\}}(\tilde\omega) \in \omega_x + V'\right\}}_{\in\mathscr{F}(\Lambda) \text{ as finite intersection of countable unions of measurable sets}}, \end{aligned}$$

where $p_{\{y\}}(\omega) = \omega_y$ is the projection to the y-coordinate in the respective W^Λ, measurable by definition of $\mathscr{F}(\Lambda)$.

Therefore, every Borel set $A \in \mathscr{F}$ has a representation as $\dot{\bigcup}_{\Lambda\in\mathbb{X}} A_\Lambda$ where $A \cap W^\Lambda = A_\Lambda \in \mathscr{F}(\Lambda)$.

Proposition 2.24. *The family $(\chi_K)_{K\in\mathscr{K}}$ is a specification on $\mathbb{Y}$.*

Proof. (S_1): The mapping $\chi_K(\,\cdot\,|\,\omega)$ is a probability measure on $(\mathbb{Y}, \mathscr{F})$ for all $\omega \in \mathbb{Y}$, because $\pi_K(\,\cdot\,|\,\omega)$ is a probability measure on $(W^{\underline{\omega}}, \mathscr{F}(\underline{\omega}))$.

(S_3): We directly use that π is a specification on each W^Λ: Because of the disjoint structure of $\mathbb{Y}$ we have for all $A \in \mathscr{F}$ and $\omega \in \mathbb{Y}$ that $\omega \in A$ if and only if $\omega \in A \cap W^{\underline{\omega}} =: A_{\underline{\omega}}$. Thus for $A \in \mathscr{T}_K$, $K \in \mathscr{K}$,

$$\chi_K(A \,|\, \omega) = \pi_K(\overbrace{A \cap W^{\underline{\omega}}}^{\in\mathscr{T}_K(\underline{\omega})} \,|\, \omega) = 1_{A_{\underline{\omega}}}(\omega) = 1_A(\omega)\,.$$

(S_4): Let $K_1, K_2 \in \mathscr{K}$ such that $K_2 \subseteq K_1$. We have to check that the composition of the kernels χ_{K_1} and χ_{K_2} behaves in the right way. Let $A \in \mathscr{F}$

and $\omega \in Y$. As before, let $A_{\underline{\omega}} = A \cap W^{\underline{\omega}}$. Then we have

$$\begin{aligned}(\chi_{K_1} \,\square\, \chi_{K_2})(A \,|\, \omega) \\ &= \int_{W^{\underline{\omega}}} \chi_{K_2}(A \,|\, \widetilde{\omega})\, \mathrm{d}\chi_{K_1}(\,\cdot\,|\,\omega)(\widetilde{\omega}) = \int_{W^{\underline{\omega}}} \pi_{K_2}(A_{\underline{\omega}} \,|\, \widetilde{\omega})\, \mathrm{d}\pi_{K_1}(\,\cdot\,|\,\omega)(\widetilde{\omega}) \\ &= (\pi_{K_1}\pi_{K_1})(A_{\underline{\omega}} \,|\, \omega) = \pi_{K_1}(A_{\underline{\omega}} \,|\, \omega) = \chi_{K_1}(A \,|\, \omega)\,.\end{aligned}$$

(S_2): We need to show that $\chi_K(A \,|\, \cdot\,)$ is $\widetilde{\mathscr{T}}_K$- and $\mathscr{F}$-measurable. The first is again a direct consequence of π being a specification: Let $I \subseteq \mathbb{R}_0^+$ an interval. Then

$$\begin{aligned}\chi_K(A \,|\, \cdot\,)^{-1}(I) &= \{\omega \in Y \,|\, \chi_K(A \,|\, \omega) \in I\} \\ &= \{\omega \in Y \,|\, \pi_K(A_{\underline{\omega}} \,|\, \omega) \in I\} = \dot{\bigcup_{\Lambda \in \mathbb{X}}} \underbrace{\{\omega \in W^\Lambda \,|\, \pi_K(A_\Lambda \,|\, \omega) \in I\}}_{\in \mathscr{T}_K(\Lambda)} \in \widetilde{\mathscr{T}}_K\,.\end{aligned}$$

To show that the specification is $\mathscr{F}$-measurable takes some more steps. The first step is to look at what happens if we replace the indicator function 1_A, respectively $1_{A_{\underline{\omega}}}$, in the definition of π by an arbitrary continuous function $h : Y \to \mathbb{R}_0^+$: Let

$$\begin{aligned}\chi_K(h \,|\, \omega) &:= \pi_K(h \,|\, \omega) \\ &:= \frac{1}{Z_K(\omega)} \int_{W^{\underline{\omega} \cap K}} h(\eta \otimes \omega_{K^\complement})\, \exp\left(-\mathcal{H}_K(\eta \otimes \omega_{K^\complement})\right)\, \mathrm{d}\lambda^{\underline{\omega} \cap K}(\eta)\,.\end{aligned}$$

We will show that $\chi_K(h \,|\, \omega)$ is continuous in ω and thus $\mathscr{F}$-measurable. Let $(\omega^n)_{n\in\mathbb{N}}$ be a sequence in $\mathbb{Y}$ converging to ω. Because of the convergence and the translation invariance of the specifications, we may safely assume that for large enough n the supports of ω and ω^n agree in K. Now since $\lambda^{\underline{\omega} \cap K}$ is a finite measure and h and exp are continuous, the question of continuity of $\chi_K(h \,|\, \omega)$ reduces to the question of continuity of $\mathcal{H}_K(\eta \otimes \omega_{K^\complement})$ in ω.

Let $\varepsilon > 0$ and let without loss of generality $\underline{\omega}$ and $\underline{\omega^n}$ agree in a ball B_n around the origin. In particular, let $\underline{\eta \otimes \omega} \cap K = \underline{\eta \otimes \omega^n} \cap K = S$. Further let $R = R(K, \frac{\varepsilon}{3})$ be the radius defined in Prop. 2.19. We may assume that $B_R \subseteq B_n$. Then

$$\begin{aligned}\left|\mathcal{H}_K(\eta \otimes \omega_{K^\complement}) - \mathcal{H}_K(\eta \otimes \omega^n_{K^\complement})\right| \\ &= \left|\sum_{x\in S,\, y\in\underline{\omega}} \beta\, \phi(\eta_x, \omega_y)\, J(x-y) - \sum_{x\in S,\, y\in\underline{\omega^n}} \beta\, \phi(\eta_x, \omega^n_y)\, J(x-y)\right| \\ &= \Bigg|\sum_{x\in S,\, y\in\underline{\omega}\cap B_R\setminus S} \beta\left(\phi(\eta_x, \omega_y) - \phi(\eta_x, \omega^n_y)\right) J(x-y) \\ &\quad + \sum_{x\in S,\, y\in\underline{\omega}\cap B_R{}^\complement} \beta\, \phi(\eta_x, \omega_y)\, J(x-y) - \sum_{x\in S,\, y\in\underline{\omega^n}\cap B_R{}^\complement} \beta\, \phi(\eta_x, \omega^n_y)\, J(x-y)\Bigg| \\ &\leqslant \left|\sum_{x\in S,\, y\in\underline{\omega}\cap B_R\setminus S} \beta\left(\phi(\eta_x, \omega_y) - \phi(\eta_x, \omega^n_y)\right) J(x-y)\right| \\ &\quad + \Delta_{\mathcal{H}}(K, R, \eta \otimes \omega_{K^\complement}) + \Delta_{\mathcal{H}}(K, R, \eta \otimes \omega^n_{K^\complement})\,.\end{aligned}$$

From the FLC property we know that $k = \#\{z \in \Gamma - \Gamma \,|\, \|z\| \leqslant 2R\} < \infty$ and also $s(B_R) = \max_{\Lambda\in\mathbb{X}} \#(\Lambda \cap B_R) < \infty$. Let also $j(R) = \max\{|J(z)| \,|\, z \in \Gamma - \Gamma,\, \|z\| \leqslant 2R\}$. Since ϕ is assumed to be continuous, we can choose N large enough so that, for all larger n, the weight differences in B_R are small enough to have $|\phi(\eta_x, \omega_y) - \phi(\eta_x, \omega_y^n)| < \frac{\varepsilon}{3\beta\, k\, s(B_R)\, j(R)}$. We then get

$$\begin{aligned}
&\left|\mathcal{H}_K(\eta \otimes \omega_{K^{\complement}}) - \mathcal{H}_K(\eta \otimes \omega^n_{K^{\complement}})\right| \\
&\qquad = \left| \sum_{x\in S,\, y\in\underline{\omega}\cap B_R\setminus S} \beta\left(\phi(\eta_x, \omega_y) - \phi(\eta_x, \omega_y^n)\right) J(x-y)\right| + \frac{2\varepsilon}{3} \\
&\qquad\qquad \leqslant s(B_R) \sum_{z\in\Gamma-\Gamma,\, \|z\|\leqslant 2R} \beta \frac{\varepsilon}{3\beta\, k\, s(B_R)\, j(R)} |J(z)| + \frac{2\varepsilon}{3} \leqslant \varepsilon\,.
\end{aligned}$$

Because we are in a metrizable space we know (see [**24**]) that every indicator function of closed sets is a point-wise limit of continuous functions. Thus for $F \subseteq \mathbb{Y}$ closed and $1_F(\omega) = \lim_{n\to\infty} h_n(\omega)$ we have

$$\begin{aligned}
&\chi_K(F \,|\, \omega) \\
&\qquad = \frac{1}{Z_K(\omega)} \int_{W^{\underline{\omega}\cap K}} 1_F(\eta \otimes \omega_{K^{\complement}})\, \exp\left(-\mathcal{H}_K(\eta \otimes \omega_{K^{\complement}})\right) \mathrm{d}\lambda^{\underline{\omega}\cap K}(\eta) \\
&\qquad = \frac{1}{Z_K(\omega)} \int_{W^{\underline{\omega}\cap K}} \lim_{n\to\infty} h_n(\eta \otimes \omega_{K^{\complement}})\, \exp\left(-\mathcal{H}_K(\eta \otimes \omega_{K^{\complement}})\right) \mathrm{d}\lambda^{\underline{\omega}\cap K}(\eta) \\
&\qquad = \lim_{n\to\infty} \frac{1}{Z_K(\omega)} \int_{W^{\underline{\omega}\cap K}} h_n(\eta \otimes \omega_{K^{\complement}})\, \exp\left(-\mathcal{H}_K(\eta \otimes \omega_{K^{\complement}})\right) \mathrm{d}\lambda^{\underline{\omega}\cap K}(\eta) \\
&\qquad\qquad = \lim_{n\to\infty} \chi_K(h_n \,|\, \omega)\,.
\end{aligned}$$

Hence $\chi_K(F \,|\, \cdot)$ is a limit of measurable (even continuous) functions and as such again measurable (see e.g. [**21**]).

We will now apply a monotone class argument to show that this property for closed sets extends to arbitrary measurable $A \subseteq \mathbb{Y}$: The set of closed sets of $\mathbb{Y}$ is a generator of the Borel σ-algebra, closed under finite intersections and contained in the set $\widehat{\mathscr{F}} := \{A \in \mathscr{F} \,|\, \chi_K(A \,|\, \cdot) \text{ is } \mathscr{F}\text{-measurable}\}$. Thus we only have to show that $\widehat{\mathscr{F}}$ is a Dynkin system, because then $\widehat{\mathscr{F}} = \mathscr{F}$ (see [**21**]): Since $\mathbb{Y}$ is closed also $\mathbb{Y} \in \widehat{\mathscr{F}}$. Suppose $A \in \widehat{\mathscr{F}}$ then

$$\chi_K\left(A^{\complement} \,|\, \cdot\,\right) = 1 - \chi_K(A \,|\, \cdot)$$

is also measurable and thus $A^{\complement} \in \widehat{\mathscr{F}}$. Now let $(A_n)_{n\in\mathbb{N}}$ be a sequence of pairwise disjoint sets in $\widehat{\mathscr{F}}$. Then

$$\chi_K\Big(\bigcup_{n\in\mathbb{N}} A_n \,|\, \cdot\,\Big) = \sum_{n\in\mathbb{N}} \chi_K(A_n \,|\, \cdot)$$

and is thus also measurable, which completes our proof. □

For the next steps we need to introduce the following restriction. This time we need to make more assumptions on the dynamical system $\mathbb{X}$. Recall that our goal is to have a 'natural' ergodic measure on $\mathbb{Y}$, where the aim is to obtain ergodicity by an extremal property of the Gibbs measure. We will achieve that by demanding a similar property of the underlying non-weighted structure:

Restriction 3. From now on we will assume that the dynamical system $(\mathbb{X}(\Gamma), T)$ is uniquely ergodic.

Remark 2.25. Restriction 3 still allows a large class of examples. In particular, the corresponding dynamical system of a regular model set is uniquely ergodic (see [**88**]).

We will denote the unique ergodic measure on $(\mathbb{X}(G), \mathscr{B})$ by ν. In the next lines we give a natural extension ϑ of this measure to the system $\mathbb{Y}$ induced by the pair potential Φ.

So let ν choose the support and then let the Gibbs measure on that particular support choose the weights:

$$\vartheta(A) := \int_{\mathbb{X}} \int_{W^\Lambda} 1_{A\cap W^\Lambda}(\omega)\, \mathrm{d}\mu_\Lambda(\omega)\, \mathrm{d}\nu(\Lambda) = \int_{\mathbb{X}} \mu_\Lambda(A \cap W^\Lambda)\, \mathrm{d}\nu(\Lambda)\,.$$

We first have to check that it is well-defined, i.e. that for all $A \in \mathscr{F}$ the map $f : \Lambda \mapsto \mu_\Lambda(A \cap W^\Lambda)$ is measurable: let $g : \mathbb{X} \to \mathbb{Y}$ be measurable, e.g. let $c \in W$ and $g(\Lambda) = (c)_{x\in\Lambda}$, further let $f_n : \Lambda \mapsto \chi_{B_n(0)}(A \,|\, g(\Lambda))$. Then f_n is measurable because $\chi_{B_n(0)}(A \,|\, \cdot\,)$ is measurable (see proof of Prop. 2.24) and we thus have a composition of measurable maps. On the other hand, due to theorem 2.23, we know that $f(\Lambda) = \lim_{n\to\infty} f_n(\Lambda)$ which also makes it measurable.

And indeed, ϑ is a Gibbs measure on $\mathbb{Y}$ specified by χ:

Lemma 2.26. *We have $\vartheta \in \mathscr{G}_0(\chi)$.*

Proof. We will first check the DLR equations and use the fact that all μ_Λ are DLR states. So let $A \in \mathscr{F}$ and $K \in \mathscr{K}$:

$$\begin{aligned}\int \chi_K(A \,|\, \omega)\, \mathrm{d}\vartheta(\omega) &= \int_{\mathbb{X}} \int_{W^\Lambda} \chi_K(A \,|\, \omega)\, \mathrm{d}\mu_\Lambda(\omega)\, \mathrm{d}\nu(\Lambda) \\ &= \int_{\mathbb{X}} \int_{W^\Lambda} \pi_K(A \cap \overbrace{W^\omega}^{=W^\Lambda} \,|\, \omega)\, \mathrm{d}\mu_\Lambda(\omega)\, \mathrm{d}\nu(\Lambda) \\ &\overset{\text{DLR}}{=} \int_{\mathbb{X}} \mu_\Lambda(A \cap W^\Lambda)\, \mathrm{d}\nu(\Lambda) = \vartheta(A)\,.\end{aligned}$$

Now we have to verify the translation invariance of ϑ:

$$\begin{aligned}\vartheta(A+t) &= \int_{\mathbb{X}} \mu_\Lambda\big((A+t) \cap W^\Lambda\big)\, \mathrm{d}\nu(\Lambda) \\ &\overset{\nu \text{ transl. inv.}}{=} \int_{\mathbb{X}} \mu_{\Lambda+t}\big((A+t) \cap W^{\Lambda+t}\big)\, \mathrm{d}\nu(\Lambda) \\ &= \int_{\mathbb{X}} \mu_{\Lambda+t}\big((A \cap W^\Lambda) + t\big)\, \mathrm{d}\nu(\Lambda) = \int_{\mathbb{X}} \mu_\Lambda(A \cap W^\Lambda)\, \mathrm{d}\nu(\Lambda) = \vartheta(A)\,.\end{aligned}$$

□

The next step is to show the uniqueness of ϑ as a translation invariant Gibbs measure. The proof for this property of ϑ is based on the uniqueness of the Gibbs measures μ_Λ and disintegration of measures which we will introduce by the following proposition.

Proposition 2.27. *Let θ be a translation invariant measure on $(\mathbb{Y}, \mathscr{F})$. Then it can be disintegrated with respect to ν, i.e. there exists a measurable mapping $\mathbb{X} \to \mathcal{M}(\mathbb{Y})$, $\Lambda \mapsto \theta_\Lambda$ such that for each positive measurable function f we have*

$$\int_{\mathbb{Y}} f(\omega)\,\mathrm{d}\theta(\omega) = \int_{\mathbb{X}}\int_{\mathbb{Y}} f(\omega)\,\mathrm{d}\theta_\Lambda(\omega)\,\mathrm{d}\nu(\Lambda)\,,$$

where the measures θ_Λ are concentrated on the fibres $\{\omega \in \mathbb{Y} \,|\, \underline{\omega} = \Lambda\} = W^\Lambda$.

Proof. We can apply Theorem 5.8 from [**43**], because the mapping $\omega \mapsto \underline{\omega}$ implies a homeomorphism (which also results in the concentration on the fibres) and $\mathbb{Y}$ is a compact metrizable space. We only need to check that for $B \in \mathscr{B}$ we have $\tilde{\nu}(B) := \theta(\{\omega \in \mathbb{Y} \,|\, \underline{\omega} \in B\}) = \nu(B)$. But that is obvious because the map $B \mapsto \tilde{\nu}(B)$ defines a measure on $(\mathbb{X}, \mathscr{B})$, the image of θ under the measurable map $\omega \mapsto \underline{\omega}$, and it is translation invariant:

$$\begin{aligned}\tilde{\nu}(B+t) &= \theta(\{\omega \in \mathbb{Y} \,|\, \underline{\omega} \in B + t\}) \\ &= \theta(\{\omega \in \mathbb{Y} \,|\, \underline{\omega} \in B\} + t) = \theta(\{\omega \in \mathbb{Y} \,|\, \underline{\omega} \in B\}) = \tilde{\nu}(B)\end{aligned}$$

But ν is supposed to be the only translation invariant measure on $(\mathbb{X}, \mathscr{B})$, so $\tilde{\nu} = \nu$. □

Now to our desired uniqueness:

Proposition 2.28. *The only translation invariant Gibbs measure specified by χ is given by ϑ, i.e. $\mathscr{G}_0(\chi) = \{\vartheta\}$.*

Proof. Let $B \in \mathscr{B}$, and $B_{\mathbb{Y}} := \{\omega \in \mathbb{Y} \,|\, \underline{\omega} \in B\}$. Note that $B_{\mathbb{Y}}$ is a measurable set, because the mapping $\omega \mapsto \underline{\omega}$ is measurable. Let us note that, for any $\theta \in \mathscr{G}_0(\chi)$, we may use 2.27. Thus, for $A \in \mathscr{F}$, we have

$$\begin{aligned}\theta(A \cap B_{\mathbb{Y}}) &= \int_{\mathbb{X}}\int_{\mathbb{Y}} 1_{A\cap B_{\mathbb{Y}}}(\omega)\,\mathrm{d}\theta_\Lambda(\omega)\,\mathrm{d}\nu(\Lambda) \\ &= \int_{\mathbb{X}}\int_{\mathbb{Y}} 1_A(\omega)\,1_{B_{\mathbb{Y}}}(\omega)\,\mathrm{d}\theta_\Lambda(\omega)\,\mathrm{d}\nu(\Lambda) \\ &= \int_{\mathbb{X}}\int_{\mathbb{Y}} 1_A(\omega)\,1_B(\underline{\omega})\,\mathrm{d}\theta_\Lambda(\omega)\,\mathrm{d}\nu(\Lambda) \\ &\overset{\theta_\Lambda \text{ conc. on } W^\Lambda}{=} \int_{\mathbb{X}}\int_{\mathbb{Y}} 1_{W^\Lambda}(\omega)\,1_A(\omega)\,1_B(\underline{\omega})\,\mathrm{d}\theta_\Lambda(\omega)\,\mathrm{d}\nu(\Lambda) \\ &= \int_{\mathbb{X}}\int_{\mathbb{Y}} 1_{A\cap W^\Lambda}(\omega)\,1_B(\Lambda)\,\mathrm{d}\theta_\Lambda(\omega)\,\mathrm{d}\nu(\Lambda) \\ &= \int_{\mathbb{X}} 1_B(\Lambda)\int_{W^\Lambda} 1_{A\cap W^\Lambda}(\omega)\,\mathrm{d}\theta_\Lambda(\omega)\,\mathrm{d}\nu(\Lambda)\,.\end{aligned}$$

On the other hand, because θ is a Gibbs measure, we also have, for any $K \in \mathscr{K}$,

$$\begin{aligned}\theta(A\cap B_{\mathbb{Y}}) &= \int_{\mathbb{Y}} \chi_K(A\cap B_{\mathbb{Y}}\,|\,\omega)\,\mathrm{d}\theta(\omega) = \int_{\mathbb{X}}\int_{\mathbb{Y}} \chi_K(A\cap B_{\mathbb{Y}}\,|\,\omega)\,\mathrm{d}\theta_\Lambda(\omega)\,\mathrm{d}\nu(\Lambda)\\ &= \int_{\mathbb{X}}\int_{\mathbb{Y}} \pi_K(A\cap B_{\mathbb{Y}}\cap W^{\underline{\omega}}\,|\,\omega)\,\mathrm{d}\theta_\Lambda(\omega)\,\mathrm{d}\nu(\Lambda)\\ &= \int_{\mathbb{X}}\int_{\mathbb{Y}} \pi_K(A\cap B_{\mathbb{Y}}\cap W^{\Lambda}\,|\,\omega)\,\mathrm{d}\theta_\Lambda(\omega)\,\mathrm{d}\nu(\Lambda)\\ &= \int_{\mathbb{X}}\int_{\mathbb{Y}} 1_{B_{\mathbb{Y}}}(\omega)\,\pi_K(A\cap W^{\Lambda}\,|\,\omega)\,\mathrm{d}\theta_\Lambda(\omega)\,\mathrm{d}\nu(\Lambda)\\ &= \int_{\mathbb{X}}\int_{W^\Lambda} 1_B(\Lambda)\,\pi_K(A\cap W^{\Lambda}\,|\,\omega)\,\mathrm{d}\theta_\Lambda(\omega)\,\mathrm{d}\nu(\Lambda)\\ &= \int_{\mathbb{X}} 1_B(\Lambda)\int_{W^\Lambda} \pi_K(A\cap W^{\Lambda}\,|\,\omega)\,\mathrm{d}\theta_\Lambda(\omega)\,\mathrm{d}\nu(\Lambda)\,.\end{aligned}$$

A standard argument from measure theory thus yields that ν-almost surely we have

$$\int_{W^\Lambda} \pi_K(A\cap W^{\Lambda}\,|\,\omega)\,\mathrm{d}\theta_\Lambda(\omega) = \int_{W^\Lambda} 1_{A\cap W^\Lambda}(\omega)\,\mathrm{d}\theta_\Lambda(\omega)\,.$$

Since any $A_\Lambda \in \mathscr{F}(\Lambda)$ can be written in the form $A\cap W^\Lambda$ for some $A\in\mathscr{F}$ we get that the restriction of θ_Λ to W^Λ solves the DLR equations for the corresponding specification π for ν-almost all Λ. Since we only have one unique Gibbs measure for any W^Λ, we know the restriction of θ_Λ to W^Λ is given by μ_Λ. Because this is true ν-almost surely, one way to write $\theta(A)$ is

$$\theta(A) = \int_{\mathbb{X}}\int_{W^\Lambda} 1_{A\cap W^\Lambda}(\omega)\,\mathrm{d}\mu_\Lambda(\omega)\,\mathrm{d}\nu(\Lambda) = \vartheta(A)\,.$$

□

Now we are able to state the main result of this section:

Theorem 2.29. *If Restrictions* 1-3 *hold then the measure ϑ is ergodic on $(\mathbb{Y},\mathscr{F})$ with respect to the $\mathbb{R}^d$-action T.*

Proof. We want to apply Theorem 2.14, so we need to check that there exists a sequence $(\mathscr{F}_n)_{n\in\mathbb{N}}$ of sub-σ-algebras of $\mathscr{F}$ such that $\mathscr{F}$ is the smallest σ-algebra containing $\bigcup_{n\in\mathbb{N}}\mathscr{F}_n$, and such that for any $n\in\mathbb{N}$, $K\in\mathscr{K}$ there exists some $t\in\mathbb{R}^d$ such that $\mathscr{F}_n + t \subseteq \mathscr{T}_K$. One can easily check that the $\mathscr{F}_{B_n}$ comply with this requirement. Thus, the extremal points of the convex set $\mathscr{G}_0(\chi)$ are ergodic. Since ϑ is the only translation invariant Gibbs measure it is an extremal one and therefore ergodic. □

Let us also make some comment on the measure ϑ from the point of view of point process theory: Consider the mapping $\delta^{(M)} : \mathbb{Y} \to \mathcal{M}(\mathbb{R}^d\times W)$, where

$$\delta^{(M)}(\omega) := \sum_{x\in\underline{\omega}} \delta_{(x,\omega_x)}\,,$$

then the image of ϑ under the (obviously measurable mapping) $\delta^{(M)}$ is a marked point process in $\mathbb{R}^d$ with marks in W.

2.3. Diffraction properties

In this section, we show that almost surely with respect to ϑ we get no singular continuous part in the diffraction of a random $\omega \in \mathbb{Y}$, as long as we stick to the prerequisites from the previous sections and additionally assume that the system $(\mathbb{X}, T)$ is pure point diffractive. To get sensible statements we will embed the diffraction of the weighted FLC sets into the theory of the diffraction of complex Radon measures.

We are interested in the diffraction of the following objects:

$$\delta^{(H)}(\omega) := \sum_{x \in \underline{\omega}} H_x(\omega)\, \delta_x \,,$$

where $\omega \in \mathbb{Y}$ and we extend the definition of the one-point functions to this specific need, $H_x(\omega) := 1_{\underline{\omega}}(x) \cdot \omega_x$.

Remark 2.30. The mapping $\omega \mapsto \delta^{(H)}(\omega)$ is continuous from $\mathbb{Y}$ to $\mathcal{M}(\mathbb{R}^d)$.

Proof. Let $(\omega^n)_{n\in\mathbb{N}}$ be a convergent sequence in $\mathbb{Y}$ with limit ω and let f be a continuous function with compact support $K \subset \mathbb{R}^d$. Then because of the convergence of the ω^n for N large enough and any $x \in \operatorname{supp}\omega \cap K^o$ there exists a sequence $(x_n)_{n>N}$ with $x_n \in \operatorname{supp}\omega^n \cap K^o$ such that $x_n \to x$ and $\omega^n \cap K^o$ consists only of the respective x_n's. Note that because of the assumed continuity of f we have $f(x) = 0$ for all $x \in \partial K$ and thus

$$\left|\delta^{(H)}(\omega)(f) - \delta^{(H)}(\omega^n)(f)\right| = \Big| \sum_{x \in \operatorname{supp}\omega \cap K^o} \left(\omega_x f(x) - \omega^n_{x_n} f(x_n)\right) \Big| \,.$$

Because f is assumed to be continuous and the weights $\omega^n_{x_n}$ necessarily also converge to ω_x (due to the convergence of the ω_n), a simple $2\,\varepsilon$-argument shows the continuity of $\delta^{(H)}$. □

So let us use the theory provided in Chapter 1 together with the following result given in [**14**]:

Theorem 2.31. *Let Λ be an FLC set, and $\mu = \sum_{x\in\Lambda} w(x)\,\delta_x$, where $w(x) \in \mathbb{C}$ and $\sup_{x\in\Lambda} |w(x)| < \infty$. The existence of the natural autocorrelation γ of μ is equivalent to the existence of the limits*

$$\eta(z) := \lim_{R\to\infty} \frac{1}{\operatorname{vol} B_R} \sum_{\substack{x \in \Lambda \cap B_R \\ x - z \in \Lambda}} w(x)\overline{w(x-z)} \,,$$

for all $z \in \Lambda - \Lambda$. The natural autocorrelation in this case is given by

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

□

If it exists, the autocorrelation of $\delta^{(H)}(\omega)$ is thus given by the measure

$$\gamma^{(H)}(\omega) := \sum_{z \in \underline{\omega} - \underline{\omega}} \eta^{(H)}(\omega, z)\, \delta_z \,,$$

where the autocorrelation coefficients are given by

$$\eta^{(H)}(\omega, z) := \lim_{R\to\infty} \frac{1}{\operatorname{vol}\left(B_R\right)} \sum_{\substack{x \in \underline{\omega} \cap B_R \\ x - z \in \underline{\omega}}} H_x(\omega)\, \overline{H_{x-z}(\omega)} \,.$$

The next steps prove the existence of those coefficients, at least almost surely with respect to ϑ. The strategy will be to show that a yet to be defined averaged version is pure point diffractive if Γ is, while the objects above differ from that average only mildly and thus lead only to an absolutely continuous part of the diffraction.

The tools to derive the diffraction properties of our objects come from the theory of dynamical systems. A natural factor map can be formulated. To check the needed properties as a factor map it is essential to ensure that the expectations of the one-point functions with respect to the Gibbs measures μ_Λ depend continuously on the respective Λ. Several small steps are necessary to get there.

At first we need to show that the specifications π_K vary not too strongly for different $\Lambda \in \mathbb{X}$. One step in that direction is the following proposition that states that we may estimate the specifications by 'more local' objects:

Proposition 2.32. *Let $\varepsilon > 0$ and $K \in \mathscr{K}$. Then there exists some $R > 0$ such that for all $\Lambda \in \mathbb{X}$, $\omega \in W^\Lambda$ and $x \in \Lambda$*

$$|\pi_K(H_x \,|\, \omega) - \pi_{K,R}(H_x \,|\, \omega)| < \varepsilon \,,$$

where

$$\begin{aligned} &\pi_{K,R}(H_x \,|\, \omega) \\ &\quad = \frac{1}{Z_{K,R}(\omega)} \int_{W^{\Lambda\cap K}} H_x(\eta \otimes \omega_{K^\complement}) \, \exp\left(-\mathcal{H}_{K,R}(\eta \otimes \omega_{K^\complement})\right) \, \mathrm{d}\lambda^{\Lambda\cap K}(\eta) \,, \end{aligned}$$

$$\mathcal{H}_{K,R}(\omega) = \sum_{\substack{x\in\Lambda\cap K,\\ y\in\Lambda\cap B_R}} \beta\, \phi(\omega_x, \omega_y)\, J(x-y)$$

and

$$Z_{K,R}(\omega) = \int_{W^{\Lambda\cap K}} \exp\left(-\mathcal{H}_{K,R}(\eta \otimes \omega_{K^\complement})\right) \mathrm{d}\lambda^{\Lambda\cap K}(\eta) \,.$$

Proof. Without loss of generality, assume $x = 0$ (otherwise consider $\Lambda - x$, $K - x$). We have

$$\begin{aligned} &\left|\pi_K(H_x \,|\, \omega) - \pi_{K,R}(H_x \,|\, \omega)\right| \\ &= \Bigg| \frac{1}{Z_K(\omega)} \overbrace{\int_{W^{\Lambda\cap K}} H_0(\eta \otimes \omega_{K^\complement}) \, \exp\big(-\mathcal{H}_K(\eta \otimes \omega_{K^\complement})\big) \, \mathrm{d}\lambda^{\Lambda\cap K}(\eta)}^{I} \\ &\qquad - \frac{1}{Z_{K,R}(\omega)} \underbrace{\int_{W^{\Lambda\cap K}} H_0(\eta \otimes \omega_{K^\complement}) \, \exp\big(-\mathcal{H}_{K,R}(\eta \otimes \omega_{K^\complement})\big) \, \mathrm{d}\lambda^{\Lambda\cap K}(\eta)}_{I_R} \Bigg| \\ &\qquad\qquad \leqslant \left|\frac{I - I_R}{Z_K(\omega)}\right| + \left| I_R \, \frac{Z_K(\omega) - Z_{K,R}(\omega)}{Z_K(\omega)\, Z_{K,R}(\omega)} \right| . \end{aligned}$$

Now

$$\begin{aligned}
&|I - I_R| \\
&\quad = \Bigg| \int_{W^{\Lambda\cap K}} H_0(\eta\otimes\omega_{K^{\complement}}) \Big(\exp\big(-\mathcal{H}_K(\eta\otimes\omega_{K^{\complement}})\big) \\
&\qquad\qquad - \exp\big(-\mathcal{H}_{K,R}(\eta\otimes\omega_{K^{\complement}})\big)\Big)\, \mathrm{d}\lambda^{\Lambda\cap K}(\eta)\Bigg| \\
&= \Bigg| \int_{W^{\Lambda\cap K}} H_0(\eta\otimes\omega_{K^{\complement}})\, \exp\big(-\mathcal{H}_K(\eta\otimes\omega_{K^{\complement}})\big) \\
&\qquad \times \Big(1 - \exp\big(\mathcal{H}_K(\eta\otimes\omega_{K^{\complement}}) - \mathcal{H}_{K,R}(\eta\otimes\omega_{K^{\complement}})\big)\Big)\, \mathrm{d}\lambda^{\Lambda\cap K}(\eta)\Bigg| \\
&\leqslant \int_{W^{\Lambda\cap K}} \Bigg| H_0(\eta\otimes\omega_{K^{\complement}})\, \exp\big(-\mathcal{H}_K(\eta\otimes\omega_{K^{\complement}})\big) \\
&\qquad \times \Big(1 - \exp\big(\mathcal{H}_K(\eta\otimes\omega_{K^{\complement}}) - \mathcal{H}_{K,R}(\eta\otimes\omega_{K^{\complement}})\big)\Big)\Bigg| \, \mathrm{d}\lambda^{\Lambda\cap K}(\eta) \\
&\leqslant \max_{c\in W} |c| \cdot \max_{\eta\in W^{\Lambda\cap K}} \Big|1 - \exp\big(\mathcal{H}_K(\eta\otimes\omega_{K^{\complement}}) - \mathcal{H}_{K,R}(\eta\otimes\omega_{K^{\complement}})\big)\Big| \cdot |Z_K(\omega)|\,.
\end{aligned}$$

We have

$$\begin{aligned}
&|\mathcal{H}_K(\eta\otimes\omega_{K^{\complement}}) - \mathcal{H}_{K,R}(\eta\otimes\omega_{K^{\complement}})| \\
&\qquad = \Bigg| \sum_{\substack{x\in K\cap\Lambda,\\ y\in\Lambda\setminus B_R}} \beta\,\phi(\eta_x,\omega_y)\, J(x-y)\Bigg| \leqslant \Delta_{\mathcal{H}}(K,R,\eta\otimes\omega_{K^{\complement}})
\end{aligned}$$

Here $\Delta_{\mathcal{H}}(K,R,\eta\otimes\omega_{K^{\complement}})$ is used as in Prop. 2.19. As shown in this proposition, $\Delta_{\mathcal{H}}(K,R,\eta\otimes\omega_{K^{\complement}})$ gets arbitrarily small for growing R, independently of η and ω.

For $|x| \leqslant 1$ we have $|\exp(x) - 1| \leqslant 2|x|$ (see [**42**, Theorem (Satz) 2, p.71]). Thus, for R large enough, we have

$$\left|\frac{I - I_R}{Z_K(\omega)}\right| \leqslant \max_{c\in W} |c| \cdot 2\,\Delta_{\mathcal{H}}(K,R,\eta\otimes\omega_{K^{\complement}}) \leqslant \frac{\varepsilon}{2}\,.$$

Basically the same calculations lead to the estimate

$$\left| I_R\, \frac{Z_K(\omega) - Z_{K,R}(\omega)}{Z_K(\omega)\, Z_{K,R}(\omega)}\right| \leqslant \frac{\varepsilon}{2}$$

for some R. We then just take the larger one. □

This proposition states that we only need to know a sufficiently large but finite sample of the boundary condition ω to get estimates for the behaviour of the one-point functions with respect to the specifications π_K. We might interpret this as close sets in $\mathbb{X}$ having close estimates for the specifications.

Theorem 2.23 states that in case of uniqueness of the μ_Λ, which we are in by our restrictions, the specifications π_K converge to the Gibbs measures μ_Λ. For the respective integrals of the one-point functions we need an estimate of this convergence that does not depend on the specific $\Lambda \in \mathbb{X}$:

Proposition 2.33. *Let $\varepsilon > 0$. Then there exists $K \in \mathscr{K}$ such that for all $\Lambda \in \mathbb{X}$, $\omega \in W^\Lambda$ and $x_0 \in \Lambda$ we have*

$$|\pi_K(H_0 \,|\, \omega - x_0) - \mu_{\Lambda - x_0}(H_0)| < \varepsilon \,.$$

Proof. Let $K \in \mathscr{K}$, $\Lambda \in \mathbb{X}$. Again we may assume $x_0 = 0$. Because we are in the Dobrushin uniqueness regime by Restriction 1, we can apply [**44**] theorem (8.23)(ii) to obtain

$$\sup_{\omega \in W^\Lambda} \left| \pi_K(A \,|\, \omega) - \mu_\Lambda(A) \right| \leqslant \sum_{y \in \Lambda \cap K^\complement} D_{0,y} \,, \tag{2.9}$$

for all $A \in \mathscr{F}_{\{0\}}(\Lambda)$, where again $D = (D_{x,y})_{x,y \in \Lambda} = \sum_{n>0} C^n$ and $C = C(\Lambda, \pi)$ is the Dobrushin interdependence matrix. We already know that the right-hand side of (2.9) is the tail of a converging series and consequently vanishes for growing K. But we still need to show that K can be chosen independent of the specific Λ. For this task, we need to apply Remark (8.26) in [**44**]: Consider the following metric on $\mathbb{R}^d$:

$$s(x,y) := \tilde{t} \, \|x - y\| \wedge \tilde{p} \, \log(1 + \|x - y\|) \,,$$

where $a \wedge b$ denotes the minimum of $a, b \in \mathbb{R}$ and $\tilde{t}, \tilde{p} > 0$ are the above constructed constants. It is easy to check that s is indeed a metric[4]. If

$$c_s(\Lambda, \pi) := \sup_{x \in \Lambda} \sum_{y \in \Lambda} C_{xy}(\Lambda, \pi) \, \mathrm{e}^{s(x,y)} < 1 \,, \tag{2.10}$$

the following estimate holds:

$$\sum_{y \in \Lambda \cap K^\complement} D_{0,y}(\Lambda, \pi) \leqslant \frac{2}{1 - c_s(\Lambda, \pi)} \exp\Big(- \min_{y \in \Lambda \cap K^\complement} s(0,y) \Big) \,. \tag{2.11}$$

Since Inequality (2.10) as well as $c_s(\Lambda, \pi)$ still depend on Λ, we need to find some c_s' such that $c_s(\Lambda, \pi) \leqslant c_s' < 1$ for all $\Lambda \in \mathbb{X}(\Gamma)$, because then the condition (2.10) still holds and we may replace $c_s(\Lambda, \pi)$ by c_s' in Inequality (2.10). Fortunately, [**44**, Rem. (8.26)] also provides a way to obtain that c_s': One has

$$\begin{aligned} c_s(\Lambda, \pi) &\leqslant \frac{1}{2} \sup_{x \in \Lambda} \sum_{y \in \Lambda \cap K^\complement} \mathrm{e}^{s(x,y)} \sup_{\omega, \widetilde{\omega} \in W^\Lambda} |\Phi_S(\omega) - \Phi_S(\widetilde{\omega})| \\ &= \frac{1}{2} \sup_{x \in \Lambda} \sum_{y \in \Lambda} \mathrm{e}^{s(x,y)} \beta \, |J(x-y)| \sup_{\omega, \widetilde{\omega} \in W^\Lambda} |\phi(\omega_x, \omega_y) - \phi(\omega_x, \omega_y)| \\ &\leqslant \beta \, m_\phi \sup_{x \in \Lambda} \sum_{y \in \Lambda} \mathrm{e}^{s(x,y)} \, |J(x-y)| \,. \end{aligned}$$

Now

$$\sum_{y \in \Lambda} \mathrm{e}^{s(x,y)} \, |J(x-y)| < \sum_{y \in \Lambda} (1 + \|x - y\|)^{\tilde{p}} \, |J(x-y)| \,,$$

and it is easy to check that there exists some $c_{\tilde{p}}$ such that $(1 + \|z\|)^{\tilde{p}} < c_{\tilde{p}} \, \|z\|^{\tilde{p}}$ for all $z \in \Gamma - \Gamma$. Thus, we have

$$c_s(\Lambda, \pi) \leqslant \beta \, m_\phi \sup_{x \in \Lambda} \sum_{y \in \Lambda} \mathrm{e}^{s(x,y)} \, |J(x-y)| \leqslant \beta \, m_\phi \, c_{\tilde{p}} \, c_\Gamma \,.$$

[4]Note that we included the $\tilde{t} \, \|x - y\|$ part only to show that this construction also works for exponential decay.

We have come to the point where the refinement constant c_β (compare Restriction 2) for the inverse temperature comes into play: If we set $c_\beta > c_{\tilde{p}}$ we get

$$c_s(\Lambda, \pi) \leqslant \beta\, m_\phi\, c_{\tilde{p}}\, c_\Gamma =: c_s' < 1$$

and by that inequality together with Inequalities (2.9), (2.11) also

$$\sup_{\omega \in W^\Lambda} \left|\pi_K(A\,|\,\omega) - \mu_\Lambda(A)\right| \leqslant \frac{2}{1 - c_s'} \exp\Big(- \min_{y \in \Lambda \cap K^\complement} s(0, y)\Big)\,, \tag{2.12}$$

for $A \in \mathscr{F}_{\{0\}}$. Since $s(0, y)$ grows at least logarithmically in $\|y\|$ a set K can be chosen independent of the specific Λ to get this estimate arbitrarily small.

We aim at an estimate for the difference of integrals of the one-point function. For that, fix some $\omega \in W^\Lambda$ and consider that $\kappa(\,\cdot\,) = \pi_K(\,\cdot\,|\,\omega) - \mu_\Lambda(\,\cdot\,)$ defines a signed measure on $(W^\Lambda, \mathscr{F}_{\{0\}}(\Lambda))$. Thus there exists a Hahn-decomposition $W^\Lambda = A^- \cup A^+$ into disjoint sets from $\mathscr{F}_{\{0\}}(\Lambda)$ such that κ is a positive finite measure on $A^+ \cap \mathscr{F}_{\{0\}}(\Lambda)$ as well as $-\kappa$ on $A^- \cap \mathscr{F}_K(\Lambda)$ (see [**21**, Theorem (Satz) 18.1]). Hence we get

$$\begin{aligned}\left|\pi_K(H_0\,|\,\omega) - \mu_\Lambda(H_0)\right| & \\ \leqslant \left|\int_{A^+} H_0(\omega)\,\mathrm{d}\kappa(\omega)\right| + \left|-\int_{A^-} H_0(\omega)\,\mathrm{d}\kappa(\omega)\right| & \\ \leqslant \max_{c \in W} |c|\,\big(|\kappa(A^+)| + |\kappa(A^-)|\big)\,. &\end{aligned}$$

Applying inequality (2.12) for A^+ and A^- and choosing K as in the considerations above then gives the desired result. □

Restriction 2.1. From now on we assume the temperature to be high enough to have

$$\beta < \frac{1}{m_\phi\, c_\Gamma\, c_{\tilde{p}}}\,,$$

where $c_{\tilde{p}}$ is such that $(1 + \|z\|)^{\tilde{p}} < c_{\tilde{p}}\, \|z\|^{\tilde{p}}$ for all $z \in \Gamma - \Gamma$.

Combining the two propositions above, we get the desired continuity of the expectations:

Proposition 2.34. *Let $(\Lambda_n)_{n\in\mathbb{N}}$ be a convergent sequence in $\mathbb{X}$ with limit Λ. Let $(t(n))_{n\in\mathbb{N}}$ be the corresponding sequence of vectors $t(n) \in \mathbb{R}^d$ such that Λ and $\Lambda_n - t(n)$ agree in a large compact set $K_n \subset \mathbb{R}^d$. Then for any $x \in \Lambda$ we have $\mu_{\Lambda_n}(H_{x-t(n)}) \to \mu_\Lambda(H_x)$ for $n \to \infty$.*

Proof. Again we may assume that $x = 0$ and due to the same translation-invariance argument that $t(n) = 0$ for all $n \in \mathbb{N}$. Now let $\varepsilon > 0$. According to Prop. 2.33 we can choose $K \in \mathscr{K}$ such that for any $\omega \in W^\Lambda$

$$|\mu_\Lambda(H_0) - \pi_K(H_0\,|\,\omega)| < \frac{\varepsilon}{4}$$

and for $\omega^n \in W^{\Lambda_n}$

$$|\mu_{\Lambda_n}(H_0) - \pi_K(H_0\,|\,\omega^n)| < \frac{\varepsilon}{4}\,.$$

Prop. 2.32 implies that there exists some $R \in \mathbb{R}^+$ such that also

$$|\pi_K(H_0\,|\,\omega) - \pi_{K,R}(H_0\,|\,\omega)| < \frac{\varepsilon}{4}$$

and

$$|\pi_K(H_0\,|\,\omega^n) - \pi_{K,R}(H_0\,|\,\omega^n)| < \frac{\varepsilon}{4}\,.$$

If we choose n large enough such that Λ and Λ_n agree on B_R and also take $\omega^n_{B_R} = \omega_{B_R}$, we have

$$\pi_{K,R}(H_0\,|\,\omega) = \pi_{K,R}(H_0\,|\,\omega^n)\,,$$

and the triangle inequality thus results in $|\mu_\Lambda(H_0) - \mu_{\Lambda_n}(H_0)| < \varepsilon$. □

We can now define the averaged autocorrelations and analyse their diffractive nature:

Let $C := \max_{c\in W}|c|$ and $V \subset \mathbb{R}^d$ an open set, such that for all $\Lambda \in \mathbb{X}$ we have $\#(\Lambda \cap V) \leqslant 1$. Such a V exists due to the FLC property of Γ. Now let

$$\begin{array}{rccl} \delta^{\mathbb{E}}: & \mathbb{X} & \longrightarrow & \mathcal{M}_{C,V}(\mathbb{R}^d) \\ & \Lambda & \longmapsto & \delta^{\mathbb{E}}_\Lambda := \displaystyle\sum_{x\in\Lambda} \mathbb{E}_{\mu_\Lambda}(H_x)\,\delta_x\,. \end{array}$$

Here we have changed the notation and have written $\mathbb{E}_{\mu_\Lambda}(H_x)$ instead of $\mu_\Lambda(H_x)$ to stress that these values really are (complex) constants (with absolute value smaller than C), only depending on the specific $\Lambda \in \mathbb{X}$ and therefore obviously $\delta^{\mathbb{E}}_\Lambda$ is a translation bounded measure in $\mathcal{M}_{C,V}(\mathbb{R}^d)$.

Proposition 2.35. *The map $\delta^{\mathbb{E}}$ is continuous and maps $\mathbb{X}$ onto the set $\overline{\{\delta^{\mathbb{E}}_\Gamma + t\,|\,t\in\mathbb{R}^d\}}$, where the closure is taken with respect to the vague topology.*

Proof. Since $\mathbb{X}$ is first countable, it is sufficient for continuity to check that for any converging sequence $(\Lambda_n)_{n\in\mathbb{N}}$, $\lim_{n\to\infty}\Lambda_n = \Lambda$ and any continuous function f with compact support also $\delta^{\mathbb{E}}_{\Lambda_n}(f)$ converges to $\delta^{\mathbb{E}}_\Lambda(f)$. Let F be the support of f. Then $\Lambda_n \cap F$ is finite for any $n \in \mathbb{N}$. We have

$$\delta^{\mathbb{E}}_{\Lambda_n}(f) = \sum_{x\in\Lambda_n} \mathbb{E}_{\mu_{\Lambda_n}}(H_x)\,\delta_x(f)) = \sum_{x\in\Lambda_n\cap F} \mathbb{E}_{\mu_{\Lambda_n}}(H_x)\,f(x)\,.$$

By the continuity of f and Prop. 2.34, this finite sum converges in the right manner.

Let $t \in \mathbb{R}^d$. Obviously we have $\delta^{\mathbb{E}}_{\Gamma+t} = \delta^{\mathbb{E}}_\Gamma + t$, because the Gibbs measures have this property. Thus $\delta^{\mathbb{E}}(\{\Gamma + t\,|\,t\in\mathbb{R}^d\}) = \{\delta^{\mathbb{E}}_\Gamma + t\,|\,t\in\mathbb{R}^d\}$. Hence from continuity of $\delta^{\mathbb{E}}$ we obtain

$$\delta^{\mathbb{E}}(\mathbb{X}) = \delta^{\mathbb{E}}(\overline{\{\Gamma + t\,|\,t\in\mathbb{R}^d\}}) \subseteq \overline{\{\delta^{\mathbb{E}}_\Gamma + t\,|\,t\in\mathbb{R}^d\}}\,.$$

On the other hand, $\mathcal{M}_{C,V}(\mathbb{R}^d)$ is Hausdorff by [**10**, Theorem 2] and $\mathbb{X}$ compact. Therefore the image of $\mathbb{X}$ under the continuous map $\delta^{\mathbb{E}}$ itself is compact, thus closed. In addition, this image contains the orbit $\{\delta^{\mathbb{E}}_\Gamma + t\,|\,t\in\mathbb{R}^d\}$. But $\overline{\{\delta^{\mathbb{E}}_\Gamma + t\,|\,t\in\mathbb{R}^d\}}$ is the smallest of such sets, which implies

$$\overline{\{\delta^{\mathbb{E}}_\Gamma + t\,|\,t\in\mathbb{R}^d\}} \subseteq \delta^{\mathbb{E}}(\mathbb{X})\,,$$

and that completes our proof. □

We now get:

Lemma 2.36. *If the dynamical system $(\mathbb{X}, T)$ is pure point diffractive, then the same holds for every $\delta^{\mathbb{E}}_{\Lambda}$. In particular, the autocorrelation coefficients exist and are given by*

$$\eta^{\mathbb{E}}_{\Lambda}(z) := \lim_{R\to\infty} \frac{1}{\operatorname{vol}\left(B_R\right)} \sum_{\substack{x\in\Lambda\cap B_R \\ x-z\in\Lambda}} \mathbb{E}_{\mu_\Lambda}(H_x)\, \mathbb{E}_{\mu_\Lambda}(\overline{H_{x-z}(\omega)})\,.$$

Proof. We know by Prop. 2.35 that $\overline{\{\delta^{\mathbb{E}}_{\Gamma} + t \,|\, t \in \mathbb{R}^d\}}$ with translation as action is a factor of the dynamical system $(\mathbb{X}, T)$. Because we assume $\mathbb{X}$ to be pure point diffractive, the elements of the factor $\overline{\{\delta^{\mathbb{E}}_{\Gamma} + t \,|\, t \in \mathbb{R}^d\}}$ inherit the spectral structure of $(\mathbb{X}, T)$, see [**11**, Thm. 4]. □

It is thus sensible to state the next restriction as follows:

Restriction 4. We assume the system $\mathbb{X}$ to be pure point diffractive.

Remark 2.37. Again, the class of regular model sets provides valid examples. Every regular model set and its complete dynamical system is pure point diffractive, see [**88**]. (Figure 3 shows the diffraction image of the Penrose vertex set as a well known example with pure point diffraction.)

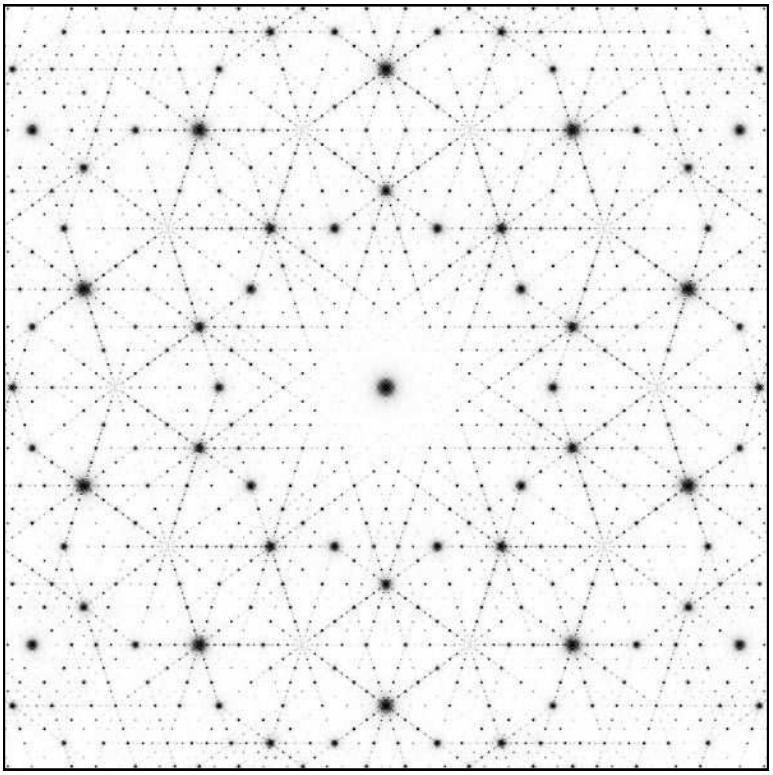


Figure 3. Central patch of the diffraction image of the Penrose vertex set; the diameter of the points corresponds to their intensity. This picture is taken from [**91**]

Now we can make use of the main result of the previous section, namely the ergodicity of the measure ϑ on $\mathbb{Y}$, to calculate some diffraction properties of a randomly weighted set.

Lemma 2.38. *The autocorrelation $\eta^{(H)}(\omega)$ exists almost surely with respect to ϑ.*

Proof. Let

$$\eta_R^{(H)}(\omega, z) := \frac{1}{\operatorname{vol}\big(B_R\big)} \sum_{\substack{x \in \underline{\omega} \cap B_R \\ x-z \in \underline{\omega}}} H_x(\omega)\, \overline{H_{x-z}(\omega)}\,.$$

For fixed z, we might interpret $\eta_R^{(H)}$ as

$$\eta_R^{(H)}(\omega, z) := \frac{\xi_\omega\big(B_R\big)}{\operatorname{vol}\big(B_R\big)}\,,$$

where ξ_ω is the stationary random measure defined by

$$\xi_\omega := \sum_{\substack{x \in \underline{\omega} \\ x-z \in \underline{\omega}}} H_x(\omega)\, \overline{H_{x-z}(\omega)}\, \delta_x\,.$$

Measurability is checked analogously to Remark 2.30 and the translation invariance is obvious. Then, due to the ergodic Theorem 12.2.IV. and preceding remarks in [**32**], by the ergodicity of ϑ, we get ϑ-almost surely

$$\lim_{R\to\infty} \frac{\xi_\omega\big(B_R\big)}{\operatorname{vol}\big(B_R\big)} = \frac{1}{\operatorname{vol}(B)} \int_{\mathbb{Y}} \xi_{\omega'}(B)\, \mathrm{d}\vartheta(\omega')\,,$$

where B is a relatively compact Borel set in $\mathbb{R}^d$ with non empty interior, e.g. the unit cube or any ball of finite radius. Before we go on with the proof, let us just make some remarks on the ergodic theorem above: Instead of shifting the testing area B to get a 'space average' as an estimate for the 'time average', we let the ergodic measure ϑ shift the underlying structure. At the end of this section we will make use of the free choice of B to obtain easier formulas for the diffraction measure.

Recall the definition of the covariance:

$$\operatorname{cov}_{\mu_\Lambda}\big(H_x, \overline{H_y}\big) = \mathbb{E}_{\mu_\Lambda}\big(H_x\, \overline{H_y}\big) - \mathbb{E}_{\mu_\Lambda}\big(H_x\big)\, \mathbb{E}_{\mu_\Lambda}\big(\overline{H_y}\big)\,.$$

Hence, we have

$$\begin{aligned}
&\int_{\mathbb{Y}} \xi_\omega(B)\, \mathrm{d}\vartheta(\omega) \\
&\quad = \int_{\mathbb{Y}} \sum_{\substack{x \in \underline{\omega} \cap B \\ x-z \in \underline{\omega}}} H_x(\omega)\, \overline{H_{x-z}(\omega)}\, \mathrm{d}\vartheta(\omega) = \int_{\mathbb{X}} \sum_{\substack{x \in \Lambda \cap B \\ x-z \in \Lambda}} \mathbb{E}_{\mu_\Lambda}\big(H_x\, \overline{H_{x-z}}\big)\, \mathrm{d}\nu(\Lambda) \\
&\qquad = \int_{\mathbb{X}} \Bigg(\sum_{\substack{x \in \Lambda \cap B \\ x-z \in \Lambda}} \mathbb{E}_{\mu_\Lambda}\big(H_x\big)\, \mathbb{E}_{\mu_\Lambda}\big(\overline{H_{x-z}}\big) + \operatorname{cov}_{\mu_\Lambda}\big(H_x, \overline{H_{x-z}}\big) \Bigg)\, \mathrm{d}\nu(\Lambda) \\
&\qquad\qquad = \int_{\mathbb{X}} \sum_{\substack{x \in \Lambda \cap B \\ x-z \in \Lambda}} \mathbb{E}_{\mu_\Lambda}\big(H_x\big)\, \mathbb{E}_{\mu_\Lambda}\big(\overline{H_{x-z}}\big)\, \mathrm{d}\nu(\Lambda) \\
&\qquad\qquad\qquad + \int_{\mathbb{X}} \sum_{\substack{x \in \Lambda \cap B \\ x-z \in \Lambda}} \operatorname{cov}_{\mu_\Lambda}\big(H_x, \overline{H_{x-z}}\big)\, \mathrm{d}\nu(\Lambda)\,.
\end{aligned}$$

Applying the same ergodic theorem backwards we get

$$\frac{1}{\mathrm{vol}(B)} \int_{\mathbb{X}} \sum_{\substack{x\in\Lambda\cap B\\ x-z\in\Lambda}} \mathbb{E}_{\mu_\Lambda}\big(H_x\big)\, \mathbb{E}_{\mu_\Lambda}\big(\overline{H_{x-z}}\big)\, \mathrm{d}\nu(\Lambda)$$

$$= \lim_{R\to\infty} \frac{1}{\mathrm{vol}\,\big(B_R\big)} \sum_{\substack{x\in\Lambda\cap B_R\\ x-z\in\Lambda}} \mathbb{E}_{\mu_\Lambda}\big(H_x\big)\, \mathbb{E}_{\mu_\Lambda}\big(\overline{H_{x-z}}\big) = \eta_\Lambda^{\mathbb{E}}(z)$$

for ν-almost all $\Lambda \in \mathbb{X}$. The measure $\vartheta \circ \mathrm{supp}^{-1}$ obviously is absolutely continuous with respect to ν (see the proof of Prop. 2.27) and we thus have, for ϑ-almost all $\omega \in \mathbb{Y}$,

$$\frac{1}{\mathrm{vol}(B)} \int_{\mathbb{X}} \sum_{\substack{x\in\Lambda\cap B\\ x-z\in\Lambda}} \mathbb{E}_{\mu_\Lambda}\big(H_x\big)\, \mathbb{E}_{\mu_\Lambda}\big(\overline{H_{x-z}}\big)\, \mathrm{d}\nu(\Lambda) = \eta_{\underline{\omega}}^{\mathbb{E}}(z)\,.$$

Therefore we get (again ϑ-almost surely)

$$\eta^{(H)}(\omega, z) = \eta_{\underline{\omega}}^{\mathbb{E}}(z) + \frac{1}{\mathrm{vol}(B)} \int_{\mathbb{X}} \sum_{\substack{x\in\Lambda\cap B\\ x-z\in\Lambda}} \mathrm{cov}_{\mu_\Lambda}\left(H_x, \overline{H_{x-z}}\right) \mathrm{d}\nu(\Lambda)\,.$$

Since $\underline{\omega} \in \mathbb{X}$, $\eta_\Lambda^{\mathbb{E}}(z)$ exists for all $\Lambda \in \mathbb{X}$ and the second part is an integral of a finite sum of bounded functions, the autocorrelation coefficient exists ϑ-almost surely. □

To exclude singular continuous diffraction we also need the next

Proposition 2.39. *We have*

$$\sum_{z\in\Gamma-\Gamma} \left| \int_{\mathbb{X}} \sum_{\substack{x\in\Lambda\cap B\\ x-z\in\Lambda}} \mathrm{cov}_{\mu_\Lambda}\left(H_x, \overline{H_{x-z}}\right) \mathrm{d}\nu(\Lambda) \right| < \infty\,.$$

Proof. Consider

$$\sum_{z\in\Gamma-\Gamma} \left| \int_{\mathbb{X}} \sum_{\substack{x\in\Lambda\cap B\\ x-z\in\Lambda}} \mathrm{cov}_{\mu_\Lambda}\left(H_x, \overline{H_{x-z}}\right) \mathrm{d}\nu(\Lambda) \right|$$

$$\leqslant \sum_{z\in\Gamma-\Gamma} \int_{\mathbb{X}} \sum_{\substack{x\in\Lambda\cap B\\ x-z\in\Lambda}} \left| \mathrm{cov}_{\mu_\Lambda}\left(H_x, \overline{H_{x-z}}\right) \right| \mathrm{d}\nu(\Lambda)$$

$$= \int_{\mathbb{X}} \sum_{z\in\Lambda-\Lambda} \sum_{\substack{x\in\Lambda\cap B\\ x-z\in\Lambda}} \left| \mathrm{cov}_{\mu_\Lambda}\left(H_x, \overline{H_{x-z}}\right) \right| \mathrm{d}\nu(\Lambda)$$

$$\leqslant \int_{\mathbb{X}} \sum_{x\in\Lambda\cap B} \sum_{y\in\Lambda} \left| \mathrm{cov}_{\mu_\Lambda}\left(H_x, \overline{H_y}\right) \right| \mathrm{d}\nu(\Lambda) \overset{(2.5)}{\leqslant} c_b \cdot \max_{\Lambda\in\mathbb{X}} |\Lambda \cap B| \leqslant \infty\,.$$

□

Finally, we can state the main result of this chapter:

Theorem 2.40. *Let Γ be an FLC set such that the dynamical system $\big(\mathbb{X}(\Gamma), T\big)$ is uniquely ergodic and its diffraction is pure point. Let ϑ be the above constructed Gibbs measure on $\mathbb{Y}$ for an algebraically ($p > d+1$)*

or exponentially decaying potential. Then, at high enough temperatures, ϑ-almost surely no singular continuous part is present in the diffraction of the randomly weighted FLC sets $\omega \in \mathbb{Y}$.

Proof. The autocorrelation coefficients exist ϑ-almost surely. The differences to the averagely weighted FLC sets are given by weighted Dirac combs whose weights are given by a sequence of absolutely summable constants (Prop. 2.39). They thus only lead to an absolutely continuous part of the diffraction (Prop. 1.3), whereas, due to Lemma 2.36, the coefficients of the averagely weighted sets lead to pure point diffraction:

$$\widehat{\gamma^{(H)}(\omega)} = \overbrace{\mathcal{F}\biggl(\sum_{z\in\underline{\omega}-\underline{\omega}} \eta^{\mathbb{E}}_{\underline{\omega}}(z)\,\delta_z\biggr)}^{\text{pure point part}} + \underbrace{\mathcal{F}\biggl(\frac{1}{\mathrm{vol}(B)} \sum_{z\in\underline{\omega}-\underline{\omega}} \Bigl(\int_{\mathbb{X}} \sum_{\substack{x\in\Lambda\cap B\\ x-z\in\Lambda}} \mathrm{cov}_{\mu_\Lambda}\bigl(H_x, \overline{H_{x-z}}\bigr)\,\mathrm{d}\nu(\Lambda)\Bigr)\,\delta_z\biggr)}_{\text{a.c. part}} . \quad (2.13)$$

□

Let us now simplify the formula for the absolutely continuous part of the diffraction in Eq. (2.13) by using the freedom to choose the sample set B. As a first step, let $B = B_\varepsilon$ be the closed ball of radius $\varepsilon > 0$ around $0 \in \mathbb{R}^d$. We may choose ε small enough so that B_ε contains at most 1 point of any $\Lambda \in \mathbb{X}$. Let

$$\mathbb{X}_\varepsilon := \bigl\{\Lambda \in \mathbb{X} \,|\, \#(\Lambda \cap B_\varepsilon) \geqslant 1\bigr\},$$

which is trivially measurable. For any $\Lambda \in \mathbb{X}_\varepsilon$, there exists a uniquely determined $x_\varepsilon(\Lambda) \in \Lambda \cap B_\varepsilon$. Thus, we have

$$\begin{aligned}
&\frac{1}{\mathrm{vol}(B)} \int_{\mathbb{X}} \sum_{\substack{x\in\Lambda\cap B\\ x-z\in\Lambda}} \mathrm{cov}_{\mu_\Lambda}\bigl(H_x, \overline{H_{x-z}}\bigr)\,\mathrm{d}\nu(\Lambda)\\
&\quad= \frac{1}{\mathrm{vol}(B_\varepsilon)} \int_{\mathbb{X}_\varepsilon} 1_\Lambda\bigl(x_\varepsilon(\Lambda) - z\bigr)\ \mathrm{cov}_{\mu_\Lambda}\bigl(H_{x_\varepsilon(\Lambda)}, \overline{H_{x_\varepsilon(\Lambda)-z}}\bigr)\,\mathrm{d}\nu(\Lambda)\\
&\quad\quad= \frac{\nu(\mathbb{X}_\varepsilon)}{\mathrm{vol}(B_\varepsilon)} \int_{\mathbb{X}} 1_\Lambda\bigl(x_\varepsilon(\Lambda) - z\bigr)\ \mathrm{cov}_{\mu_\Lambda}\bigl(H_{x_\varepsilon(\Lambda)}, \overline{H_{x_\varepsilon(\Lambda)-z}}\bigr)\,\mathrm{d}\nu_\varepsilon(\Lambda)\,,
\end{aligned}$$

where ν_ε is the conditional probability measure

$$\nu_\varepsilon(\,\cdot\,) := \nu(\,\cdot\,|\,\mathbb{X}_\varepsilon) = \frac{\nu(\,\cdot\,\cap\,\mathbb{X}_\varepsilon)}{\nu(\mathbb{X}_\varepsilon)}\,.$$

To further simplify this formula, the idea is to look at a suitable limit of this quantity as $\varepsilon \to 0$. Again, we may interpret the measures ν and ν_ε as stationary point processes. In this interpretation, for any sequence $(\varepsilon_n)_{n\in\mathbb{N}}$, such that $\varepsilon_n \to 0$ for $n \to \infty$, the sequence $(\nu_{\varepsilon_n})_{n\in\mathbb{N}}$ is known to converge

weakly[5] to the *Palm measure* ν_0, which is concentrated on the set

$$\mathbb{X}_0 := \{\Lambda \in \mathbb{X} \,|\, 0 \in \Lambda\}\,,$$

see [**58**]. For a definition of the Palm measure in the stationary case see Chapter 3, for a definition in the general case see [**58**]. Now consider that, for $\Lambda \in \mathbb{X}_\varepsilon$ and $B \subset \mathbb{R}^d$ small enough to contain at most one point from any $\Lambda \in \mathbb{X}$, we have

$$\begin{aligned} h(\Lambda) := \sum_{\substack{x\in\Lambda\cap B\\ x-z\in\Lambda}} \operatorname{cov}_{\mu_\Lambda}\left(H_x, \overline{H_{x-z}}\right) \\ = 1_\Lambda\big(x_\varepsilon(\Lambda) - z\big)\, \operatorname{cov}_{\mu_\Lambda}\left(H_{x_\varepsilon(\Lambda)}, \overline{H_{x_\varepsilon(\Lambda)-z}}\right). \end{aligned}$$

Since h is a bounded continuous function, we obtain

$$\begin{aligned} \lim_{n\to\infty} \int_{\mathbb{X}} h(\Lambda)\,\mathrm{d}\nu_{\varepsilon_n}(\Lambda) \\ = \int_{\mathbb{X}} h(\Lambda)\,\mathrm{d}\nu_0(\Lambda) = \int_{\mathbb{X}_0} 1_\Lambda\big(-z\big)\, \operatorname{cov}_{\mu_\Lambda}\left(H_0, \overline{H_{-z}}\right) \mathrm{d}\nu_0(\Lambda)\,. \end{aligned}$$

Note that we may replace $-z$ by z in the above equation, because for $\Lambda \in \mathbb{X}_0$ and $-z \in \Lambda$ also $\Lambda + z \in \mathbb{X}_0$. Further, by the ergodicity of ν and by the same ergodic theorem as used above, we get for ν-almost all $\widetilde{\Lambda} \in \mathbb{X}$

$$\lim_{n\to\infty} \frac{\#(\widetilde{\Lambda} \cap B_n)}{\operatorname{vol}(B_n)} = \frac{1}{\operatorname{vol}(B)} \int_{\mathbb{X}} \#(\Lambda \cap B)\,\mathrm{d}\nu(\Lambda) =: \operatorname{dens}(\Gamma)\,,$$

independent of the choice of the relatively compact B with non-empty interior. For ε small enough, we have

$$1_{\mathbb{X}_\varepsilon}(\Lambda) = \#(\Lambda \cap B_\varepsilon)$$

and thus

$$\frac{\nu(\mathbb{X}_\varepsilon)}{\operatorname{vol}(B_\varepsilon)} = \frac{1}{\operatorname{vol}(B_\varepsilon)} \int_{\mathbb{X}} \#(\Lambda \cap B_\varepsilon)\,\mathrm{d}\nu(\Lambda) = \operatorname{dens}(\Gamma)\,.$$

Combining the above observations, we get the following corollary.

Corollary 2.41. *Under the prerequisites of Theorem* 2.40*, the absolutely continuous part of the diffraction for ϑ-almost all $\omega \in \mathbb{Y}$ is given by*

$$\begin{aligned} \widehat{\gamma^{(H)}(\omega)}_{\mathrm{ac}} \\ = \operatorname{dens}(\Gamma) \cdot \mathcal{F}\left(\sum_{z\in\underline{\omega}-\underline{\omega}} \left(\int_{\mathbb{X}_0} 1_\Lambda\big(z\big) \operatorname{cov}_{\mu_\Lambda}\left(H_0, \overline{H_z}\right) \mathrm{d}\nu_0(\Lambda) \right) \delta_z \right), \end{aligned}$$

where the absolute continuity again follows from the absolute summability of the involved covariance functions. □

[5] A sequence $(P_n)_n$ of point processes in $\mathbb{R}^d$ converges weakly to the point process P if and only if, for all bounded continuous $h : \mathcal{N}(\mathbb{R}^d) \to \mathbb{R}_0^+$, one has $\lim_{n\to\infty} P_n(h) = P$, see [**24**].

2.4. Further thoughts

2.4.1. Conclusions. The constructed class of randomised FLC sets can be interpreted as a model for quasicrystals with structural disorder in equilibrium. It is assumed that the effective interaction is short-ranged. The absence of a singular continuous part of the diffraction spectrum for this class fits into the general picture that modelling physical structures and their diffraction often need not include such a part. Other models of structural disorder (e.g. models in [**6, 16, 17**]) also (mostly) lead to a pure point part if the structure is close to a (quasi)crystalline one with pure point diffraction, e.g. lattices or more generally regular model sets, only adding an absolutely continuous part to the diffraction that results from the covariances of the weights (for instance in [**17**]) or the distribution of displacements (e.g. in [**91, 51, 52**]) of the atoms. In this sense the results of Chapter 2 extend results of [**16, 17, 97**], where Gibbs measures at high temperatures on lattices or with finite weight sets, respectively, are considered.

2.4.2. Outlook. The topology on $\mathbb{Y}$ is a natural candidate for a topology on families of weighted FLC sets since it is essentially the LRT. One could therefore ask if other measures on $(\mathbb{Y}, \mathscr{F})$ share the diffraction results of the Gibbs measure ϑ. Two major components are used to show the absence of singular continuous diffraction in the given model: The first is the ergodicity of ϑ, because the thermodynamic limits then lead to known quantities. Other ergodic (Gibbs) measures, where the ergodicity does not come from a high temperature regime are also possible. The second component is given by the estimate of the covariances of the one-point functions. In our case this estimate is strongly related to the short range potential. It would be interesting to investigate if there are other ways to obtain similarly strong knowledge about the covariances. A first attempt could be to introduce some random displacements of the atoms in the randomly chosen FLC set and still stick to a short range potential. Another extension would be to look into non-compact weight sets, although this could lead to issues of integrability in the context of the local energies.

For the theory of point processes, measures such as ν and ϑ, as given in this chapter, also provide a way to construct stationary point processes that are completely different from Poisson and related processes. In particular, they are concentrated on (marked) Delone configurations, i.e. configurations that obey a hard-core condition and have no big gaps, similar to the process constructed by Kallenberg [**56**]. In addition, there are still hardly explored variations of the well-known model sets, e.g. by changing the windows.

CHAPTER 3

Diffraction of the Matérn hard-core point process

The treatment of the diffraction of stationary, ergodic point processes in $\mathbb{R}^d$ in general has been simplified by Goueré [**46**] by identifying the intensity of the so called Palm distribution with the autocorrelation of almost all realisations. But the exact calculations remain difficult and can only be achieved in certain situations. This is the case in the Matérn hard-core process, thanks to calculations by Stoyan and Stoyan [**94**]. We give a detailed treatment on this case building on observations and claims given in [**6**]. Stochastic geometry knows a tool for the spectral analysis of point processes that is very similar to the diffraction measure, namely the Bartlett spectrum (for a definition see [**18, 19, 31**], for a hint at the connection [**6, 60**]). We are not going to talk about the latter in detail but show how to derive one object from the other in ergodic cases.

3.1. Moments of point processes and diffraction

The Palm distribution of a point process is a so-called second order property of point processes, i.e. a property strongly related to second moments of the process. To prepare and explain the calculations in later sections, we need to introduce some objects. At the end of this section, we also give a precise statement of the above mentioned result that relates these objects to autocorrelation and diffraction, respectively.

In the following we only consider simple point processes in $\mathbb{R}^d$, although the objects defined also make sense for general point processes and random measures. For reasons of completeness we also give the definition of the most important first order object, the *intensity measure* or *first moment* of a point process. Let P be a point process in $\mathbb{R}^d$. Then the intensity measure $\vartheta_P^{(1)} =: \vartheta_P$ is given by

$$\vartheta_P^{(1)}(f) := \int_{\mathcal{N}} \int_{\mathbb{R}^d} f(x)\, \mathrm{d}\mu(x)\, \mathrm{d}P(\mu)\,,$$

for every measurable function f from $\mathbb{R}^d$ to $\mathbb{R}_0^+$, where $\mathcal{N} = \mathcal{N}(\mathbb{R}^d)$ denotes the space of counting measures in $\mathbb{R}^d$. This measure need not be σ-finite. In case it is, we will call P a *first order* or *integrable* point process.

In the case of a stationary process, the intensity measure is always a multiple of the Lebesgue measure, i.e. $\vartheta_P = \kappa\, \lambda^d$, where $\kappa \in \mathbb{R}_0^+$. In this case also κ is called the *intensity*.

The definition of the first moment measure extends naturally to the *n-th moment measure* given by

$$\vartheta_P^{(n)}(h) := \int_{\mathcal{N}} \int_{\mathbb{R}^d}^{n} \cdots \int_{\mathbb{R}^d} h(x_1, \ldots, x_n) \, \mathrm{d}\mu^n(x_1, \ldots, x_n) \, \mathrm{d}P(\mu) \\ = \int_{\mathcal{N}} \sum_{x_1, \ldots, x_n \in \operatorname{supp} \mu} h(x_1, \ldots, x_n) \, \mathrm{d}P(\mu) \,,$$

where $h : \mathbb{R}^d \times \overset{n\text{-times}}{\cdots} \times \mathbb{R}^d \to \mathbb{R}_0^+$ is assumed measurable. In particular,

$$\vartheta_P^{(n)}(B_1 \times \cdots \times B_n) = \mathbb{E}_P(\zeta_{B_1} \cdot \ldots \cdot \zeta_{B_n}) \,,$$

for $B_1, \ldots, B_n \in \mathscr{B}_0(\mathbb{R}^d)$, where ζ_B again denotes the random variable defined by $\zeta_B(\mu) = \mu(B)$. If the measure is locally finite on $(\mathbb{R}^d)^n$, we will call P an *n-th order* or *n-times integrable* point process.

A close relative of the n-th moment measure is the n-th factorial moment measure given by

$$\alpha_P^{(n)}(h) := \int_{\mathcal{N}} \sum_{\substack{x_1, \ldots, x_n \in \operatorname{supp} \mu \\ x_i \neq x_j \text{ for } i \neq j}} h(x_1, \ldots, x_n) \, \mathrm{d}P(\mu) \,.$$

Thus the difference to the n-th moment is that the factorial moment only counts the evaluation of h where the n-tuples $(x_1, \ldots, x_n)$ consist of distinct points x_i. Note that permutations are still counted. If $B_1, \ldots, B_n$ are pairwise disjoint Borel sets in $\mathbb{R}^d$, then $\vartheta_P^{(n)}(B_1 \times \cdots \times B_n) = \alpha_P^{(n)}(B_1 \times \cdots \times B_n)$.

From now on, we restrict ourselves to the case where n is at most two. Suppose that $\alpha_P^{(2)}$ is absolutely continuous with respect to the Lebesgue measure, i.e. there exists $\rho_P^{(2)} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}_0^+$ such that

$$\alpha_P^{(2)}(h) := \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} h(x, y) \, \rho_P^{(2)}(x, y) \, \mathrm{d}\lambda^d(x) \, \mathrm{d}\lambda^d(y) \,,$$

then $\rho_P^{(2)}$ is called the *second-order product density*. In case of a translation and rotation invariant process P, the density (if it exists) can always be written in the form $\rho_P^{(2)}(x, y) = \rho_P(\|x - y\|)$, see [**59**]. We will also call ρ_P the second-order product density.

We can now define the important Palm distribution or Palm measure. Let P be a stationary point process in $\mathbb{R}^d$ with finite intensity κ. The Palm measure P_0 of P can be defined in the following way: for $F \in \mathscr{F}(\mathbb{R}^d)$ let

$$P_0(F) := \frac{1}{\kappa \cdot \lambda^d(B)} \int_{\mathcal{N}} \sum_{x \in \operatorname{supp} \mu \cap B} 1_F(\mu - x) \, \mathrm{d}P(\mu) \,, \tag{3.14}$$

where B is an arbitrary Borel set with non-empty volume. The definition does not depend on the specific B and defines a probability on $\mathscr{F}(\mathbb{R}^d)$, concentrated on counting measures with an atom at 0. There is a direct connection to the second order factorial measure: let B_1, B_2 be Borel sets in $\mathbb{R}^d$ then

$$\alpha_P^{(2)}(B_1 \times B_2) = \kappa^2 \int_{B_1} \mathcal{K}(B_2 - x) \, \mathrm{d}\lambda^d(x) \tag{3.15}$$

where $\mathcal{K}$ is the *second reduced moment measure*, defined with the Palm measure by

$$\mathcal{K}(B) := \frac{1}{\kappa} \int_{\mathcal{N}} \mu(B \smallsetminus \{0\}) \, \mathrm{d}P_0(\mu) \, .$$

The equation (3.15) then follows from the refined Campbell theorem (see [**59**]). This also yields λ^d-almost surely the equation

$$\mathcal{K}(B) = \frac{1}{\kappa^2} \int_{\mathbb{R}^d} 1_B(x) \, \rho_P(\|x\|) \, \mathrm{d}\lambda^d(x) \, ,$$

if the density ρ_P exists. But the above relation also gives us the possibility to calculate the intensity of the Palm measure by means of the second order product density: for a Borel set $B \subset \mathbb{R}^d$ we get

$$\begin{aligned} \vartheta_{P_0}(B) &= \int \mu(B) \, \mathrm{d}P_0(\mu) \\ &= \int \mu(B \smallsetminus \{0\}) \, \mathrm{d}P_0(\mu) + 1_B(0) \int \mu(\{0\}) \, \mathrm{d}P_0(\mu) = \kappa \mathcal{K}(B) + 1_B(0) \\ &= \frac{1}{\kappa} \int 1_B(x) \, \rho_P(\|x\|) \, \mathrm{d}\lambda^d(x) + 1_B(0) \, , \end{aligned}$$

and thus

$$\vartheta_{P_0} = \frac{1}{\kappa} \rho_P(\|\cdot\|) \, \lambda^d + \delta_0 \, .$$

The connection of ϑ_{P_0} and the autocorrelation of point sets realized by certain point processes is given by the following theorem:

Theorem 3.1. *Let P be a second order stationary ergodic point process in $\mathbb{R}^d$ with intensity κ. Then for P-almost all $\mu \in \mathcal{M}(\mathbb{R}^d)$ the natural autocorrelation measures $\gamma(\mu)$ exist and are the same, given by*

$$\gamma(\mu) = \gamma_P = \kappa \, \vartheta_{P_0} \, .$$

Proof. For a proof see [**46**] or, with more details, [**6**]. □

In terms of the second order product density this translates to the following:

Corollary 3.2. *Let P be a second order stationary ergodic point process in $\mathbb{R}^d$ with intensity κ such that the second order product density ρ_P exists. Then P-almost surely the natural autocorrelation measure for a configuration μ exists and is given by*

$$\gamma(\mu) = \rho_P(\|\cdot\|) \, \lambda^d + \kappa \, \delta_0 \, .$$

□

This also gives us an easy example, namely the natural autocorrelation of the stationary Poisson point process:

Example 3.3. The Poisson Process P_κ is known to have the simple constant second order product density $\rho_{P_\kappa}(r) = \kappa^2$, compare e.g. [**59**]. This leads to an almost sure autocorrelation of $\gamma_{P_\kappa} = \kappa^2 \, \lambda^d + \kappa \, \delta_0$ and thus to diffraction $\widehat{\gamma_{P_\kappa}} = \kappa^2 \, \delta_0 + \kappa \, \lambda^d$.

The next example is an example about what can go wrong, if the point process is not ergodic.

Example 3.4. Let $0 < p < 1$ and let $\kappa_1, \kappa_2 > 0$ and $P_1 = P_{\kappa_1}, P_2 = P_{\kappa_2}$ be the corresponding stationary Poisson point processes. The *mixed* Poisson process given by $P := p\,P_1 + (1-p)\,P_2$ then is the easiest version of a Cox-process, a process where the intensity is chosen at random, see for instance [**58**]. It is not ergodic as a non trivial convex combination of two ergodic processes (see [**58**, 6.2.6.]). The intensity of P is given by the same convex combination of the two respective intensities. Analogously, its Palm measure is a mixture of the Palm measures $P_{1,0}, P_{2,0}$ of the original Poisson processes

$$P_0 = \frac{1}{\kappa}\big(p\,\kappa_1\,P_{1,0} + (1-p)\,\kappa_2\,P_{2,0}\big)\,,$$

by directly applying the definition of the Palm measure, (3.14). This necessarily leads to the same linear combination for the intensity of P_0. If the construction would also work in this non ergodic case we would get the autocorrelation to be almost surely

$$\begin{aligned}\kappa\,\vartheta_{P_0} &= p\,\kappa_1\,\vartheta_{P_{1,0}} + (1-p)\,\kappa_2\,\vartheta_{P_{2,0}}\\ &= p\,\kappa_1\,(\kappa_1\,\lambda^d + \delta_0) + (1-p)\,\kappa_2\,(\kappa_2\,\lambda^d + \delta_0)\\ &= \big(p\,{\kappa_1}^2 + (1-p){\kappa_2}^2\big)\,\lambda^d + \kappa\,\delta_0\end{aligned}$$

and the diffraction

$$\big(p\,{\kappa_1}^2 + (1-p){\kappa_2}^2\big)\,\delta_0 + \kappa\,\lambda^d\,.$$

This cannot be the P-almost sure diffraction as, with probability $p < 1$, a configuration is a Poisson realisation with intensity κ_1, and thus has diffraction ${\kappa_1}^2\,\delta_0 + \kappa_1\,\lambda^d$.

Before we turn to the examination of the Matérn hard-core point process, let us give the connection between the diffraction measure and the before mentioned Bartlett spectrum:

Proposition 3.5. *Let P be a second order stationary point process in $\mathbb{R}^d$ with intensity κ. Let further ξ_P be the* reduced covariance measure *of P, defined for Schwartz functions φ as*

$$\xi_P(\varphi) := \int_{\mathbb{N}}\int_{\mathbb{U}^d} (\mu - x)(\varphi)\,\mathrm{d}\mu(x)\,\mathrm{d}P(\mu) - \kappa^2\,\lambda^d(\varphi)\,,$$

where $\mathbb{U}^d$ is the unit cube in $\mathbb{R}^d$ (which can again be replaced by any Borel set of Lebesgue measure 1). Then there exists a symmetric, translation-bounded measure $\beta_P \in \mathcal{M}(\mathbb{R}^d)$, such that for all $\varphi \in \mathcal{S}(\mathbb{R}^d)$

$$\xi_P(\varphi) = \beta_P(\check{\varphi})\,.$$

Proof. See [**31**, Prop. 8.2.I]. Note that the inverse Fourier transform of a Schwartz function φ in [**31**] is defined by

$$\int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\,x\cdot y}\varphi(x)\,\mathrm{d}x$$

and thus might lead to differences in the form of missing constant factors $1/(2\pi)^d$ in our calculations compared to the quoted sources. □

This proposition suggests the following definition:

Definition 3.6. Let P be a second order stationary point process in $\mathbb{R}^d$. A measure β_P that is associated to P in the sense of Prop. 3.5 is called the *Bartlett spectrum* of P.

The Bartlett spectrum is unique, since the inverse Fourier transform of a tempered distribution is unique (see [**83**]).

Example 3.7. The Bartlett spectrum of the stationary Poisson process with intensity κ is given by $\beta_{P_\kappa} = \kappa\lambda^d$, see [**31**, Ex. 8.2(a)].

The example above gives some intuition for the following connection between the Bartlett spectrum and diffraction measure:

Proposition 3.8. *Let P be a stationary ergodic point process with intensity κ. Then we have*

$$\widehat{\gamma_P} = \beta_P + \kappa^2\,\delta_0\,.$$

Proof. Let φ be a Schwartz function and consider

$$\begin{aligned}\widehat{\gamma_P}(\breve{\varphi}) &= \gamma_P(\widehat{\breve{\varphi}}) = \gamma_P(\varphi) = \kappa\,\vartheta_{P_0}(\varphi)\\ &= \int_{\mathcal{N}}\int_{\mathbb{U}^d} (\mu - x)(\varphi)\,\mathrm{d}\mu(x)\,\mathrm{d}P(\mu) = \xi_P(\varphi) - \kappa^2\,\lambda^d(\varphi)\\ &= \xi_P(\varphi) + \kappa^2\,\lambda^d(\widehat{\breve{\varphi}}) = \xi_P(\varphi) + \kappa^2\,\widehat{\lambda^d}(\breve{\varphi}) = \xi_P(\varphi) + \kappa^2\,\delta_0(\breve{\varphi})\,.\end{aligned}$$

□

Note that a connection between the Bartlett spectrum and diffraction is also mentioned in [**60**] and used for structural analysis.

3.2. The Matérn hard-core point process

Theorem 3.1 will give us the opportunity to calculate the diffraction of almost all the counting measures with respect to the point process that we are going to introduce in the sequel. Of course all the prerequisites need to be checked. The idea to the process we regard was first introduced by Matérn in his PhD thesis in 1960 to model repulsive action between random points, see [**72**].

Let P be the stationary, independently marked Poisson point process in $\mathbb{R}^d$ with marks in $(0,1)$. That is, the marks are uniformly distributed in $I = (0,1)$, and the underlying point process is given by the Poisson point process P_κ, $\kappa > 0$. Let π be the projection from the marked point configurations to the unmarked ones. The *Matérn hard core point process* P_R with hard-core radius R is given as the image of P under the mapping

$$\begin{array}{rccc}\varphi_R\colon & \mathcal{N}(\mathbb{R}^d\times I) & \longrightarrow & \mathcal{N}(\mathbb{R}^d)\\ & \mu & \longmapsto & \mu_R = \displaystyle\sum_{x\in\operatorname{supp}\mu_R}\delta_x\,,\end{array}$$

where for $\mu = \sum_{x\in\operatorname{supp}\pi(\mu)}\delta_{(x,m_x)}$

$$\begin{aligned}&\operatorname{supp}\mu_R\\ &= \big\{x\in\operatorname{supp}\pi(\mu)\,\big|\,m_x < m_y,\ \text{for all } y\in\big(\operatorname{supp}\pi(\mu)\cap B_R(x)\big)\smallsetminus\{x\}\big\}\,.\end{aligned}$$

So $P_R := \varphi_R(P)$ picks the points of a realization μ that have the smallest mark in a ball of radius R around them. The basic concepts of the process are illustrated in the sequence of images of Figure 4.

Note that the thinning is simultaneous, so that even a thinned out point might thin out another one. Thus, the interaction of one point in a configuration is limited to the points within the distance R. This, together with the stationarity of the Poisson process and the independent marking, directly results in the stationarity of the Matérn process. It is also the key ingredient for the proof of ergodicity of P_R:

Proposition 3.9. *The process P_R is mixing, hence also ergodic.*

Proof. Every mixing process is ergodic (see e.g. [**89**, p. 194]) so we can concentrate on that property. The strategy will be to use the mixing property of the underlying Poisson point process. Since the hard-core condition only acts locally, points far from each other do not interact due to the simultaneous thinning. Thus the random variables ζ_{K_1} and ζ_{K_2} become independent if the two sets K_1, K_2 are far away from each other.

According to [**89**, Theorem (Satz) 5.2.3], to check if P_R is mixing is equivalent to checking the following property: for all compact $K_1, K_2 \subset \mathbb{R}^d$

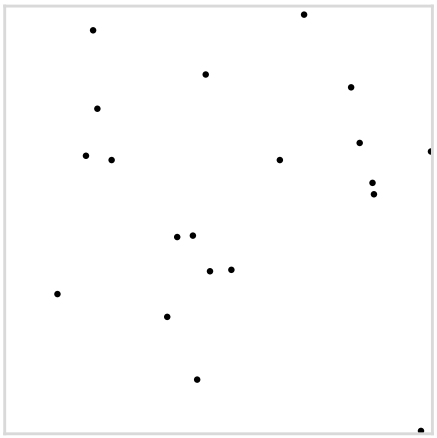
$$\lim_{\|x\|\to\infty} \Big(1 - P_R\Big(\Big\{\mu \in \mathcal{N}(\mathbb{R}^d) \,\Big|\, \mu\big(K_1 \cup (K_2 - x)\big) > 0\Big\}\Big)\Big) = \Big(1 - P_R\big(\{\zeta_{K_1} > 0\}\big)\Big)\Big(1 - P_R\big(\{\zeta_{K_2} > 0\}\big)\Big)$$

or equivalently

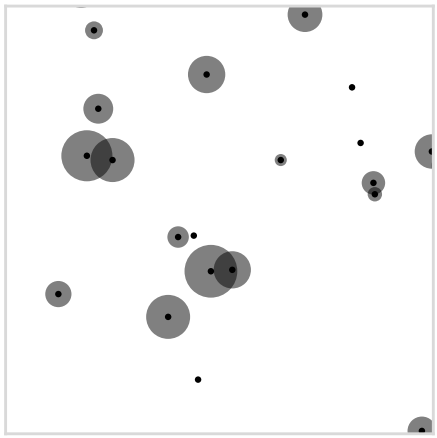
$$\lim_{\|x\|\to\infty} P_R\Big(\Big\{\mu \in \mathcal{N}(\mathbb{R}^d) \,\Big|\, \mu\big(K_1 \cup (K_2 - x)\big) = 0\Big\}\Big) = P_R\big(\{\zeta_{K_1} = 0\}\big) \cdot P_R\big(\{\zeta_{K_2} = 0\}\big)\,.$$

(Recall $\zeta_B(\mu) = \mu(B)$.) For $K \in \mathscr{K}(\mathbb{R}^d)$ let $K^{(R)} := K + B_R(0)$. Then by the definition of φ_R we get $\varphi_R(\nu)(K) = \varphi_R(\nu|_{K^{(R)}})(K)$, because the thinning is done simultaneously and only the marks of points at distance at most R from K influence the thinning in K. (Here $\nu|_{K^{(R)}}$ denotes the restriction of ν to $K^{(R)}$.) Now let $\|x\|$ be large enough such that $K_1^{(R)}$ and $K_2^{(R)}$ do not intersect. Then

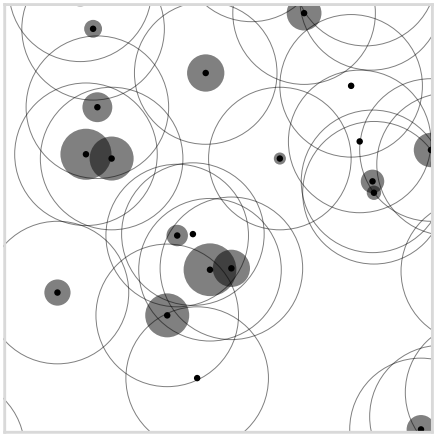
$$\begin{aligned}
&P_R\Big(\Big\{\mu \in \mathcal{N}(\mathbb{R}^d) \,\Big|\, \mu\big(K_1 \cup (K_2 - x)\big) = 0\Big\}\Big) \\
&\quad = P_R\Big(\Big\{\mu \in \mathcal{N}(\mathbb{R}^d) \,\Big|\, \mu(K_1) = 0,\, \mu(K_2 - x) = 0\Big\}\Big) \\
&\quad = P\Big(\Big\{\nu \in \mathcal{N}(\mathbb{R}^d \times I) \,\Big|\, \varphi_R(\nu)(K_1) = 0,\, \varphi_R(\nu)(K_2 - x) = 0\Big\}\Big) \\
&= P\Big(\Big\{\nu \in \mathcal{N}(\mathbb{R}^d \times I) \,\Big|\, \varphi_R(\nu|_{K_1^{(R)}})(K_1) = 0,\, \varphi_R(\nu|_{K_2^{(R)} - x})(K_2 - x) = 0\Big\}\Big)
\end{aligned}$$



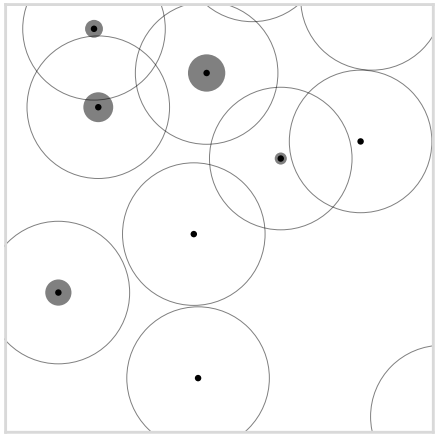
(a) First the Poisson process realises some random point set in $\mathbb{R}^2$



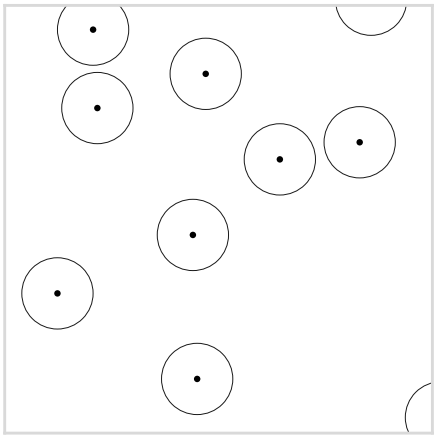
(b) Now the marks are choosen independently for each point of the realisation, illustrated by the radii of the grey disks



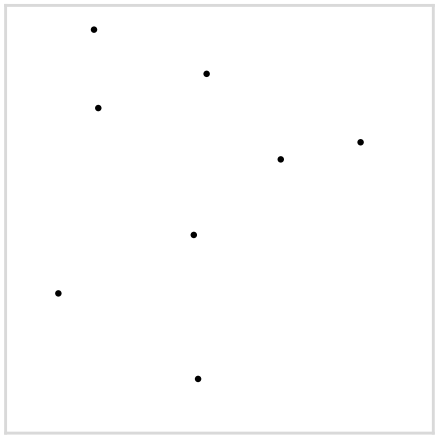
(c) Within each hard-core radius, the marks are compared



(d) Only the points with the smallest mark within each hard-core radius 'survive'



(e) This image is meant to show why the process has 'hard cores' by drawing circles of half the hard-core radius around the remaining points



(f) The last image illustrates the resulting outcome of the Matérn process for the sample realisation

FIGURE 4. An illustration of the Matérn hard-core point process

Because the restrictions of a Poisson process to disjoint sets are independent we get

$$\begin{aligned}
&P_R\Big(\Big\{\mu\in\mathcal{N}(\mathbb{R}^d)\,\Big|\,\mu\big(K_1\cup(K_2-x)\big)=0\Big\}\Big)\\
&\qquad= P\Big(\Big\{\nu\in\mathcal{N}(\mathbb{R}^d\times I)\,\Big|\,\varphi_R(\nu|_{K_1^{(R)}})(K_1)=0\Big\}\Big)\\
&\qquad\qquad\times P\Big(\Big\{\nu\in\mathcal{N}(\mathbb{R}^d\times I)\,\Big|\,\varphi_R(\nu|_{K_2^{(R)}-x})(K_2-x)=0\Big\}\Big)\\
&\quad= P_R\big(\{\mu\in\mathcal{N}(\mathbb{R}^d)\,|\,\mu(K_1)=0\}\big)\cdot P_R\big(\{\mu\in\mathcal{N}(\mathbb{R}^d)\,|\,\mu(K_2-x)=0\}\big)\\
&\qquad= P_R\big(\{\mu\in\mathcal{N}(\mathbb{R}^d)\,|\,\mu(K_1)=0\}\big)\cdot P_R\big(\{\mu\in\mathcal{N}(\mathbb{R}^d)\,|\,\mu(K_2)=0\}\big)\,,
\end{aligned}$$

because P_R is stationary. □

Thanks to the calculations in [**94**] and [**59**], we know that the intensity of the process P_R is

$$\kappa_R=\frac{1-\exp(-\kappa\,b_R)}{b_R}$$

and that the second order product density $\rho_R:=\rho_{P_R}$ is given by

$$\rho_R(r)=\begin{cases}0\,, & \text{if } r\leqslant R\,,\\[2ex] 2\,\dfrac{G_R(r)\big(1-\exp(-\kappa\,b_R)\big)-b_R\big(1-\exp(-\kappa\,G_R(r))\big)}{b_R\,G_R(r)\,(G_R(r)-b_R)}, & \text{if } r>R\,,\end{cases}$$

where $b_R=b_{d,R}=\frac{\pi^{d/2}}{\Gamma((d/2)+1)}R^d$ is the volume of a d-dimensional ball with radius R in $\mathbb{R}^d$ and

$$G_R(r)=\lambda^d(B_R(0)\cup B_R(x_r))=2\,b_R-\overbrace{\lambda^d(B_R(0)\cap B_R(x_r))}^{=:g_R(r)}\,,$$

where x_r is an arbitrary vector of length r. Now obviously $G_R(r)=2\,b_R$ for $r\geqslant 2\,R$ and one thus has after an easy calculation that $\rho_R(r)={\kappa_R}^2$ in that case. So, outside a ball of radius $2\,R$, the second order product density looks exactly like the respective one of a Poisson process with intensity κ_R. It is therefore reasonable to regard the second order density, and also the autocorrelation of the process, as being the second order product density of a slightly refined Poisson point process by writing

$$\rho_R(r)={\kappa_R}^2+\widetilde{\rho}_R(r)\,,$$

with

$$\widetilde{\rho}_R(r)=-1_{[0,2R]}(r)\,{\kappa_R}^2+1_{[R,2R]}(r)\,\rho_R(r)\,,$$

Note that $\widetilde{\rho}_R(\|\cdot\|)$ obviously has compact support $B_{2R}(0)$ and is bounded, which allows us to calculate its Fourier transform. Since it is also obviously a function in $L^1(\mathbb{R}^d)$, we also know that its transform vanishes at infinity by the Riemann-Lebesgue Lemma (see e.g. [**80**, Thm. 2.2.4]). We will refer to $\widetilde{\rho}_R(\|\cdot\|)$ as the refined second order (product) density.

The intensity κ_R gives the average packing density of the process, i.e. the average ratio of the space filled by non overlapping spheres (in our case, they have a radius of $R/2$) around the points of the realisation an the 'total space'. Some easy calculations give a maximal packing density of $(1/2)^d$,

which is far of from a dense packing, compare e.g. [**73**]. In $d = 3$ in a face-centred cubic lattice the spheres occupy $\pi/\sqrt{18} = 0.74\ldots$ of the total space, see [**29**].

Before we go deeper into the examination of the diffraction, let us consider the point-wise limit of the densities for $\kappa \to \infty$: Obviously we have

$$\lim_{\kappa\to\infty} \kappa_R = \frac{1}{b_R}$$

and

$$\lim_{\kappa\to\infty} \rho_R(r) = 1_{(R,\infty)}(r)\, \frac{2}{b_R\, G_R(r)} =: \rho_R^\infty(r)\,.$$

Analogously we define

$$\widetilde{\rho}_R^\infty(r) := -1_{[0,2R]}(r)\, \frac{1}{{b_R}^2} + 1_{[R,2R]}(r)\, \rho_R^\infty(r)\,.$$

These limits are reached exponentially fast and thus provide a good estimate for the calculations of the diffraction for large κ, as we will see in various figures. It is not obvious that those point-wise limits belong to some point process that is the limit of the corresponding Matérn point processes in some sense. Nevertheless, for any sequence of Poisson intensities $(\kappa^{(n)})_{n\to\infty}$, the sequence $(P_{R,n})$ of corresponding Matérn processes has the the property that, for any bounded Borel set $B \subset \mathbb{R}^d$,

$$\lim_{t\to\infty} \limsup_{n\to\infty} P_{R,n}(\zeta_B > t) = 0\,, \tag{3.16}$$

because $P_{R,n}$-almost surely, for all n, the counting function ζ_B is obviously bounded by $\lambda^d(B_R)$ times the maximal number of non-intersecting $(R/2)$-balls in the set $B + B_{R/2}$. Due to [**55**, Lemma 4.4], Equation 3.16 implies that the sequence $(P_{R,n})_{n\in\mathbb{N}}$ is relatively compact in the vague topology and thus has at least one accumulation point.

The limit $\kappa \to 0$ leads to the process that almost surely realizes the empty space. In this case, also $\kappa_R = 0$, and the product density is also constantly 0.

Since one can always adjust the intensity κ to get qualitatively the same but scaled process for different R, we set $R = 1$ in the following figures without loss of generality. (We will give an argument for that later on.)

3.3. Diffraction properties

Since we know the autocorrelation of a Poisson process and the Fourier transform is linear, we can concentrate on the diffraction part coming from $\widetilde{\rho}_R$: The autocorrelation of P_R is given by

$$\begin{aligned}\gamma_{P_R} &= \rho_R(\|\cdot\|)\,\lambda^d + \kappa_R\,\delta_0 \\ &= {\kappa_R}^2\,\lambda^d + \kappa_R\,\delta_0 + \widetilde{\rho}_R(\|\cdot\|)\,\lambda^d = \gamma + \widetilde{\rho}_R(\|\cdot\|)\,\lambda^d\,,\end{aligned}$$

where γ is the autocorrelation of the Poisson process P_{κ_R}, and thus the diffraction is

$$\widehat{\gamma_{P_R}} = \widehat{\gamma} + \mathcal{F}\big(\widetilde{\rho}_R(\|\,\cdot\,\|)\big)\,\lambda^d\,,$$

where we used that by an application of the Fubini Theorem, for a test-function $\varphi \in \mathcal{S}(\mathbb{R}^d)$, we have

$$\begin{aligned}
&\mathcal{F}\big(\widetilde{\rho}_R(\|\cdot\|)\,\lambda^d\big)(\varphi)\\
&\quad = \big(\widetilde{\rho}_R(\|\cdot\|)\,\lambda^d\big)(\widehat{\varphi}) = \int_{\mathbb{R}^d} \widetilde{\rho}_R(\|y\|) \int_{\mathbb{R}^d} \varphi(x)\,\mathrm{e}^{-2\pi\mathrm{i}\,x\cdot y}\,\mathrm{d}\lambda^d(x)\,\mathrm{d}\lambda^d(y)\\
&= \int_{\mathbb{R}^d} \varphi(x) \int_{\mathbb{R}^d} \widetilde{\rho}_R(\|y\|)\,\mathrm{e}^{-2\pi\mathrm{i}\,y\cdot x}\,\mathrm{d}\lambda^d(y)\,\mathrm{d}\lambda^d(x) = \Big(\mathcal{F}\big(\widetilde{\rho}_R(\|\cdot\|)\big)\,\lambda^d\Big)(\varphi)\,.
\end{aligned}$$

So the main task is to compute, or at least analyse, the Fourier transform of $\widetilde{\rho}_R(\|\cdot\|)$.

In dimension $d = 1$ the function $g_R(r)$ is simply given by $g_R(r) = 2R - r$ and allows us to compute the diffraction of P_R explicitly. In higher dimensions, we can give only formulas containing special integrals and discuss the results by comparing different intensities κ of the underlying Poisson process and dimensions.

3.3.1. Diffraction in dimension $d = 1$. As mentioned above, we have $g_R(r) = 2R - r$, $b_R = 2R$ and thus $G_R(r) = 2R + r$ for $R \leqslant r \leqslant 2R$. So the product density for those radii is given by

$$\begin{aligned}
\rho_R(r) &= 2\,\frac{(2R+r)\big(1-\exp(-\kappa\,2R)\big) - 2R\big(1-\exp(-\kappa\,(2R+r))\big)}{2R\,(2R+r)\,(2R+r-2R)}\\
&= \frac{2\kappa_R}{r} - \frac{2}{(2R+r)r} + \frac{2\exp(-\kappa\,(2R+r))}{(2R+r)r}
\end{aligned}$$

and the corresponding point-wise limit for $\kappa \to \infty$ by

$$\rho_R^{\infty}(r) = \frac{1}{R(r+2R)}\,.$$

Thus we have for $R \leqslant r \leqslant 2R$ (see Figure 5)

$$\widetilde{\rho}_R(r) = -{\kappa_R}^2 + \frac{2\kappa_R}{r} - \frac{2}{(2R+r)r} + \frac{2\exp(-\kappa\,(2R+r))}{(2R+r)r}\,.$$

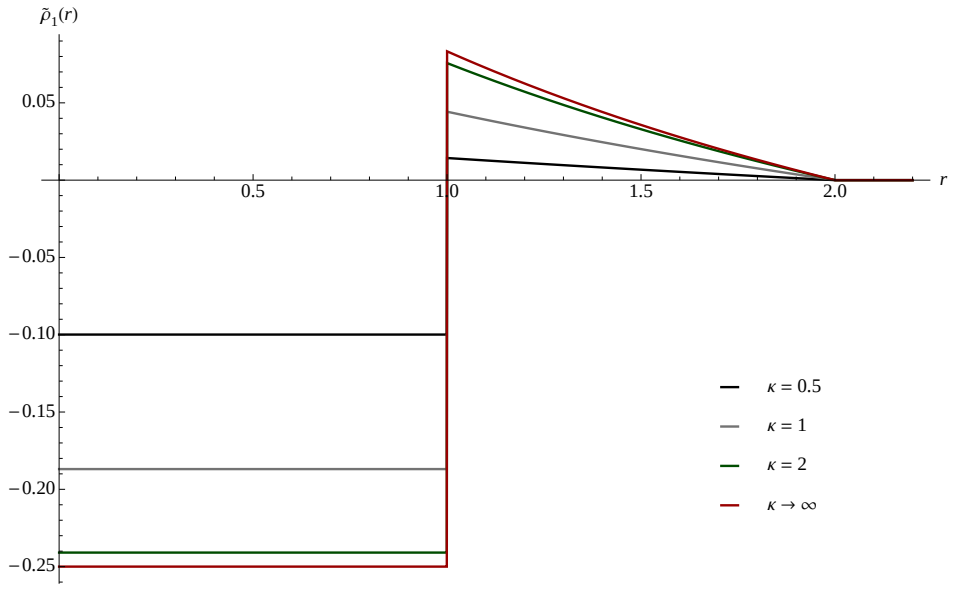


FIGURE 5. $\widetilde{\rho}_R(r)$ in $d = 1$ for $R = 1$ and different intensities κ including the limit $\kappa \to \infty$

The Fourier transform of $\widetilde{\rho}_R(|\cdot|)$ can be computed explicitly (by elementary calculations) and is given by

$$\begin{aligned}
\widehat{\gamma}_{\mathrm{ref}}(y) &:= \mathcal{F}\big(\widetilde{\rho}_R(|x|)\big)(y) \\
&= -{\kappa_R}^2 \frac{\sin(4\pi R\, y)}{\pi\, y} + 4\,\kappa_R\big(\operatorname{Ci}(4\pi R y) - \operatorname{Ci}(2\pi R y)\big) \\
&\quad - \frac{2}{R}\Big(\operatorname{Ci}(4\pi R y) - \operatorname{Ci}(2\pi R y) + \cos(4R\pi y)\big(\operatorname{Ci}(6R\pi y) - \operatorname{Ci}(8R\pi y)\big) \\
&\qquad + \sin(4R\pi y)\big(\operatorname{Si}(6R\pi y) - \operatorname{Si}(8R\pi y)\big)\Big) \\
&\quad + \frac{\exp(-2R\kappa)}{R}\Big[\operatorname{Ei}\big(-2R(\kappa + 2\pi \mathrm{i}\, y)\big) - \operatorname{Ei}\big(-R(\kappa + 2\pi \mathrm{i}\, y)\big) \\
&\qquad + \operatorname{Ei}\big(-2R(\kappa - 2\pi \mathrm{i}\, y)\big) - \operatorname{Ei}\big(-R(\kappa - 2\pi \mathrm{i}\, y)\big)\Big] \\
&\quad - \frac{\exp(4R\pi \mathrm{i}\, y)}{R}\Big[\operatorname{Ei}\big(-4R(\kappa + 2\pi \mathrm{i}\, y)\big) - \operatorname{Ei}\big(-3R(\kappa + 2\pi \mathrm{i}\, y)\big)\Big] \\
&\quad - \frac{\exp(-4R\pi \mathrm{i}\, y)}{R}\Big[\operatorname{Ei}\big(-4R(\kappa - 2\pi \mathrm{i}\, y)\big) - \operatorname{Ei}\big(-3R(\kappa - 2\pi \mathrm{i}\, y)\big)\Big], \qquad (3.17)
\end{aligned}$$

and also the limit for $\kappa \to \infty$

$$\begin{aligned}
&\mathcal{F}\big(\widetilde{\rho}_R^{\,\infty}(|x|)\big)(y) \\
&\quad = -\frac{\sin(4\pi R y)}{4R^2} + \frac{2}{R}\Big(\cos(4R\pi y)\big(\operatorname{Ci}(8R\pi y) - (\operatorname{Ci}(6R\pi y)\big) \\
&\qquad + \sin(4R\pi y)\big(\operatorname{Si}(8R\pi y) - (\operatorname{Si}(6R\pi y)\big)\Big),
\end{aligned}$$

which are both plotted in Figure 6. Unfortunately, the author has not found a way to express this result for $\widehat{\gamma}_{\mathrm{ref}}$ in a shorter formula. Note that one has

$\mathcal{F}\big(\widetilde{\rho}_R(|\,\cdot\,|)\big)(y) = \mathcal{F}\big(\widetilde{\rho}_R(|\,\cdot\,|)\big)(|y|)$, because the transformed function also only depends on the absolute value of its argument. Since $\mathrm{Ci}(x) \sim \sin(x)/x$, $\mathrm{Si}(x) \sim -\cos(x)/x$ for real $x \to +\infty$, and $\mathrm{Ei}(z) \sim \exp(-z)/z$ for complex $z \to \infty$, we get that at least $|\mathcal{F}\big(\widetilde{\rho}_R(|\,\cdot\,|)\big)(y)| = \mathcal{O}(1/|y|)$. But we will also give some general argument to verify such a result for all dimensions. If we add the refined intensity κ_R to $\mathcal{F}\big(\widetilde{\rho}_R(|\,\cdot\,|)\big)$, we get the absolutely continuous part of the diffraction of the 1-dimensional Matérn hard-core point process. This density is illustrated in Figure 7.

Let us state the above results in summary:

Proposition 3.10. *The diffraction of the Matérn hard core point process in dimension $d = 1$ is almost surely given by*

$$\widehat{\gamma_R} = {\kappa_R}^2\, \delta_0 + (\widehat{\gamma}_{\mathrm{ref}} + \kappa_R)\, \lambda^1\,,$$

where $\widehat{\gamma}_{\mathrm{ref}}$ is the density given in Eq. (3.17) *with $|\widehat{\gamma}_{\mathrm{ref}}(y)| = \mathcal{O}(1/|y|)$ for $|y| \to \infty$.* □

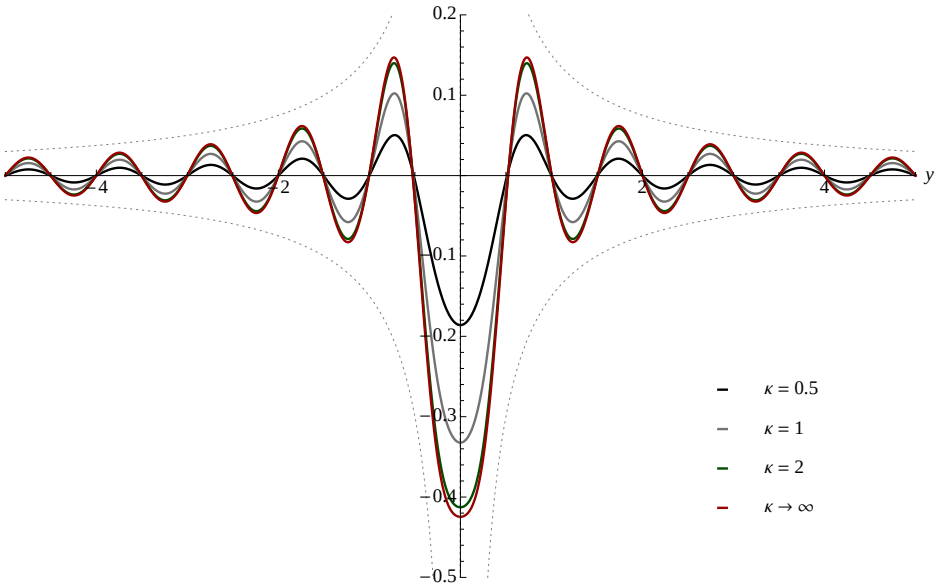


FIGURE 6. Part $\widehat{\gamma}_{\mathrm{ref}}$ of the diffraction of the Matérn process in $d = 1$, including the limit $\kappa \to \infty$. The dotted curves are given by $\pm 0.15\, y^{-1}$ to illustrate the decay

3.3.2. Diffraction in dimension $d \geqslant 1$. The Fourier transform of a function depending only on the norm of its argument can be expressed as a one-dimensional Hankel transform, as

$$\mathcal{F}\big(f(\|\,\cdot\,\|)\big)(y) = \frac{2\pi}{\|y\|^{d/2-1}} \int_0^\infty r^{d/2}\, f(r)\, J_{(d/2)-1}(2\pi r\|y\|)\,\mathrm{d}r\,,$$

see [**68**] for a simple proof in $d = 2$ and [**92**] for the general case. For a definition of the Bessel functions see e.g. [**1**, Chap. 9].

The next step is to look at the functions G_R or g_R, respectively. It is easy to see that $g_R(r)$ is the volume of two spherical caps of height $R - \dfrac{r}{2}$ of

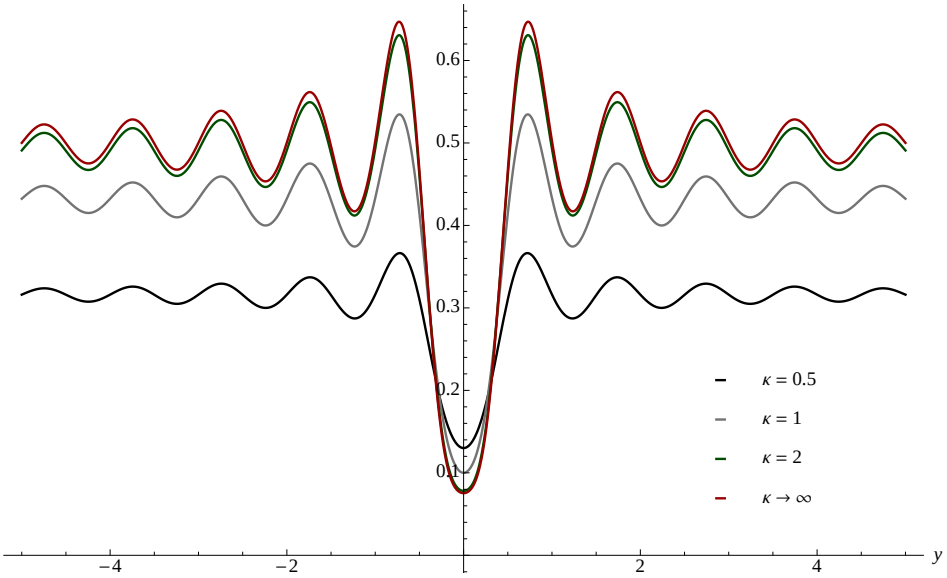


FIGURE 7. Absolutely continuous part of the diffraction of the 1-dimensional Matérn hard-core point process including the limit $\kappa \to \infty$, in other words: its Bartlett spectrum

spheres with radius R. This volume can be computed explicitly: Let $s_R(h)$ be the volume of a d-dimensional spherical cap of height $h < R$; then by an easy calculation one has

$$\begin{aligned} s_R(h) = \int_{R-h}^{R} b_{(d-1),\sqrt{R^2-r^2}}\,\mathrm{d}r = b_{(d-1),R} \int_{R-h}^{R} {}_1F_0\Big(-\frac{d-1}{2}, \Big(\frac{r}{R}\Big)^2\Big)\,\mathrm{d}r \\ = b_R\left[\frac{1}{2} - c_d\,\frac{R-h}{R}\,{}_2F_1\Big(\frac{1-d}{2}, \frac{1}{2}; \frac{3}{2}; \Big(\frac{R-h}{R}\Big)^2\Big)\right], \end{aligned}$$

where $c_d = \dfrac{\Gamma(\frac{d}{2}+1)}{\sqrt{\pi}\,\Gamma(\frac{d+1}{2})}$ and $b_{d,r}$ is the volume of the d-dimensional ball of radius r. The integral involved is evaluated using properties of hypergeometric functions, given e.g. in [**1**]. Thus for $R \leqslant r \leqslant 2R$ we get

$$\begin{aligned} G_R(r) = 2\,b_R - g_R(r) = 2\,b_R - 2\,s_R\Big(R - \frac{r}{2}\Big) \\ = b_R\left(1 + c_d\,\frac{r}{R}\,{}_2F_1\Big(\frac{1-d}{2}, \frac{1}{2}; \frac{3}{2}; \Big(\frac{r}{2R}\Big)^2\Big)\right). \end{aligned}$$

In odd dimensions, $G_R(r)$ reduces to polynomials in r, while in even dimensions also arcsin and square root parts are present. Let us have a look at

the resulting function $G_R(r)$ in the lower dimensions for $R \leqslant r \leqslant 2R$:

$$G_R(r) = \begin{cases} b_{2,R} + R\,r\sqrt{1-\left(\frac{r}{2R}\right)^2} + 2\,R^2 \arcsin\left(\frac{r}{2R}\right), & \text{for } d=2\,, \\ b_{3,R} + \pi\,R^2\,r - \frac{\pi}{12}\,r^3\,, & \text{for } d=3\,, \\ b_{4,R} + \frac{5\,\pi}{6}\,R^3\,r\sqrt{1-\left(\frac{r}{2R}\right)^2} - \frac{\pi}{12}\,R\,r^3\sqrt{1-\left(\frac{r}{2R}\right)^2} \\ \qquad +\pi\,R^4\,\arcsin\left(\frac{r}{2R}\right), & \text{for } d=4\,, \\ b_{5,R} + \frac{\pi^2}{2}\,R^4\,r - \frac{\pi^2}{12}\,R^2\,r^3 + \frac{\pi^2}{160}\,r^5\,, & \text{for } d=5\,, \end{cases}$$

Let us now give the argument why it is essentially enough to restrict oneself to the case $R = 1$, at least in pictures: First note, that G_R is of the form $G_R(r) = R^d \cdot G_1(r/R)$. Also $\rho_R(r) = \rho(\kappa,\, R,\, r)$. In this notation, we have for $R \leqslant r \leqslant 2R$

$$\begin{aligned} &\frac{\rho(R^d\cdot\kappa,\,1,\,r/R)}{R^{2d}} \\ &\quad = 2\,\frac{G_1(r/R)\big(1-\exp(-R^d\cdot\kappa\,b_1)\big) - b_1\big(1-\exp(-R^d\cdot\kappa\,G_1(r/R))\big)}{R^{2d}\,b_1\,G_1(r/R)\,(G_1(r/R)-b_1)} \\ &\quad = 2\,\frac{G_R(r)\big(1-\exp(-\kappa\,b_R)\big) - b_R\big(1-\exp(-\kappa\,G_R(r))\big)}{b_R\,G_R(r)\,(G_R(r)-b_R)} = \rho(\kappa,\,R,\,r)\,. \end{aligned}$$

This 'rescaling' translates naturally to the diffraction by linearity and scaling property of the Fourier transform.

Let us have a look at the part of the diffraction that can be analytically computed, even in higher dimensions. The piecewise constant part of the (refined) second order density has the following Fourier transform:

$$\begin{aligned} &\mathcal{F}\big(1_{[0,2R]}(\|\cdot\|)\big)(y) \\ &\qquad = \frac{2\pi}{\|y\|^{d/2-1}}\int_0^{2R} r^{d/2}\,J_{(d/2)-1}(2\pi r\|y\|)\,\mathrm{d}r = \frac{(2R)^{d/2}}{\|y\|^{d/2}}\,J_{(d/2)}(4\pi R\|y\|)\,, \end{aligned}$$

for the integration see [**47**]. For ν fixed and $|z| \to \infty$, $|\arg z| < \pi$, one has

$$J_\nu(z) \sim \sqrt{\frac{2}{\pi}}\,z^{-1/2}\left(\cos\left(z-\frac{\pi}{2}\,\nu-\frac{\pi}{4}\right) + \mathrm{e}^{|\mathrm{Im}(z)|}\,\mathcal{O}\big(|z|^{-1}\big)\right), \tag{3.18}$$

see [**1**], thus we have

$$\mathcal{F}\big(1_{[0,2R]}(\|x\|)\big)(y) = \mathcal{O}\big(\|y\|^{-(d+1)/2}\big)\,,$$

for $\|y\| \to \infty$.

Since $\widetilde{\rho}_R(r)$ is bounded and supported in $[0, 2R]$, the decay of the Fourier integral for large arguments can be estimated by the same asymptotic behaviour of the Bessel function given in (3.18) that we used for the constant

part of the density:

$$\begin{aligned}\bigl|\mathcal{F}\bigl(\widetilde{\rho}_R(\|\cdot\|)\bigr)(y)\bigr| &= \left|\frac{2\pi}{\|y\|^{d/2-1}}\int_0^{2R}\widetilde{\rho}_R(r)r^{d/2}\,J_{(d/2)-1}(2\pi r\|y\|)\,\mathrm{d}r\right| \\ &\leqslant \sup_{r\in[0,2R]}|\widetilde{\rho}_R(r)|\left|\frac{(2R)^{d/2}}{\|y\|^{d/2}}\,J_{(d/2)}(4\pi R\|y\|)\right|.\end{aligned}$$

Thus, also this part of the diffraction is $\mathcal{O}\bigl(\|y\|^{-(d+1)/2}\bigr)$, which we already saw for $d = 1$. Hence, we have proved the following result:

Theorem 3.11. *The diffraction of the Matérn hard core point process is almost surely given by*

$$\widehat{\gamma_R} = {\kappa_R}^2\,\delta_0 + (\widehat{\gamma}_{\mathrm{ref}} + \kappa_R)\,\lambda^d\,,$$

where $\widehat{\gamma}_{\mathrm{ref}}$ is the Fourier transform of the refined second order product density $\widetilde{\rho}_R(\|\cdot\|)$. Furthermore, we have $|\widehat{\gamma}_{\mathrm{ref}}(y)| = \mathcal{O}\bigl(\|y\|^{-(d+1)/2}\bigr)$ for $\|y\| \to \infty$. □

Let us finally compare and analyse the functions involved for some dimensions. A plot for the refined second order product density in several different dimensions is given in Figure 8. Quantitatively, some of the differ-

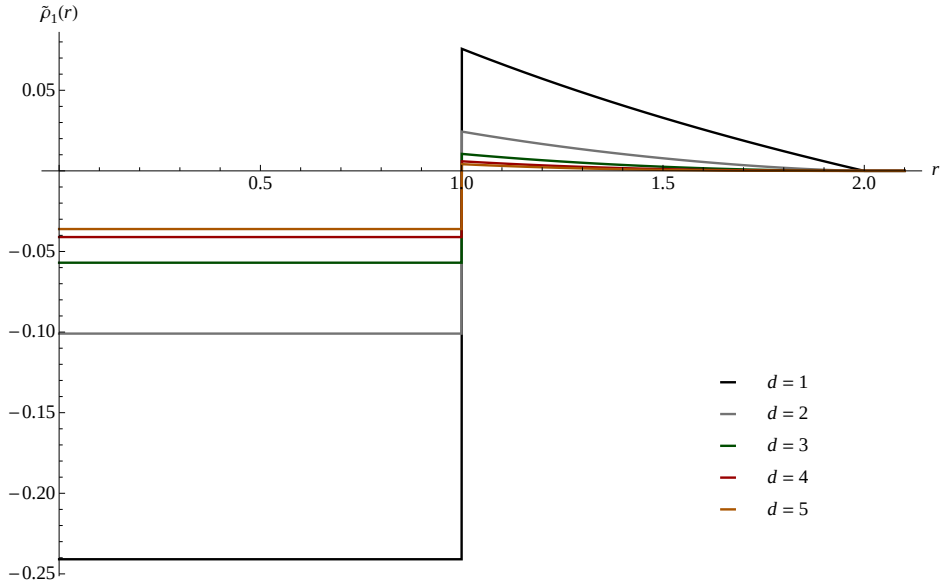


FIGURE 8. Refined second order product density for intensity $\kappa = 2$ of the underlying Poisson process in several dimensions.

ences for small arguments originate from the different volumes of the unit balls.

It is easy to check and to understand that in any dimension, and for any intensity of the underlying Poisson process, the intensity of the Matérn process is lower than that of the corresponding Poisson process, because almost surely the function φ_R removes points from the realisations. This

also results in a lower second order product density for all values. It is also obvious that the higher the intensity κ, the greater the number of points that have to be removed, and the greater the differences to the Poisson product densities become, as is illustrated in Figure 9. In any dimension, and for any intensity of the underlying Poisson process, one finds the refined second order product density to be higher than 0 at the point of discontinuity. Since the product density measures appearance of relative distances between points, that might be interpreted as the Matérn process being closer to the original Poisson process for relative distances close to the hard-core radius.

If we look at the diffraction properties in odd dimensions, at least the Fourier transform of $\widetilde{\rho}_R^{\infty}$ can be computed analytically, due to the polynomial form of $G_R(r)$ for $d = 3$ one explicitly gets

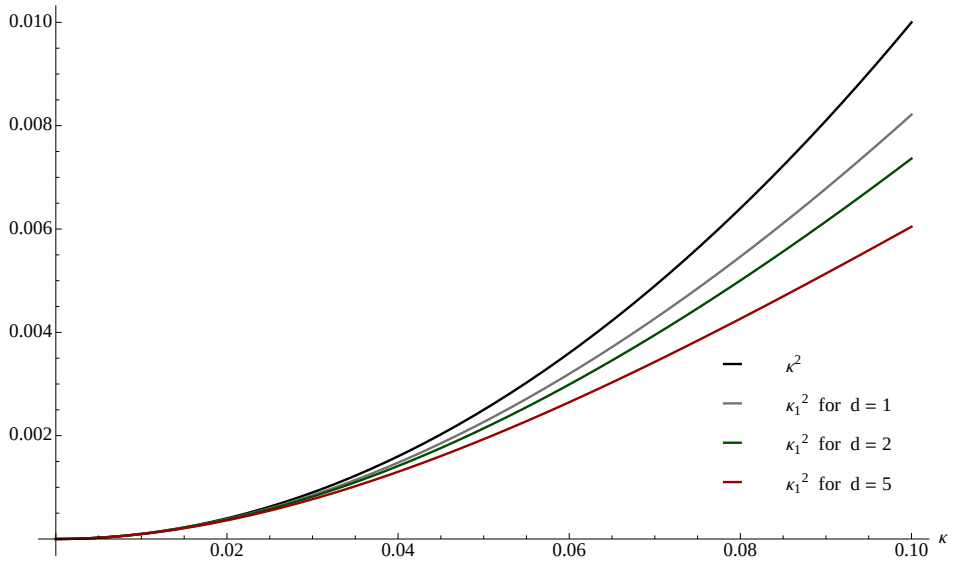
$$\begin{aligned}
&\mathcal{F}\big(\widetilde{\rho}_R^{\infty}(\|\cdot\|)\big)(y)\\
&= \frac{9}{8\,\pi^3\,R^5\,y^2}\cos(4\pi R\,y) - \frac{9}{32\,\pi^4\,R^6\,y^3}\sin(4\pi R\,y) - \frac{9}{\pi^2\,R^4\,y}\Big(3\sin(4\pi R\,y)\\
&\quad - 4\sin(2\pi R\,y) + 4\,\mathrm{Ci}(6\pi R\,y)\,\sin(4\pi R\,y) - 4\,\mathrm{Ci}(8\pi R\,y)\,\sin(4\pi R\,y)\\
&\quad + 4\,\mathrm{Ci}(-6\pi R\,y)\,\sin(8\pi R\,y) - 4\,\mathrm{Ci}(-4\pi R\,y)\,\sin(8\pi R\,y)\\
&\quad + 4\cos(8\pi R\,y)\,\mathrm{Si}(4\pi R\,y) - 4\cos(4\pi R\,y)\,\mathrm{Si}(6\pi R\,y) - 4\cos(8\pi R\,y)\,\mathrm{Si}(6\pi R\,y)\\
&\quad + 4\cos(4\pi R\,y)\,\mathrm{Si}(8\pi R\,y) + 24\pi R\,y\big(\cos(4\pi R\,y)\,\mathrm{Ci}(6\pi R\,y)\\
&\quad - \cos(4\pi R\,y)\,\mathrm{Ci}(8\pi R\,y) + \sin(4\pi R\,y)\,\mathrm{Si}(6\pi R\,y) - \sin(4\pi R\,y)\,\mathrm{Si}(8\pi R\,y)\big)\Big).
\end{aligned}$$

Plots, derived numerically, as to be expected, give pictures of the diffraction densities that are very similar to the pictures in the one dimensional case. The Fourier transform of the refined density in $d = 3$ is shown in Figure 10, and the decay is hinted at within this image, too. Figure 11 gives a plot of the absolutely continous part of the diffraction of the Matérn hard-core process in that dimension. Note that this is also its Bartlett spectrum.

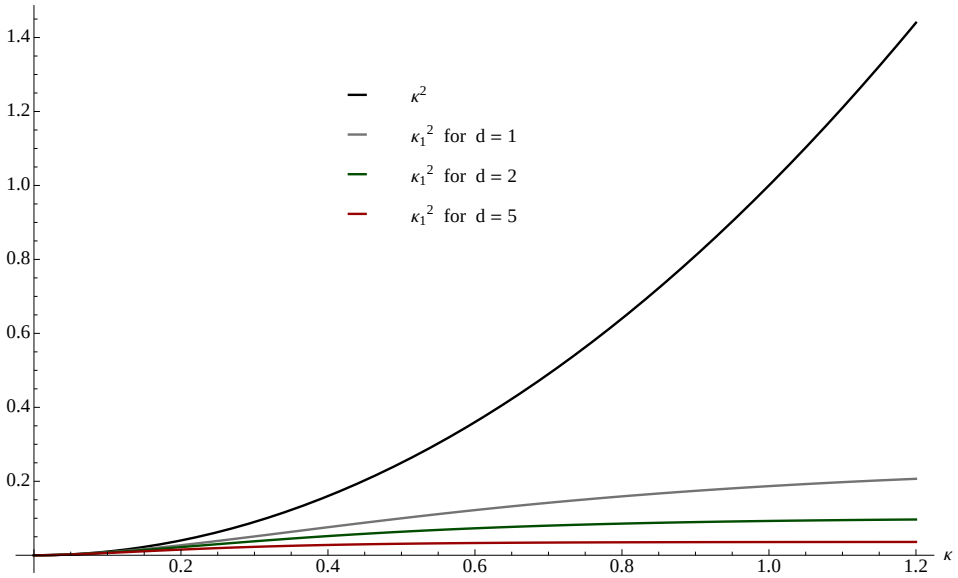
Qualitatively, there are no big differences except the speed of decay for large arguments of the non-constant part of the diffraction as stated above, namely the absolutely continuous part of the diffraction oscillates around ${\kappa_R}^2$ with decaying amplitudes. Figures 12 and 13 show plots of numerically derived diffraction densities.

The observed oscillation is a result of the radial symmetric structure of the process and governed by the respective Bessel function, the decay to the squared refined intensity is analogous to the decay of the transformed support function $1_{B_{2R}}$ (compare Figures 12 and 13).

We simulated a 2-dimensional Matérn process with hard-core radius 1 in a disk of radius 800. The intensity of the underlying Poisson point process was set to 2. The theoretical diffraction pattern can only be guessed from the simulated diffraction with a lot of goodwill, because the sample is much to small (about 170.000 points), see Figure 14. But a look at a radially averaged version, where samples at 100 different angles were taken for the average, shows stronger hints to the right shape of the diffraction pattern, see Figure 15.



(a) Small intensities



(b) Bigger intensities - the differences grow quickly

FIGURE 9. This picture shows the squared intensities of the Matérn process in several dimensions compared to the second order product density of the underlying Poisson process depending on the intensity of the Poisson process. One can observe the small differences for small intensities. The hard-core radius is chosen to be 1

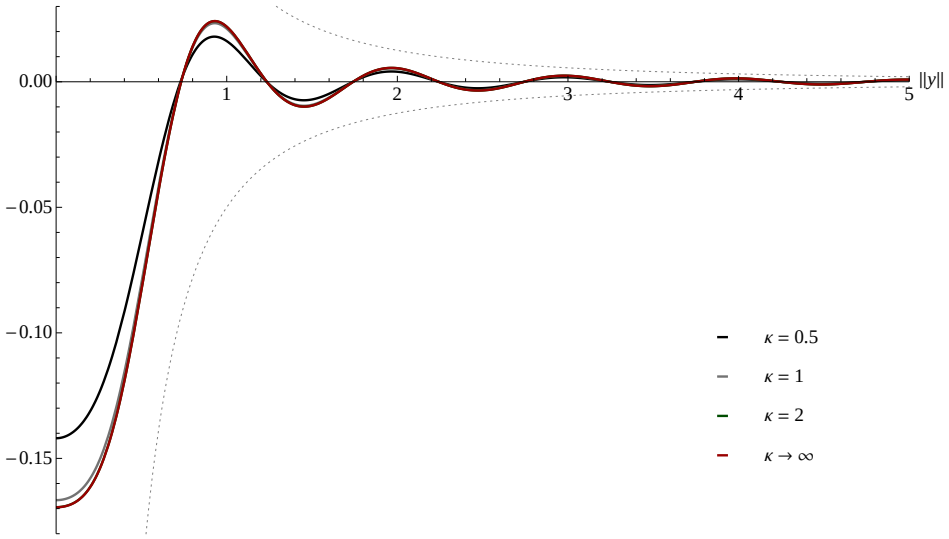


FIGURE 10. $\widehat{\gamma}_{\mathrm{ref}}$ in $d = 3$ for several intensities, including the limit $\kappa \to \infty$. Decay is hinted by the dotted graph of $\pm 0.05\|y\|^{-2}$

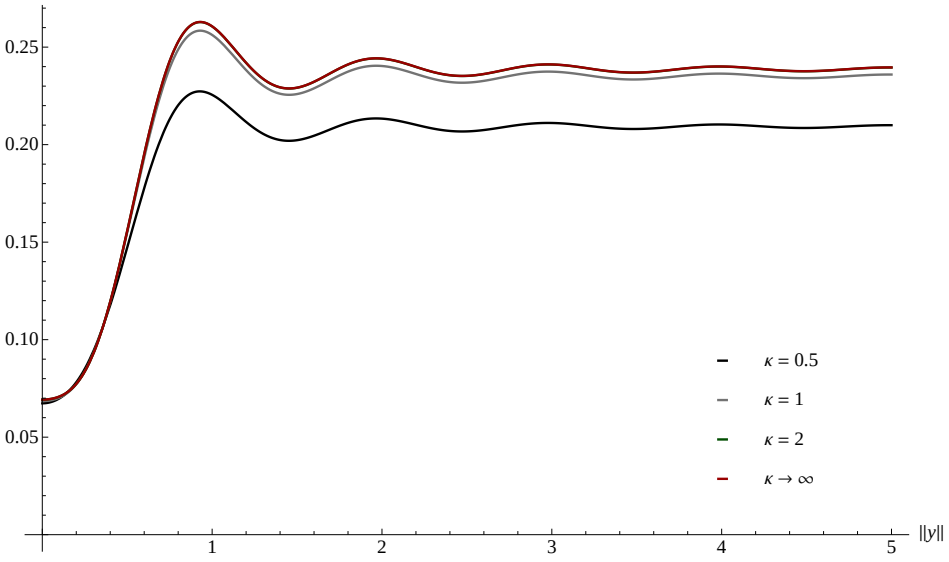


FIGURE 11. Absolutely continuous part of the diffraction of the Matérn process in dimension $d = 3$ for different intensities

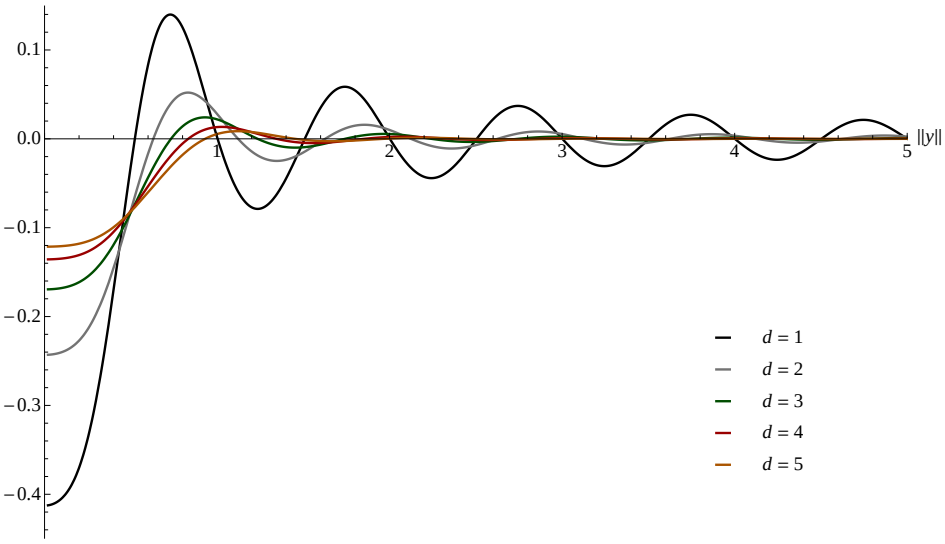


FIGURE 12. Part $\widehat{\gamma}_{\mathrm{ref}}$ of the diffraction of the Matérn hard-core point process; the underlying Poisson intensity is fixed to $\kappa = 2$ while dimension d varies

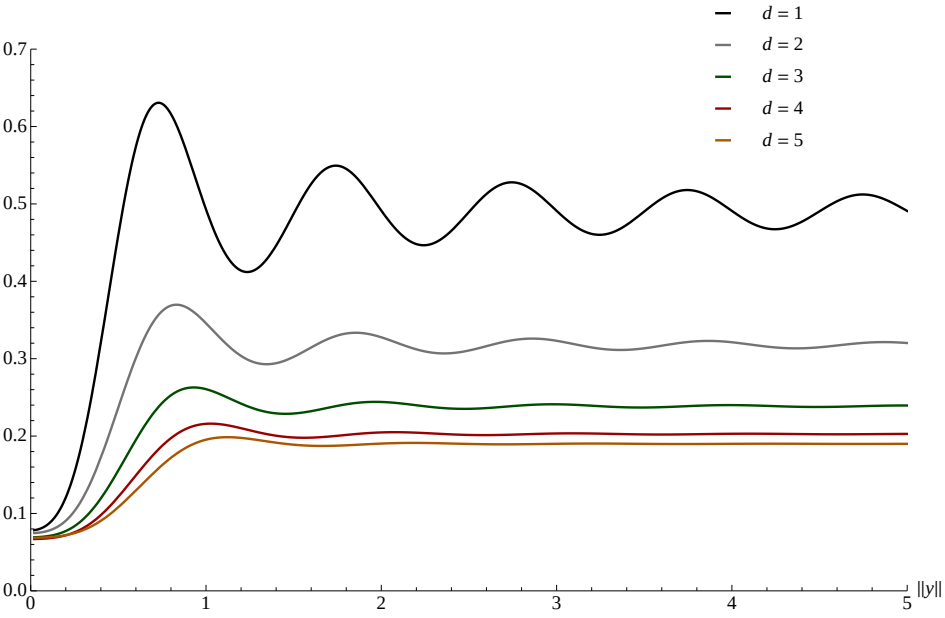
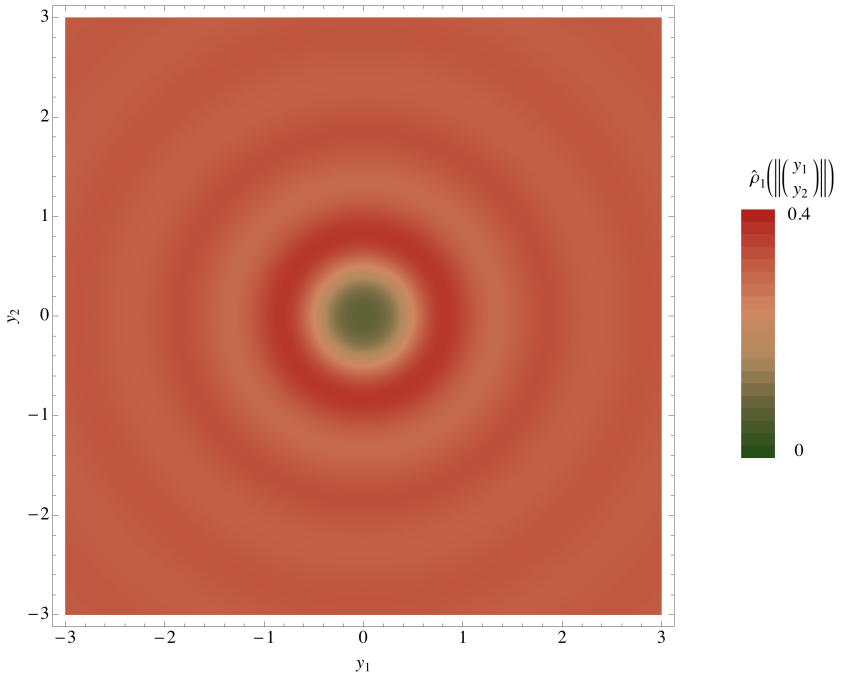
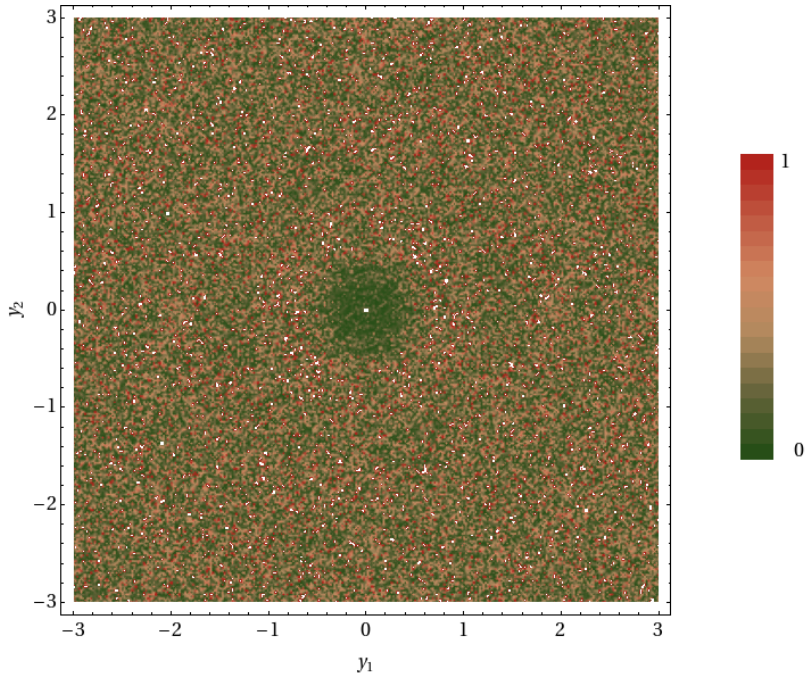


FIGURE 13. Absolutely continuous part of the diffraction of the Matérn hard-core point process with underlying Poisson intensity $\kappa = 2$ for several dimensions



(a) Theoretical absolutely continuous part of the diffraction of the Matérn hard-core process in $d = 2$



(b) Diffraction of a large sample of a simulation of the Matérn hard-core process with underlying Poisson intensity, fitted to the theoretical counterpart

FIGURE 14. Comparison between theoretical and simulated diffraction of the Matérn hard-core process. Not much of the theoretical structure is visible in the simulation, since the sample size is too small

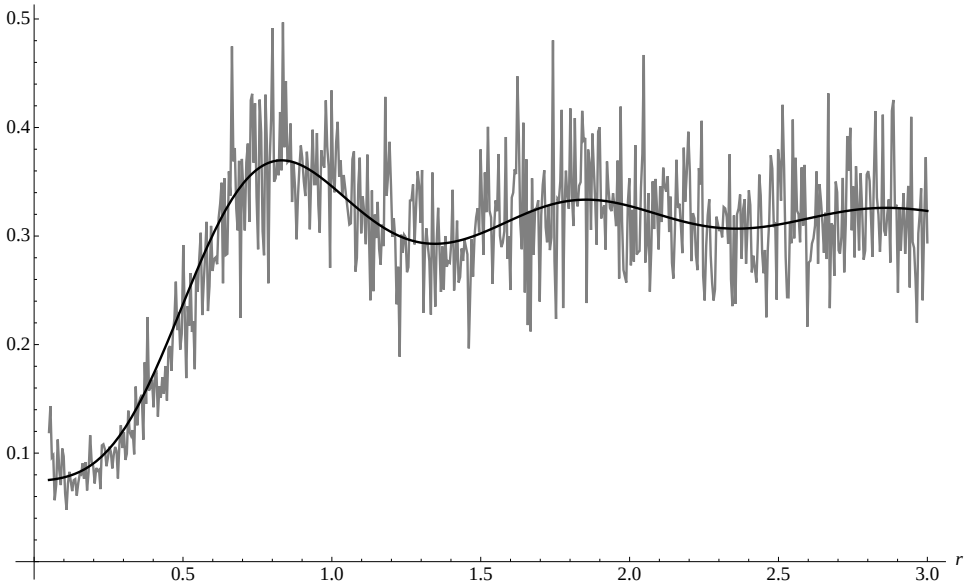


FIGURE 15. The gray curve is given by a radial average of the simulated diffraction, avoiding the Bragg peak in 0. It is fitted to the theoretical a.c. part of the diffraction of the Matérn process, which is given by the black curve.

3.4. Concluding thoughts

3.4.1. Conclusions. This chapter shows one example where the method introduced by Goueré [**46**] helps to calculate the diffraction of almost all realisations of a specific process, the Matèrn hard-core point process. Although we could not compute the Fourier transforms of the involved functions of the Matérn process in dimension $d > 1$ analytically, the structure of the diffraction gets visible.

3.4.2. Outlook. In the paper of Stoyan and Stoyan [**94**], a second model for a hard-core point process is given, where the hard-core radius is randomly chosen. An integral formula for the resulting second order product density is given within this paper, too. One could also analyse the diffraction structure of that model, although the necessary Fourier transforms get even more difficult.

It would also be interesting to examine the vague accumulation points of the family of Matérn processes for limits $\kappa \to \infty$. These limit processes might have the nice properties of keeping the hard cores while also reducing the gaps between points. Some considerations in that direction regarding the Matérn type III process have been made in [**73**]. The problem of convergence may be related to limits of hard-core Gibbs point processes for increasing activity-parameter. They have been studied in [**71**].

The method of the Palm measure to almost surely determine autocorrelation and thus diffraction measures of a process is limited to ergodic point processes and random measures. The calculation of the second order product densities (or Palm intensities) stay difficult, even in that case. Nevertheless, it would be nice to have more methods to obtain results on the diffraction of more general (stationary) point processes and random measures. As no almost sure statements are to be expected in that situation, probability distributions for diffraction patterns would be the objects of interest.

Bibliography

[1] Abramowitz, M. & I. A. Stegun, eds.: *Handbook of Mathematical Functions with Formulas, Graphs and Mathematical tables.* 10th printing. National Bureau of Standards Applied Mathematics Series, Vol. **55**, 1972.

[2] Argabright, L. & J. G. de Lamadrid: *Fourier Analysis of Unbounded Measures on Locally Compact Abelian Groups.* Memoirs of the AMS, No. 145, AMS, Providence, Rhode Island 1974.

[3] Baake, M.: *Diffraction of weighted lattice subsets.* Canadian Math. Bulletin **45** (2002) 483–498; arXiv:math.MG/0106111

[4] Baake, M.: *A Guide to Mathematical Quasicrystals.* In: *Quasicrystals*, eds. Suck, J.-B., M. Schreiber & P. Häussler, Springer Series in Materials Science, Vol. **55**, Springer, Berlin 2002.

[5] Baake, M.: *Mathematical Diffraction in Euclidean Spaces.* Lecture Notes EPFL Lausanne, 2004.

[6] Baake, M., M. Birkner & R. V. Moody: *Diffraction of stochastic point sets: explicitly computable examples.* Commun. Math. Phys. **293** (2010) 611-660; arXiv:math-ph/0803.1266

[7] Baake, M., U. Grimm & R. V. Moody: *Die verborgene Ordnung der Quasikristalle.* Spektrum der Wissenschaft (February 2002), 64–74; arXiv:math/0203252

[8] Baake, M. & M. Höffe: *Diffraction of random tilings: some rigorous results.* J. Stat. Phys. **99** (2000) 219–261; arXiv:math-ph/9904005

[9] Baake, M., P. Kramer, M. Schlottmann, & D. Zeidler: *Planar patterns with fivefold symmetry as sections of periodic structures in* 4*-space* Internat. J. Modern Phys. B **4** (1990) 2217–2268.

[10] Baake, M. & D. Lenz: *Dynamical systems on translation bounded measures: Pure point dynamical and diffraction spectra.* Ergodic Th. & Dynam. Syst. **24** (2004) 1867–1893; arXiv:math.DS/0302061

[11] Baake, M. & D. Lenz: *Deformation of Delone dynamical systems and pure point diffraction.* J. Four. Anal. Appl. **11** (2005) 125–150.

[12] Baake, M., D. Lenz & R. V. Moody: *Characterisation of models sets by dynamical systems.* Ergodic Th. & Dynam. Syst. **27** (2007) 341–382; arXiv:math.DS/0511648

[13] Baake, M. & R. Moody: *Diffractive point sets with entropy.* J. Phys. A: Math. Gen. **31**, 9023–9039; arXiv:math-ph/9809002

[14] Baake, M. & R. Moody: *Weighted Dirac combs with pure point diffraction.* J. reine & angew. Math. (Crelle) **573** (2004) 61–94; arXiv:math.MG/0203030

[15] Baake, M., R. V. Moody, C. Richard, & B. Sing: *Which distributions of matter diffract? – Some answers* In: *Quasicrystals: Structure and Physical Properties*, H.-R. Trebin (ed.), Wiley-VCH, Berlin 2003, pp. 188–207; arXiv:math-ph/0301019

[16] Baake, M. & B. Sing: *Diffraction spectrum of lattice gas models above* T_c. Lett. Math. Phys. **68** (2004) 165–173; arXiv:math-ph/0405064

[17] Baake, M. & N. Zint: *Absence of singular continuous diffraction for discrete multicomponent particle models.* J. Stat. Phys. **130** (2008) 727–740.

[18] Bartlett, M. S.: *The spectral analysis of point processes.* J. R. Statist. Soc. B **29** (1963) 264–296.

[19] Bartlett, M. S.: *An Introduction to Stochastic Processes with Special References to Methods and Applications.* 3rd ed., Cambridge University Press, Cambridge 1978.

[20] Bauer, H.: *Wahrscheinlichkeitstheorie.* 4th ed., De Gruyter, Berlin 1991.

[21] Bauer, H.: *Maß- und Integrationstheorie.* 2nd ed., De Gruyter, Berlin 1992.

[22] Beenker, F. P. M. *Algebraic theory of non-periodic tilings of the plane by two simple building blocks: a square and a rhombus.* Eindhoven University of Technology, 1982, TH-Report, 82-WSK04.
[23] Berg, C. & G. Forst: *Potential Theory on Locally Compact Abelian Groups.* Springer, Berlin 1975.
[24] Billingsley, P.: *Convergence of Probability Measures.* Wiley, New York 1968.
[25] Billingsley, P.: *Probability and Measure* 3rd edn., Wiley, New York 1995.
[26] Bombieri, E. & J. E. Taylor: *Which distributions of matter diffract? An initial investigation.* J. Physique Coll. C3 **47** (1986) 19–28.
[27] Bourbaki, N.: *General Topology.* Part 1, Hermann, Paris 1966.
[28] Bourbaki, N.: *General Topology.* Part 2, Hermann, Paris 1966.
[29] Conway, J. H. & N. J. A. Sloane: *Sphere Packings, Lattices and Groups.* 2nd ed., Springer, New York 1993.
[30] Cowley, J. M.: *Diffraction Physics.* 3rd ed., North-Holland, Amsterdam 1995.
[31] Daley, D. J. & D. Vere-Jones: *An Introduction to the Theory of Point Processe, Vol. I: Elementary Theory and Methods.* 2nd ed., Springer, New York 2005.
[32] Daley, D. J. & D. Vere-Jones: *An Introduction to the Theory of Point Processe, Vol. II: General theory and structure.* 2nd ed., Springer, New York 2008.
[33] de Bruijn, N. G.L: *Algebraic theory of Penrose's nonperiodic tilings of the plane. I.* Nederl. Akad. Wetensch. Indag. Math. **43** (1981) 39–52.
[34] de Bruijn, N. G.L: *Algebraic theory of Penrose's nonperiodic tilings of the plane. II.* Nederl. Akad. Wetensch. Indag. Math. **43** (1981) 53–66.
[35] Dieudonné, J.: *Treatise on Analysis.* Vol. II, Academic Press, New York 1970.
[36] Dobrushin, R. L.: *Description of random fields by means of conditional probabilities and the conditions governing its regularity.* Theory Prob. and its Appl. **13** (1968) 197–224.
[37] Dobrushin, R. L.: *Gibbsian random fields for lattice systems with pairwise interactions.* Funct. Anal. and its Appl. **2** (1968) 292–301.
[38] Dobrushin, R. L.: *The problem of uniqueness of a Gibbsian random field and the problem of phase transition.* Funct. Anal. and its Appl. **2** (1968) 302–312.
[39] Dobrushin, R. L.: *Gibbsian random fields. The general case.* Funct. Anal. and its Appl. **3** (1969) 32–28.
[40] Donoghue, W. F., Jr.: *Distributions and Fourier Transforms.* Academic Press, New York 1969.
[41] Dworkin, S.: *Spectral theory and X-ray diffraction.* J. Math. Phys. **34** (1993) 2965–2967.
[42] Forster, O.: *Analysis 1.* 5th ed., Vieweg, Braunschweig 1999.
[43] Furstenberg, H.: *Recurrence in Ergodic Theory and Combinatorial Number Theory.* Princeton University Press, Princeton 1981.
[44] Georgii, H.-O.: *Gibbs Measures and Phase Transitions.* De Gruyter, Berlin 1988.
[45] Godrèche, C.: *Non Pisot tilings and singular scattering.* Phase Transitions **32** (1991) 45–79.
[46] Gouéré, J.-B.: *Diffraction et mesure de Palm des processus ponctuels.* C. R. Math. Acad. Sci. Paris **336** (2003) 57–62.
[47] Gradshteyn, I. S. & I. M. Ryzhig: *Tables of Integrals, Series, and Products.* 6th ed., Academic Press, San Diego 2000.
[48] Guinier, A.: *X-Ray Diffraction in Crystals, Imperfect Crystals and Amorphous Bodies.* Reprint, Dover, New York 1994.
[49] Hof, A.: *Quasicrystals, Aperiodicity and Lattice Systems.* PhD thesis, University of Groningen, 1992.
[50] Hof, A.: *On diffraction by aperiodic structures.* Commun. Math. Phys. **169** (1995) 25–43.
[51] Hof, A.: *Diffraction by aperiodic structures at high temperatures.* J. Phys. A: Math. Gen. **28** (1995) 57–62.
[52] Hof, A.: *Diffraction by aperiodic structures.* In: *The Mathematics of Long-Range Aperiodic Order*, R. V. Moody (ed.), NATO ASI Series C **489**, Kluwer, Dodrecht 1997, 239–268.

[53] Höffe, M. & M. Baake: *Surprises in diffuse scattering.* Z. Krist. **215** (2000) 441–444.
[54] Höffe, M.: *Diffraktionstheorie stochastischer Parkettierungen.* PhD thesis, Tübingen University, 2001.
[55] Kallenberg, O.: *Random Measures.* Akademie-Verlag, Berlin 1975.
[56] Kallenberg, O.: *A counterexample to R. Davidson's conjecture on line processes.* Math. Proc. Camb. Phil. Soc. **82** (1977) 301–307.
[57] Kelley, J. L.: *General Topology.* Reprint, Springer, New York 1975.
[58] Kerstan, J., K. Matthes & J. Mecke: *Infinitely Divisible Point Processes.* Wiley, Chichester 1978.
[59] Kendal, W., J. Mecke & D. Stoyan: *Stochastic Geometry and its Applications.* 2nd ed., Wiley, Chichester 1995.
[60] Koch, K., J. Ohser & K. Schladitz:*Spectral theory for random closed sets and estimating the covariance via frequency space.* Adv. in Appl. Probab. **35** (2003) 603–61.
[61] Kramer, P. & R. Neri: *On periodic and non-periodic space fillings of $\mathbb{E}^m$ obtained by projection.* Acta Cryst. **A40** (1984) 580–587.
[62] Kramer, P. & R. Neri: *On periodic and non-periodic space fillings of $\mathbb{E}^m$ obtained by projection. Erratum.* Acta Cryst. **A41** (1985) 619.
[63] Külske, C.: *Concentration inequalities for functions of Gibbs fields with applications to diffraction and random Gibbs measures.* Commun. Math. Phys. **239** (2003) 29–51.
[64] Külske, C.: *Universal bounds on the selfaveraging of random diffraction measures.* Probab. Theory Relat. Fields **126** (2003) 29–50.
[65] Lagarias, J. C.: *Geometric models for quasicrystals I. Delone sets of finite type.* Discrete Comp. Geom. **21** (1999) 161–191.
[66] Lagarias, J. C.: *Mathematical quasicrystals and the problem of diffraction.* In: *Directions in Mathematical Quasicrystals,* eds. M. Baake and R. V. Moody, CRM Monograph Series, vol. **13**, AMS, Providence RI 2000, pp. 61–94.
[67] Lanford, O. E. & D. Ruelle: *Observables at infinity and states with short range correlations in statistical mechanics.* Commun. Math. Physics **13** (1970) 194–215.
[68] Lang, S.: *Real and Functional Analysis.* 3rd ed., Springer, New York 1993.
[69] Lenz, D.: *Aperiodic order via dynamical systems: diffraction for sets of finite local complexity.* Contemp. Math. **485** (Ergodic Theory, Idris Assani, ed), (2009) 91–112.
[70] Luke, Y. L.: *The Special Functions and Their Approximations.* Vol. 1, Academic Press, New York 1969.
[71] Mase, S., J. Møller, D. Stoyan, R. P. Waagepetersen & G. Döge: *Packing densities and simulated tempering for hard core Gibbs point processes.* Ann. Inst. Statist. Math. **53** (2001) 661–680.
[72] Matérn, B.: *Spatial Variation.* 2nd ed., Springer, Berlin 1986.
[73] Møller, J., M. L. Huber & R. L. Wolpert: *Perfect simulation and moment properties for the Matérn type III process.* Conditionally accepted for publication in Stochastic Processes and teir Applications.
[74] Moody, R. V. : *Model sets: A survey,* in: *From Quasicrystals to More Complex Systems*, eds. F. Axel, F. Dénoyer and J. P. Gazeau, EDP Sciences, Les Ulis, and Springer, Berlin 2000, pp. 145–166; arXiv:math.MG/0002020.
[75] Olver, F. W. J.: *Asymptotics and Special Functions.* AKP Classics, Natick 1997.
[76] Papangelou, F.: *On the Palm probabilities of processes of points and processes of lines.* In *Stochastic Geometry. A Tribute to the Memory of Rollo Davidson*, eds. E. F. Harding & D. G. Kendall, Wiley, London 1974, pp. 114–147.
[77] Parthasarathy, K. R.: *Introduction to Probability and Measure.* The Macmillan Co. of India, Ltd., Delhi, 1977.
[78] Pedersen, G. K.: *Analysis Now.* Revised printing, Springer, New York 1995.
[79] Penrose, R.: *The role of aesthetics in pure and applied mathematical research.* Bull. Inst. Math. Appl. **10** (1974) 266–271.
[80] Pinsky, M. A.: *Introduction to Fourier Analysis and Wavelets.* Brooks/Cole, Pacific Grove, CA, 2002.
[81] Preston, C.: *Random Fields.* Springer, Berlin 1976.
[82] Querenburg, B. v.: *Mengentheoretische Topologie.* 2nd ed., Springer, Berlin 1979.

[83] Reed, M. & B. Simon: *Functional Analysis.* Revised and Enlarged Edn., Academic Press, San Diego 1980.
[84] Rudin, W.: *Fourier Analysis on Groups.* Intersience Publishers, New York 1967.
[85] Rudin, W.: *Functional Analysis.* McGraw-Hill, New York 1973.
[86] Ruelle, D.: *Superstable interactions in statistical mechanics.* Commun. Math. Phys. **18** (1970), 127–159.
[87] Schlottmann, M.: *Cut-and-project sets in locally compact Abelian groups.* In: *Quasicrystals and Discrete Geometry*, ed. J. Patera, Fields Institute Monographs, vol. **10**, AMS, Providence RI 1998, pp. 247–264.
[88] Schlottmann, M.: *Generalized model sets and dynamical systems.* In: *Directions in Mathematical Quasicrystals*, eds. M. Baake and R. V. Moody, CRM Monograph Series, vol. **13**, AMS, Providence RI 2000, pp. 143–159.
[89] Schneider, R. & W. Weil: *Stochastische Geometrie.* Teubner, Stuttgart 2000.
[90] Shechtman, D., I. Blech, D. Gratias & J. W. Cahn: *Metallic phase with long-range orientational order and no translation symmetry.* Phys. Rev. Lett. **53** (1984) 1951–1953.
[91] Sing, B. & T. R. Welberry: *Deformed model sets and distorted Penrose tilings.* Z. Krist. **221** (2006) 621–634; mp_arc/06-199
[92] Sneddon, I. N.: *Fourier Transforms.* McGraw-Hill, New York 1951.
[93] Solomyak, B.: *Spectrum of dynamical systems arising from Delone sets.* In: *Quasicrystals and Discrete Geometry*, ed. J. Patera, Fields Institute Monographs, vol. **10**, AMS, Providence RI 1998, pp. 265–275.
[94] Stoyan, D. & H. Stoyan: *On one of Matérn's hard-core Point Process Models.* Math. Nachr. **122** (1985) 205–214.
[95] Steurer, W. et. al.: *What is a crystal?* Z. Krist. **222** (2007) 308–319.
[96] Welberry, T. R.: *Diffuse X-ray Scattering and Models of Disorder.* Clarendon Press, Oxford 2004.
[97] Zint, N.: *Influence of randomness in mathematical models for diffraction and T-cell recognition.* PhD thesis, Bielefeld University, 2009.