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Diffraction of stochastic point sets: Exactly solvable examples

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Abstract. Stochastic point sets are considered that display a diffraction spectrum of mixed type, with special emphasis on explicitly computable cases together with a unified approach of reasonable generality. Several pairs of autocorrelation and diffraction measures are discussed that show a duality structure that may be viewed as analogues of the Poisson summation formula for lattice Dirac combs.

1. Introduction

The discoveries of quasicrystals [44], aperiodic tilings [39, 34], and complex metallic alloys [49] have greatly increased our awareness that there is a substantial difference between the notions of periodicity and long-range order. Although pinning an exact definition to the concept of long-range order is not yet possible (nor perhaps desirable at this intermediate stage, compare the discussion in [47]), there is still some general agreement that the appearance of a substantial point-like component in the diffraction of a structure is a strong, though not necessary, indicator of the phenomenon.

Mathematically, the diffraction – say of a point set $\varLambda$ in $\mathbb{R}^3$ – is the measure $\widehat{\gamma}$ on $\mathbb{R}^3$ which is the Fourier transform of the volume averaged autocorrelation γ of $\varLambda$ (or, more precisely, of its Dirac comb $\delta_{\varLambda} = \sum_{x\in\varLambda} \delta_x$). Over the past 20 years or so, considerable effort has been put into understanding the mathematics of diffraction, especially conditions under which $\varLambda$ is pure point diffractive, in the sense that $\widehat{\gamma}$ is a pure point measure, compare [27, 14, 46, 2, 8, 24]. At this point in time, we have a good number of models for producing pure point diffraction, particularly the cut and project sets (or model sets) and, under certain types of discreteness conditions, one can even go as far as to say that these types of sets essentially characterise the pure point diffractive point sets [6].

But the reality is that real life structures are not perfectly pure point diffractive, and in order to gain further insight into the possible structures of materials, and more generally into the whole concept of long-range order, it is necessary to widen the scope of this study to include mixed diffraction spectra – i.e., to consider structures whose diffraction measure contains at least some continuous part.

When it comes to mixed spectra, much less is known, although there are many particular examples [18, 13, 4, 28, 35, 25, 51, 17]. Even deterministic sets can have mixed diffraction spectra, and once any randomness is introduced, this is the norm. Determining the exact nature of the diffraction is usually difficult and often simply not known. No doubt the possibilities, both in Nature and in mathematics, for structures with long-range order is well beyond what we have presently imagined. This is also apparent by systems like the pinwheel tiling, compare [41] and references therein, which looks like an amorphous structure in spite of being completely regular.

It would seem desirable then, as a first step, to establish methods, capable of being exactly computable, that would cover many of these examples and also suggest ways in which to generalise what is known, and even move into yet unexplored territory. This is the purpose of this paper. As already suggested, it is based on the approach to diffraction set out by A. Hof in [27, 28], namely via autocorrelations and their measures. The paper is primarily guided by examples, set in as great a generality as we can manage, with the consistent theme that they are exactly computable. Briefly, the types of situations that we consider are these:

(i) renewal processes on the real line (Sec. 3);
(ii) randomisation of an arbitrary pre-given point set $\varLambda$ whose diffraction is known, by identically distributed random complex finite measures, which are independently centred at each point of $\varLambda$ (Sec. 4);
(iii) randomisation of a random point process $\varPhi$ whose law is known by indentically distributed random finite measures (positive or signed) which are independently centred at each point of each realisation of $\varPhi$ (Sec. 5.1–5.4);
(iv) equilibria of critical branching Brownian motions (Sec. 5.5).

2. Some recollections from Fourier analysis

Let μ be a finite regular (complex) Borel measure on $\mathbb{R}^d$. Its Fourier (or Fourier-Stieltjes) transform is a uniformly continuous function on $\mathbb{R}^d$, defined by

$$\widehat{\mu}(k) \;=\; \int_{\mathbb{R}^d} e^{-2\pi i k x} \,\mathrm{d}\mu(x),$$

see [43] for details. This definition includes the Fourier transform of Schwartz functions and continuous functions of compact support (the corresponding spaces being denoted by $\mathcal{S}(\mathbb{R}^d)$ and $C_{\mathsf{c}}(\mathbb{R}^d)$) by viewing them as Radon-Nikodym densities for Lebesgue measure λ, hence as a finite measure. If μ is an unbounded measure that still defines a tempered distribution, via $\mu(\varphi) = \int_{\mathbb{R}^d} \varphi \,\mathrm{d}\mu$ for $\varphi \in \mathcal{S}(\mathbb{R}^d)$, it is called a *tempered measure*. Its Fourier transform is then defined via $\widehat{\mu}(\varphi) = \mu(\widehat{\varphi})$ as usual [42], so that $\widehat{\mu}$ is a tempered distribution. Below, we only consider situations where $\widehat{\mu}$ is also a measure, meaning a linear functional on $C_{\mathsf{c}}(\mathbb{R}^d)$. Recall that a (complex) measure μ is called *translation bounded* when, for arbitrary compact sets $K \subset \mathbb{R}^d$ and for all $t \in \mathbb{R}^d$, $|\mu|(t+K) \le c_K$ with constants c_K that depend only on K. Here, $|\mu|$ denotes the total variation measure of μ. Translation boundedness is a sufficient criterion for a measure to be tempered, see [42] for details.

If $\varGamma \subset \mathbb{R}^d$ is a *lattice* (meaning a discrete subgroup of $\mathbb{R}^d$ with compact factor group $\mathbb{R}^d/\varGamma$), we write $\delta_{\varGamma} := \sum_{x\in\varGamma} \delta_x$ for the corresponding Dirac comb, with δ_x the normalised point measure at x. It is well-known that $\delta_{\varGamma}$ is a tempered measure, whose Fourier transform is again a tempered measure. The latter is explicitly given by the Poisson summation formula (PSF) in its version for lattice Dirac combs [11, Ex. 6.22],

$$\widehat{\delta_{\varGamma}} \;=\; \mathrm{dens}(\varGamma)\, \delta_{\varGamma^*}, \tag{1}$$

where $\varGamma^* := \{x \in \mathbb{R}^d \mid x\cdot y \in \mathbb{Z} \text{ for all } y \in \varGamma\}$ is the dual lattice of $\varGamma$, see [14] for details. The density of $\varGamma$ is well-defined and given by $\mathrm{dens}(\varGamma) = 1/|\det(\varGamma)|$, where $\det(\varGamma)$ is the oriented volume of a (measurable) fundamental domain of $\varGamma$. It can most easily be calculated as the determinant of a lattice basis. Observing $|\det(\varGamma^*)| = 1/|\det(\varGamma)|$, a more symmetric version of the PSF reads

$$\Big(\sqrt{|\det(\varGamma)|}\;\delta_{\varGamma}\Big)^{\widehat{}} \;=\; \sqrt{|\det(\varGamma^*)|}\;\delta_{\varGamma^*}. \tag{2}$$

In particular, one has $\widehat{\delta_{\mathbb{Z}^d}} = \delta_{\mathbb{Z}^d}$, so that the lattice Dirac comb of $\mathbb{Z}^d$ is self-dual in this sense.

As a result of independent interest, let us recall the following related formula for a radially symmetric situation in $\mathbb{R}^d$, which emerges from a simplified model of powder diffraction [3]. Let $\varGamma$ and $\varGamma^*$ be as before, and let $\eta_{\varGamma}(r)$ and $\eta_{\varGamma^*}(r)$ denote the numbers of points of $\varGamma$ and $\varGamma^*$ on centred spheres $\partial B_r(0)$ of radius r. The (non-zero) numbers $\eta_{\varGamma}(r)$ are also called the *shelling numbers* of the lattice $\varGamma$. If μ_r denotes the uniform probability measure on $\partial B_r(0)$, one has the following radial analogue of the PSF in (1),

$$\Big(\sum_{r\in\mathcal{D}_{\varGamma}} \eta_{\varGamma}(r)\,\mu_r\Big)^{\widehat{}} \;=\; \mathrm{dens}(\varGamma) \sum_{r\in\mathcal{D}_{\varGamma^*}} \eta_{\varGamma^*}(r)\,\mu_r, \tag{3}$$

where $\mathcal{D}_{\varGamma} = \{r \geq 0 \mid \eta_{\varGamma}(r) > 0\}$ and analogously for $\mathcal{D}_{\varGamma^*}$, see [3] for a proof and further details. Clearly, the formula can again be brought to a more symmetric form, as in Eq. (2).

Another simple, but important example of a dual pair of mutual Fourier transforms follows from the relations $\widehat{\delta_0} = \lambda$ and $\widehat{\lambda} = \delta_0$, with λ being Lebesgue measure, so that we have

$$\big(\delta_0 + \lambda\big)^{\widehat{}} \;=\; \delta_0 + \lambda. \tag{4}$$

We shall meet this self-dual pair of measures below in Examples 1 and 9.

A little less obvious is the following result.

Lemma 1. *Let λ denote Lebesgue measure on $\mathbb{R}^d$ and $0 < \alpha < d$. The function $x \mapsto 1/|x|^{d-\alpha}$ is locally integrable and, when seen as a Radon-Nikodym density for λ, defines an absolutely continuous and translation bounded measure on $\mathbb{R}^d$. This measure satisfies the identity*

$$\left(\frac{\Gamma\big(\frac{d-\alpha}{2}\big)}{\pi^{\frac{d-\alpha}{2}}}\,\frac{\lambda}{|x|^{d-\alpha}}\right)^{\widehat{}} \;=\; \frac{\Gamma\big(\frac{\alpha}{2}\big)}{\pi^{\frac{\alpha}{2}}}\,\frac{\lambda}{|k|^{\alpha}},$$

where the transformed measure is again translation bounded and absolutely continuous. Moreover, both measures are positive and positive definite.

Proof. Local integrability of both measures on $\mathbb{R}^d$ rests upon that of their densities around 0, which follows from rewriting the volume element in polar coordinates, $\mathrm{d}\lambda(x) = r^{d-1}\,\mathrm{d}r\,\mathrm{d}\varOmega$, with $\mathrm{d}\varOmega$ the standard surface element of the unit sphere in $\mathbb{R}^d$. Absolute continuity and translation boundedness are then clear, while the Fourier identity follows from a calculation with the heat kernel, see [40, Sec. 2.2.3]. As both measures are clearly positive, they are also positive definite by the Bochner-Schwartz theorem, compare [42, Thm. IX.10]. □

Incidentally, dividing the identity in Lemma 1 by $\Gamma(\alpha/2)/\pi^{\alpha/2}$ shows that

$$\frac{\Gamma\big(\frac{d-\alpha}{2}\big)\,\pi^{\frac{\alpha}{2}}}{\Gamma\big(\frac{\alpha}{2}\big)\,\pi^{\frac{d-\alpha}{2}}}\,\frac{\lambda}{|x|^{d-\alpha}} \;\xrightarrow{\alpha\to 0}\; \delta_0$$

in the vague topology, which follows from the corresponding Fourier transforms converging vaguely to λ.

3. Renewal processes in one dimension

An interesting class of examples is provided by the classical renewal process on the real line, defined by a probability measure ϱ on $\mathbb{R}_+$ of finite mean as follows. Starting from some initial point, at an arbitrary position, a machine moves to the right with constant speed and drops another point on the line with a random waiting time that is distributed according to ϱ. When this happens, the clock is reset and the process resumes. In what follows, we assume that both the velocity of the machine and the expectation value of ϱ are 1, so that we end up (in the limit that we let the initial point move to $-\infty$) with realisations that are almost surely point sets in $\mathbb{R}$ of density 1.

Clearly, this defines a stationary Markov process, which can be analysed by considering all realisations which contain the point 0. Moreover, there is a clear symmetry around this point, so that we can determine the autocorrelation of almost all realisations from studying what happens to the right of 0. Indeed, if we want to know what the frequency per unit length of the occurrence of two points with distance x is (or the corresponding density), we need to sum the contributions that x is the first point after 0, the second point and so on. In other words, we almost surely obtain the autocorrelation

$$\gamma \;=\; \delta_0 + \nu + \widetilde{\nu} \tag{5}$$

with $\nu = \varrho + \varrho * \varrho + \varrho * \varrho * \varrho + \ldots$ and $\widetilde{\nu}(g) := \overline{\nu(\widetilde{g})}$, where $\widetilde{g}(x) = \overline{g(-x)}$ for continuous functions of compact support, provided that the sum in Eq. (5) converges properly. Note that the point measure at 0 simply reflects that the almost sure density of the resulting point set is 1.

Lemma 2. *Let ϱ be a probability measure on $\mathbb{R}_+ \cup \{0\}$, with $\varrho(\mathbb{R}_+) > 0$. Then, $\nu_n := \varrho + \varrho * \varrho + \ldots + \varrho^{*n}$ with $n \in \mathbb{N}$ defines a sequence of positive measures that converges towards a translation bounded measure ν in the vague topology.*

Proof. Note that the condition $\varrho(\mathbb{R}_+) > 0$ implies $0 \le \varrho(\{0\}) < 1$, hence excludes the case $\varrho = \delta_0$. It is thus possible to choose some $a \in \mathbb{R}_+$ with $\varrho(\{a\}) = 0$ and $0 < \varrho([0,a)) = p < 1$, so that also $\varrho([a,\infty)) = 1 - p < 1$. Since the sequence ν_n is monotonically increasing, it suffices to show that $\limsup_{n\to\infty} \nu_n([0,x))$ is bounded by $C_1 + C_2 x$ for some constants C_1, C_2, as this implies both vague convergence of the sequence and translation boundedness of the limit. As there are at most countably many points y with $\varrho(\{y\}) > 0$, it is sufficient to establish this property for all $x \in \mathbb{R}_+$ with $\varrho(\{x\}) = 0$.

If $(X_i)_{i\in\mathbb{N}}$ denotes a family of i.i.d. random variables, with common distribution according to ϱ (and thus values in $\mathbb{R}_+ \cup \{0\}$), one has

$$\mathbb{P}\big(X_1 + \ldots + X_m < x\big) \;=\; \varrho^{*m}([0,x)).$$

On the other hand, for the a chosen above, one has the inequality

$$\mathbb{P}(X_1 + \ldots + X_m < x) \;\le\; \mathbb{P}\big(\mathrm{card}\{1 \le i \le m \mid X_i \ge a\} \le x/a\big) \;=\; \sum_{\ell=0}^{[x/a]} \binom{m}{\ell} (1-p)^{\ell}\, p^{m-\ell},$$

where $\binom{m}{\ell} = 0$ whenever $\ell > m$. Observing $\sum_{m=1}^{\infty} p^m = p/(1-p)$ and

$$\sum_{m=1}^{\infty} \binom{m}{\ell} (1-p)^{\ell}\, p^{m-\ell} \;=\; (1-p)^{\ell}\, \frac{1}{\ell!} \frac{\mathrm{d}^{\ell}}{\mathrm{d}p^{\ell}} \sum_{m=0}^{\infty} p^m \;=\; \frac{1}{1-p}$$

for all $\ell \geq 1$, the previous inequality implies, for arbitrary $n \in \mathbb{N}$,

$$\nu_n([0,x)) \;\leq\; \sum_{m=1}^{\infty} \sum_{\ell=0}^{[x/a]} \binom{m}{\ell} (1-p)^{\ell}\, p^{m-\ell} \;=\; \frac{p+[x/a]}{1-p} \;\leq\; \frac{p}{1-p} + \frac{1}{a(1-p)}\, x,$$

which establishes the claim. □

Proposition 1. *Consider the renewal process on the real line, defined by a probability measure ϱ of mean 1 on $\mathbb{R}_+$. This is a stationary stochastic process, whose realisations are point sets that almost surely possess the autocorrelation measure $\gamma = \delta_0 + \nu + \widetilde{\nu}$ of (5). Here, $\nu = \sum_{n=1}^{\infty} \varrho^{*n}$ is a translation bounded positive measure. It satisfies the renewal equations*

$$\nu \;=\; \varrho + \varrho * \nu \qquad \textit{and} \qquad (1-\widehat{\varrho})\, \widehat{\nu} \;=\; \widehat{\varrho}\,,$$

where $\widehat{\varrho}$ is a uniformly continuous function on $\mathbb{R}$. In this setting, the measure γ is both positive and positive definite.

Proof. The renewal process is a classic stochastic process on the real line which is known to be stationary and ergodic, compare [20, Ch. VI.6] for details. Consequently, the measure of occurrence of a pair of points at distance $x + \mathrm{d}x$ (or the corresponding density) can be calculated by fixing one point at 0 (due to stationarity) and then determining the ensemble average for another point at $x + \mathrm{d}x$ (due to ergodicity). This is the justification for the heuristic reasoning given above, prior to Eq. 5.

By Lemma 2, ν is a translation bounded measure, so that the convolution $\varrho * \nu$ is well defined, see [11, Prop. 1.13]. The first renewal identity is then clear from the structure of ν as a limit, while the second follows by Fourier transform and the convolution theorem. The autocorrelation is a positive definite measure by construction, though this is not immediate here on the basis of its form as a sum, see [1] for a related discussion. It follows from the previous argument how to determine it. □

The autocorrelation γ is an important intermediate step in the calculation of the diffraction measure, which is $\widehat{\gamma}$. The latter is a well-defined translation bounded positive measure, provided that γ is translation bounded and positive definite. It is then an interesting first question what the spectral type of $\widehat{\gamma}$ is, i.e., what one can say about the spectral decomposition

$$\widehat{\gamma} \;=\; \bigl(\widehat{\gamma}\bigr)_{\mathsf{pp}} + \bigl(\widehat{\gamma}\bigr)_{\mathsf{sc}} + \bigl(\widehat{\gamma}\bigr)_{\mathsf{ac}} \tag{6}$$

of $\widehat{\gamma}$ into its pure point, singular continuous and absolutely continuous parts relative to λ. For the class of point sets generated by a renewal process, this requires a distinction on the basis of the support of ϱ.

The second identity of Proposition 1 is helpful here, because one has

$$\widehat{\nu}(k) \;=\; \frac{\widehat{\varrho}(k)}{1-\widehat{\varrho}(k)} \tag{7}$$

at all positions k with $\widehat{\varrho}(k) \neq 1$. This is in line with summing $\widehat{\nu}$ as a geometric series, which gives the same formula for $\widehat{\nu}(k)$ for all k with $|\widehat{\varrho}(k)| < 1$ and has (7) as the unique continuous extension to all k with $|\widehat{\varrho}(k)| = 1 \neq \widehat{\varrho}(k)$. In fact, one sees that $\widehat{\nu}(k)$ is a continuous function on the complement of the set $\{k \in \mathbb{R} \mid \widehat{\varrho}(k) = 1\}$. For most ϱ, the latter set happens to be the singleton set $\{0\}$.

In general, a probability measure μ on $\mathbb{R}$ is called *lattice-like* when its support is a subset of a translate of a lattice, see [22] for details. We need a slightly stronger property here, and call μ *strictly lattice-like* when its support is a subset of a lattice. So, the difference is that we do not allow any translates here, see [2] for related results.

Lemma 3. *If μ is a probability measure on $\mathbb{R}$, its Fourier transform, $\widehat{\mu}(k)$, is a uniformly continuous and positive definite function on $\mathbb{R}$, with $|\widehat{\mu}(k)| \le \widehat{\mu}(0) = 1$.*

Moreover, the following three properties are equivalent.

(i) $\mathrm{card}\{k \in \mathbb{R} \mid \widehat{\mu}(k) = 1\} > 1$;
(ii) $\mathrm{card}\{k \in \mathbb{R} \mid \widehat{\mu}(k) = 1\} = \infty$;
(iii) $\mathrm{supp}(\mu)$ *is contained in a lattice.*

Proof. One has $\widehat{\mu}(k) = \int_{\mathbb{R}} e^{-2\pi i k x} \, \mathrm{d}\mu(x)$, whence the first claims are standard consequences of Fourier analysis, compare [40, Prop. 5.2.1] and [43, Sec. 1.3.3].

If $\mu = \sum_{x\in\varGamma} p(x)\delta_x$ for a lattice $\varGamma \subset \mathbb{R}$, with $p(x) \ge 0$ and $\sum_{x\in\varGamma} p(x) = 1$, one has

$$\widehat{\mu}(k) \; = \; \sum_{x\in\varGamma} p(x)\, e^{-2\pi i k x},$$

so that $\widehat{\mu}(k) = 1$ for any $k \in \varGamma^*$. In particular, $\varGamma^* \subset \{k \in \mathbb{R} \mid \widehat{\mu}(k) = 1\}$, so that we have the implications (iii) $\Rightarrow$ (ii) $\Rightarrow$ (i).

Conversely, if $\widehat{\mu}(k) = 1$ for some $k \ne 0$, one has $\int_{\mathbb{R}} e^{-2\pi i k x} \, \mathrm{d}\mu(x) = 1$ and hence

$$\int_{\mathbb{R}} \bigl(1 - \cos(2\pi k x)\bigr) \, \mathrm{d}\mu(x) \; = \; \int_{\mathrm{supp}(\mu)} \bigl(1 - \cos(2\pi k x)\bigr) \, \mathrm{d}\mu(x) \; = \; 0, \tag{8}$$

where $\mathrm{supp}(\mu)$, the support of the probability measure μ, is a closed subset of $\mathbb{R}$ and measurable. The integrand is a continuous non-negative function that, due to $k \ne 0$, vanishes precisely on the set $\frac{1}{k}\mathbb{Z}$, which is a lattice.

Write $\mathrm{supp}(\mu) = A \dot{\cup} B$ as a disjoint union of measurable sets, with $A = \mathrm{supp}(\mu) \cap \frac{1}{k}\mathbb{Z}$ and $B = \mathrm{supp}(\mu) \cap (\mathbb{R} \setminus \frac{1}{k}\mathbb{Z})$. We can now split the second integral in (8) into an integral over A, which vanishes because the integrand does, and one over the set B, which would give a positive contribution by standard arguments, unless $B = \varnothing$. But this means $\mathrm{supp}(\mu) = A \subset \frac{1}{k}\mathbb{Z}$, so that (i) $\Rightarrow$ (iii), which establishes the result. $\square$

Theorem 1. *Let ϱ be a probability measure on $\mathbb{R}_+$ with mean 1, and assume that ϱ is not strictly lattice-like. Assume further, that a moment of ϱ of order $1+\varepsilon$ exists for some $0 < \varepsilon < 1$. Then, the point sets obtained from the stationary renewal process based on ϱ almost surely has a diffraction measure of the form*

$$\widehat{\gamma} \; = \; \delta_0 + \bigl(\widehat{\gamma}\bigr)_{\mathsf{ac}} \; = \; \delta_0 + (1-h)\,\lambda,$$

where h is a continuous function on $\mathbb{R} \setminus \{0\}$ that is locally integrable. It is given by

$$h(k) \; = \; \frac{2\bigl(|\widehat{\varrho}(k)|^2 - \mathrm{Re}(\widehat{\varrho}(k))\bigr)}{|1 - \widehat{\varrho}(k)|^2}\,.$$

Proof. As usual, the central peak of intensity 1 reflects the fact that the point set almost surely has density 1. Due to the assumption that $\mathrm{supp}(\varrho)$ is not contained in a lattice, we may invoke Lemma 3 to see that $\widehat{\varrho}(k) \neq 1$ whenever $k \neq 0$, so that we have pointwise convergence

$$\widehat{\nu}_n(k) \xrightarrow{n\to\infty} \widehat{\nu}(k) \; = \; \frac{\widehat{\varrho}(k)}{1-\widehat{\varrho}(k)}$$

on $\mathbb{R} \setminus \{0\}$, and similarly for $\widehat{\widetilde{\nu}}$. Since $\widehat{\varrho}$ is uniformly continuous on $\mathbb{R}$ and $\widehat{\varrho}(k) \neq 1$ on $\mathbb{R} \setminus \{0\}$, both ν and $\widetilde{\nu}$ are represented, on $\mathbb{R} \setminus \{0\}$, by continuous Radon-Nikodym densities. As $1-h$ is the sum of the Fourier transforms of these two densities, the formula for h now follows from $\widehat{\widetilde{\nu}} = \overline{\widehat{\nu}}$.

It remains to show that $1-h$ is locally integrable near 0. Let X be a random variable with distribution ϱ. Since the latter has mean 1 and our assumption guarantees that $\langle X^{1+\varepsilon}\rangle = \int_0^\infty x^{1+\varepsilon} \,\mathrm{d}\varrho(x) < \infty$, we have the Taylor series expansion

$$\widehat{\varrho}(k) \; = \; 1 - 2\pi i k + \mathcal{O}\bigl(|k|^{1+\varepsilon}\bigr), \quad \text{as } |k| \to 0,$$

by an application of [50, Thm. 1.5.4]. Inserting this into the expression for h results in

$$h(k) \; = \; 2 + \mathcal{O}(k^{-1+\varepsilon}), \quad \text{as } |k| \to 0,$$

which establishes integrability around 0, and thus absolute continuity of the measure $(1-h)\lambda$.

As the contribution to the central peak is already completely accounted for by the term δ_0, the claim follows. $\square$

Remark 1. When, under the general assumptions of Theorem 1, the second moment of ϱ exists, one obtains from [50, Thm. 1.5.3] the slightly stronger expansion

$$\widehat{\varrho}(k) \; = \; 1 - 2\pi i k - 2\pi^2 \langle X^2\rangle\, k^2 + \, o\bigl(|k|^2\bigr), \quad \text{as } |k| \to 0.$$

This leads to the asymptotic behaviour

$$h(k) \; = \; 2 - \langle X^2 \rangle + o(1), \quad \text{as } |k| \to 0,$$

which implies that h is bounded and can continuously be extended to $h(0) = 2 - \langle X^2\rangle = 1 - \sigma^2$, where σ^2 is the variance of ϱ. Clearly, the existence of higher moments implies stronger smoothness properties. $\Diamond$

The following examples permit a simpler formulation by means of the Heavyside function,

$$\Theta(x) \; := \; \begin{cases} 1, & \text{if } x > 0, \\ \frac{1}{2}, & \text{if } x = 0, \\ 0, & \text{if } x < 0. \end{cases} \tag{9}$$

This formulation of Θ has some advantage for formal calculations around generalised functions and their Fourier transforms.

Example 1. Poisson process on the real line. The probably best-known stochastic process is the classical (homogeneous) Poisson process on the line, with intensity 1, where $\varrho = f\lambda$ is given by the density

$$f(x) \; = \; e^{-x}\, \Theta(x).$$

It is easy to check that the convolution of n copies of this function yields $e^{-x}x^n\Theta(x)/n!$, which results in $\nu = \Theta\lambda$. As the intensity is 1, this results in the autocorrelation

$$\gamma \;=\; \delta_0 + \nu + \widetilde{\nu} \;=\; \delta_0 + \lambda$$

and thus in the diffraction $\widehat{\gamma} = \gamma$, compare Eq. (4). ◊

Remark 2. Let N denote a homogeneous Poisson process on the real line, so that, for any measurable $A \subset \mathbb{R}$, $N(A)$ is the number of renewal points that fall into A. It is well-known that $N(A)$ is then Poisson-$(\lambda(A))$-distributed, i.e.,

$$\mathbb{P}(N(A) = k) \;=\; \frac{e^{-\lambda(A)}\,(\lambda(A))^k}{k!}$$

with $k \in \mathbb{N}_0$, and that, for any collection of pairwise disjoint sets $A_1, A_2, \dots, A_m$, the random numbers $N(A_1), \dots, N(A_m)$ are independent. In fact, this property characterises the Poisson process (compare [16, Ch. 2.1]), and it can serve as a definition in higher dimensions or in more general measure spaces, to which the renewal process cannot be extended. ◊

Example 2. Renewal process with repulsion. A perhaps more interesting example in this spirit is given by the density

$$f(x) \;=\; 4x\,e^{-2x}\,\Theta(x).$$

It is normalised and has mean 1, as in Example 1, but models a repulsion of points for small distances. Note that this distribution can be realised out of Example 1 by taking only every second point, followed by a rescaling of time.

By induction (or by using well-known properties of the gamma distributions, compare [20, Sec. II.2]), one checks that

$$f^{*n}(x) \;=\; \tfrac{4^n}{(2n-1)!}\,x^{2n-1}\,e^{-2x}\Theta(x),$$

which finally results in the autocorrelation

$$\gamma \;=\; \delta_0 + (1 - e^{-4|x|})\,\lambda \;=\; \delta_0 + \lambda - e^{-4|x|}\,\lambda$$

and in the diffraction measure

$$\widehat{\gamma} \;=\; \delta_0 + \frac{2 + (\pi k)^2}{4 + (\pi k)^2}\,\lambda \;=\; \delta_0 + \lambda - \frac{2\lambda}{4 + (\pi k)^2}.$$

This is illustrated in Figure 1. The "dip" in the absolutely continuous part around 0, and thus the deviation from the previous example, reflects the effectively repulsive nature of the stochastic process when viewed from the perspective of neighbouring points. ◊

Example 3. Renewal process with gamma law of mean 1. The previous two examples are special cases of the gamma family of measures. For fixed mean 1, they are parametrised with a real number $\alpha > 0$ via $\varrho_\alpha = f_\alpha\lambda$ and the density

$$f_\alpha(x) \;:=\; \frac{\alpha^\alpha}{\Gamma(\alpha)}\,x^{\alpha-1}\,e^{-\alpha x}\,\Theta(x). \tag{10}$$

While $\alpha = 1$ is the "interaction-free" Poisson process, the density implies an effectively attractive (repulsive) nature of the process for $0 < \alpha < 1$ (for $\alpha > 1$).

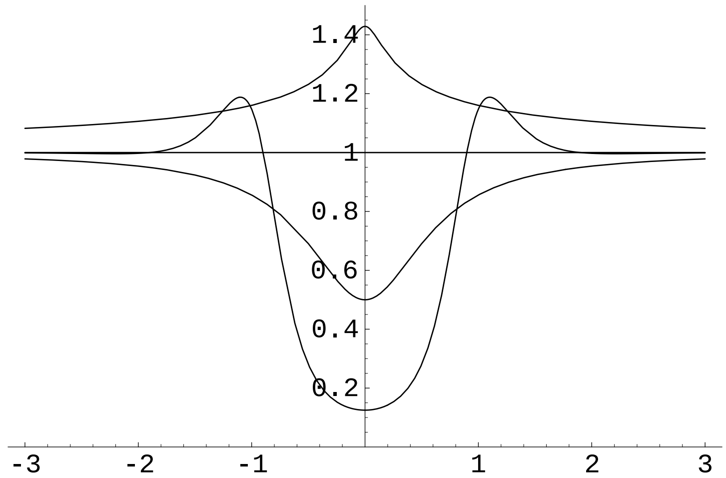

FIGURE 1. Absolutely continuous part of the diffraction measure from Example 3, for $\alpha = 0.7$ (upmost curve), $\alpha = 1$ (horizontal line, which also represents Example 1), $\alpha = 2$ (see also Example 2) and $\alpha = 8$ (overshooting curve).

Observing $f_\alpha^{*n}(x) = \frac{\alpha^{n\alpha}}{\Gamma(n\alpha)}\, x^{n\alpha-1}\, e^{-\alpha x}\, \Theta(x)$, for $n \in \mathbb{N}$, this leads to the measure

$$\nu_\alpha \;=\; g_\alpha \, \Theta \, \lambda \qquad \text{with} \qquad g_\alpha(x) \;=\; \alpha\, e^{-\alpha x} \sum_{n=1}^{\infty} \frac{(\alpha x)^{n\alpha-1}}{\Gamma(n\alpha)} \, . \tag{11}$$

Note that, for fixed α, one has $\lim_{x\to\infty} g_\alpha(x) = 1$. The calculations result in the autocorrelation

$$\gamma_\alpha \;=\; \delta_0 + g_\alpha(|x|)\, \lambda$$

and in the diffraction $\widehat{\gamma}_\alpha = \delta_0 + (1 - h_\alpha)\, \lambda$, where h_α is the symmetric function defined by

$$h_\alpha(k) \;=\; \frac{2\left(1 - \mathrm{Re}((1 + 2\pi i k/\alpha)^\alpha)\right)}{\left|1 - (1 + 2\pi i k/\alpha)^\alpha\right|^2} \, .$$

The latter follows from the general form of h in Theorem 1, together with the observation that $\widehat{f_\alpha}(k) = (1 + 2\pi i k/\alpha)^{-\alpha}$.

It is easy to see that $\lim_{k\to\pm\infty} h_\alpha(k) = 0$, for any fixed $\alpha > 0$, which makes the role of h_α as the deviation from the Poisson process diffraction more transparent, where $\alpha = 1$ and $h_1 \equiv 0$. Note also that $\lim_{\alpha\to\infty} \widehat{\gamma}_\alpha = \delta_{\mathbb{Z}}$ in the vague topology, in line with the limits mentioned before. This can nicely be studied in a series of plots of the diffraction with growing value of the parameter α. Figure 1 shows some initial cases. $\Diamond$

Remark 3. Of particular interest in the applications are Delone sets, because points (representing atoms, say) should neither be too close nor too far apart. Such sets can also arise from a renewal process. In fact, if one considers a probability measure ϱ on $\mathbb{R}_+$, the resulting point sets are always Delone sets when $\mathrm{supp}(\varrho) \subset [a,b]$ with $0 < a \le b < \infty$, and conversely. This equivalence does not depend on the nature of ϱ on $[a,b]$, while the local complexity of the resulting point sets does. In particular, if ϱ is absolutely continuous, the point sets will not have finite local complexity (see below for a definition). $\Diamond$

It is clear that no absolutely continuous ϱ is lattice-like, hence certainly not strictly lattice-like, so that all these examples match Theorem 1. But also for probability measures ϱ with $\mathrm{supp}(\varrho)$ contained in a lattice more can be said. They are of interest because they form a link to tilings of finite local complexity. Let us consider some examples.

Example 4. DETERMINISTIC LATTICE CASE. The simplest case is $\varrho = \delta_1$. From $\delta_1 * \delta_1 = \delta_2$, one sees that $\nu = \delta_{\mathbb{N}}$ and hence

$$\gamma \; = \; \delta_0 + \delta_{\mathbb{N}} + \delta_{-\mathbb{N}} \; = \; \delta_{\mathbb{Z}} \, ,$$

which is a lattice Dirac comb, with Fourier transform

$$\widehat{\gamma} \; = \; \delta_{\mathbb{Z}}$$

according to the Poisson summation formula (1). This is the deterministic case of the integer lattice, covered in this setting. $\Diamond$

Remark 4. Example 4 can also be seen as a limiting case of the measure ϱ_α defined by Eq. (10). In particular, one has $\lim_{\alpha\to\infty} \varrho_\alpha = \delta_1$ and $\lim_{\alpha\to\infty} \nu_\alpha = \delta_{\mathbb{N}}$, with ν_α as in (11) and both limits to be understood in the vague topology. This can also be seen by means of the strong law of large numbers. For each $n \in \mathbb{N}$, by well-known divisibility properties of the family of Gamma distributions, ϱ_n is the distribution of

$$\frac{1}{n} \sum_{i=1}^{n} X_i \, ,$$

where the X_i are independent and exponentially distributed random variables with mean 1. This sum then concentrates around 1, with a variance of order $1/\sqrt{n}$. $\Diamond$

Example 5. RANDOM TILINGS WITH FINITELY MANY PROTOTILES. Consider the measure

$$\varrho \; = \; \alpha \delta_a + (1{-}\alpha)\delta_b,$$

with $\alpha \in (0,1)$ and $a, b > 0$, subject to the restriction $\alpha a + (1{-}\alpha) b = 1$ to ensure density 1. Each realisation of the corresponding renewal process results in a point set that can also be viewed as a random tiling on the line with two prototiles, of lengths a and b. As before, place a normalised point measure at each point of the realisation. Then, the diffraction (almost surely) has a pure point and an absolutely continuous part, but no singular continuous one. The pure point part can be just δ_0 (when b/a is irrational) or a lattice comb, the details are given in [4], including an explicit formula for the AC part.

This has a straight-forward generalisation to any finite number of proto-tiles, with a similar result. Also in this case, there is an explicit formula for the diffraction measure, which was derived in [4] by a direct method, without using the renewal process. $\Diamond$

Remark 5. Looking back at Lemma 3, one realises that Example 5 revolves around the lattice condition in an interesting way. Namely, even if ϱ is *not* strictly lattice-like, the $\mathrm{supp}(\varrho)$ for a random tiling example with finitely many prototiles is a finite set, and thus a subset of a Meyer set. We then know from the harmonic analysis of Meyer sets, compare [37] and references therein, that $\widehat{\varrho}(k)$ will come ε-close to 1 with bounded gaps in k. This means that the diffraction measure, though it is absolutely continuous apart from the central peak at $k = 0$, will develop sharp "needles" that are close to point measures in the vague topology — a phenomenon that was also observed in [4] on the basis of the explicit solution. $\Diamond$

4. Arbitrary dimensions: Elementary approach

Let us now develop some intuition for the influence of randomness on the diffraction of point sets and certain structures derived from them in Euclidean spaces of arbitrary dimension. In this section, our point of view is from a single point set $\varLambda \subset \mathbb{R}^d$ that is being modified randomly, while Section 5 revisits this situation coming from a stationary ergodic point process approach, which treats almost all of its realisations at once.

Let $\varLambda \subset \mathbb{R}^d$ be a fixed point set, which we assume to be of finite local complexity (FLC). This property is equivalent to saying that the difference set $\varLambda - \varLambda$ is locally finite [46]. In particular, $\varLambda$ is uniformly discrete. Attached to $\varLambda$ is its *Dirac comb* $\delta_{\varLambda} = \sum_{x\in\varLambda} \delta_x$, which is a translation bounded measure. In order to introduce a diffraction measure for $\delta_{\varLambda}$, we need to define an autocorrelation measure first. As this requires a volume weighted limiting process, we fix an *averaging sequence* $\mathcal{A} = \{A_n \mid n \in \mathbb{N}\}$ of relatively compact open sets A_n subject to the conditions $\overline{A_n} \subset A_{n+1}$ and $\bigcup_{n\in\mathbb{N}} A_n = \mathbb{R}^d$. In addition, we require that $\mathcal{A}$ is also a van Hove sequence, which essentially means that the surface to volume ratio of A_n tends to 0 as $n \to \infty$, see [46] for details on this. Such sequences clearly exist, and natural ones could be of the form $A_n = B_{r_n}(0)$, with $B_r(0)$ denoting the open ball of radius r around 0, for a non-decreasing series of radii with $r_n \xrightarrow{n\to\infty} \infty$, or similarly with nested cubes.

Set $\varLambda_n = \varLambda \cap A_n$ (so that $\varLambda_n \nearrow \varLambda$ in the obvious local topology [46]) and consider the measure

$$\begin{aligned}\gamma_{\varLambda,n} \; &:= \; \frac{\delta_{\varLambda_n} * \widetilde{\delta_{\varLambda}}}{\mathrm{vol}(A_n)} \; = \; \sum_{x\in\varLambda_n}\sum_{y\in\varLambda} \delta_{x-y} \; = \; \sum_{z\in\varLambda-\varLambda} \Bigl(\frac{1}{\mathrm{vol}(A_n)} \sum_{\substack{x\in\varLambda_n,\, y\in\varLambda \\ x-y=z}} 1\Bigr)\, \delta_z \\ &= \; \sum_{z\in\varLambda-\varLambda} \frac{\mathrm{card}\{x\in\varLambda_n \mid x-z \in \varLambda\}}{\mathrm{vol}(A_n)}\, \delta_z \; =: \; \sum_{z\in\varLambda-\varLambda} \eta_n(z)\, \delta_z \,,\end{aligned}$$

which is well-defined by [11, Prop. 1.13]. This also defines the approximating autocorrelation coefficients $\eta_n(z)$. We now make the assumption that the limit

$$\lim_{n\to\infty} \gamma_{\varLambda,n} \; =: \; \gamma_{\varLambda} \tag{12}$$

exists in the vague topology, which means that $\lim_{n\to\infty} \gamma_{\varLambda,n}(g) = \gamma_{\varLambda}(g)$ for all continuous functions g with compact support. Due to the van Hove property of $\mathcal{A}$, one also has

$$\lim_{n\to\infty} \frac{1}{\mathrm{vol}(A_n)}\, \delta_{\varLambda_n} * \widetilde{\delta_{\varLambda_n}} \; = \; \gamma_{\varLambda}, \tag{13}$$

see [46, Lemma 1.2] for a proof. The difference between the two approximating measures in (12) and (13) is a "surface term" that vanishes in the infinite volume limit $n \to \infty$. The formulation in (13) explicitly shows that the measure $\gamma_{\varLambda}$ is positive definite.

Since $\varLambda - \varLambda$ is locally finite by assumption, and thus countable, Eq. (12) implies that also all the limits

$$\lim_{n\to\infty} \eta_n(z) \; =: \; \eta(z) \tag{14}$$

exist. Clearly, the measure $\gamma_{\varLambda}$ as well as the coefficients $\eta(z)$ may (and generally will) depend on the averaging sequence, though we suppress this dependence in the notation. The measure $\gamma_{\varLambda}$ is positive definite, and hence Fourier transformable [11]. The measure

$\widehat{\gamma}_{\Lambda}$ is then a translation bounded, positive measure on $\mathbb{R}^d$, which is called the *diffraction measure* of Λ, relative to the averaging sequence $\mathcal{A}$.

Remark 6. Since δ_{Λ} is translation bounded, the sequence of measures $\gamma_{\Lambda,n}$ always has points of accumulation, by [27, Prop. 2.2]. Consequently, one can always select a subsequence of $\mathcal{A}$ for which the assumption (12) is satisfied. In this sense, when the autocorrelation is not unique, we have simply selected *one* of the possible autocorrelations by a suitable choice of $\mathcal{A}$. This is now fixed, and our results below apply to any autocorrelation of this kind separately. In this sense, the assumption made in (12) or in (13) is not restrictive. $\Diamond$

The next step consists in modifying Λ by a random process in a local way. To come to a reasonably general formulation that includes several notions of randomness known from lattice theory, compare [25, 51], we employ a formulation with finite random complex measures. Let Ω denote a measure-valued random variable, and Q the corresponding law, which is itself a probability measure on $\mathcal{M}_{\mathsf{bd}} = \mathcal{M}_{\mathsf{bd}}(\mathbb{R}^d)$, the space of finite complex measures on $\mathbb{R}^d$. It is viewed as the continuous linear functionals on the space of bounded continuous functions, and coincides with the finite Borel measures by the Riesz-Markov representation theorem [42, Thm. IV.18].

To keep the notation compact, we use the symbol $\mathbb{E}_Q$ for the various expectation values. In particular, we write $\mathbb{E}_Q(\Omega) = \int_{\mathcal{M}_{\mathsf{bd}}} \omega \, \mathrm{d}Q(\omega)$, where ω refers to the realisations of Ω as usual.

To proceed, we need a version of the strong law of large numbers (SLLN) for measures.

Lemma 4. *Let $(\Omega_i)_{i\in\mathbb{N}}$ be a sequence of integrable finite i.i.d. random measures, with common law Q. Then, with probability* 1, *one has*

$$\frac{1}{n}\sum_{i=1}^{n} \Omega_i \xrightarrow{\; n\to\infty \;} \mathbb{E}_Q(\Omega_1)$$

in the vague topology.

Proof. Integrability means that $\mathbb{E}_Q(|\Omega_i|)$, which is independent of $i \in \mathbb{N}$, is a finite measure. As the space of continuous functions is separable, the almost sure convergence of the measures follows from the almost sure convergence of $\frac{1}{n}\sum_{i=1}^{n} \Omega_i(\varphi)$ for an arbitrary, but fixed bounded continuous function φ. This, in turn, follows from the conventional SLLN [19], possibly after splitting the sums into their real and imaginary parts and applying the SLLN twice. $\square$

Recall that $\widetilde{\omega}$ is the measure defined by $\widetilde{\omega}(\varphi) = \overline{\omega(\widetilde{\varphi})}$. Let Ω and Ω' be two independent random measures, with the same law Q, and such that $\mathbb{E}_Q(|\Omega|)$ is a finite measure, together with the second moment condition $\mathbb{E}_Q(|\Omega(\mathbb{R}^d)|^2) < \infty$. Then, the convolution $\Omega * \Omega'$ is well defined, and one obtains the important relations

$$\mathbb{E}_Q(\widetilde{\Omega}) = \widetilde{\mathbb{E}_Q(\Omega)} \quad \text{and} \quad \mathbb{E}_Q(\Omega * \widetilde{\Omega}') = \mathbb{E}_Q(\Omega) * \widetilde{\mathbb{E}_Q(\Omega')}, \tag{15}$$

which follow from elementary calculations, the second due to the assumed independence.

Let us now consider the random measure $\delta_{\Lambda}^{(\Omega)} = \sum_{x\in\Lambda} \Omega_x * \delta_x$ derived from the fixed point set Λ introduced above, where the Ω_x are integrable finite i.i.d. complex random measures, with common law Q and the restrictions mentioned above. When $\varOmega$ is any of these measures, $\mathbb{E}_Q(|\varOmega|)$ is a finite measure by assumption, and the measure-valued expectations $\mathbb{E}_Q(\varOmega)$ and $\mathbb{E}_Q(\varOmega * \widetilde{\varOmega})$ exist (note that also $\mathbb{E}_Q(|\varOmega * \widetilde{\varOmega}|)$ is a finite measure, due to the condition on the second moment). Observing

$$\widetilde{\delta_{\varLambda}^{(\varOmega)}} \; = \; \sum_{y\in\varLambda} \widetilde{\varOmega}_y * \delta_{-y},$$

it is easy to see that the modified autocorrelation approximant reads

$$\begin{aligned}
\gamma_{\varLambda,n}^{(\varOmega)} \; &= \; \frac{1}{\mathrm{vol}(A_n)} \Big(\sum_{x\in\varLambda_n} \varOmega_x * \delta_x \Big) * \Big(\sum_{y\in\varLambda} \widetilde{\varOmega}_y * \delta_{-y} \Big) \\
&= \; \sum_{z\in\varLambda-\varLambda} \Big(\frac{1}{\mathrm{vol}(A_n)} \sum_{\substack{x\in\varLambda_n \\ x-z\in\varLambda}} \varOmega_x * \widetilde{\varOmega}_{x-z} \Big) * \delta_z \; =: \; \sum_{z\in\varLambda-\varLambda} \zeta_{z,n}^{(\varOmega)} * \delta_z \, ,
\end{aligned} \tag{16}$$

where we now need to analyse the behaviour of the random measures $\zeta_{z,n}^{(\varOmega)}$.

Let us first look at $z = 0$, where we obtain

$$\zeta_{0,n}^{(\varOmega)} \; = \; \frac{\mathrm{card}(\varLambda_n)}{\mathrm{vol}(A_n)} \frac{1}{\mathrm{card}(\varLambda_n)} \sum_{x\in\varLambda_n} \varOmega_x * \widetilde{\varOmega}_x \xrightarrow{\; n\to\infty \;} \mathrm{dens}(\varLambda) \cdot \mathbb{E}_Q(\varOmega * \widetilde{\varOmega}) \qquad \text{(a.s.)}$$

by an application of Lemma 4. Note that $\mathrm{dens}(\varLambda) = \eta(0)$ as introduced in (14). Next, assume $z \in \varLambda - \varLambda$ with $z \neq 0$. Then, we split $\zeta_{z,n}^{(\varOmega)}$ into 2 sums,

$$\zeta_{z,n}^{(\varOmega)} \; = \; \frac{1}{\mathrm{vol}(A_n)} \Big(\sum_{\substack{x\in\varLambda_n \\ x-z\in\varLambda}}^{(1)} \varOmega_x * \widetilde{\varOmega}_{x-z} \; + \sum_{\substack{y\in\varLambda_n \\ y-z\in\varLambda}}^{(2)} \varOmega_y * \widetilde{\varOmega}_{y-z} \Big),$$

where the upper index stands for the following additional restriction. For a fixed n, the total summation set is partitioned into maximal linear chains of the form $(x, x-z, x-2z, \ldots, x-kz)$, $k \in \mathbb{N}$, with all points lying in $\varLambda$ and all except possibly the last one lying in $\varLambda_n$. The k random measures $\varOmega_{x-(m-1)z} * \widetilde{\varOmega}_{x-mz}$, for $1 \le m \le k$, are identically distributed, but not independent (due to the index overlap). However, those with m odd (type (1)) are mutually independent, as are those with m even (type (2)). Consequently, we alternatingly distribute them to the two sums, according to their type. Now, we split

$$\mathrm{card}\{x \in \varLambda_n \mid x - z \in \varLambda\} \; = \; N_n^{(1)} + N_n^{(2)}$$

accordingly, where we then have that $N_n^{(1)} \ge N_n^{(2)}$ (note that all chains with k odd contribute one term more to sum (1) than to sum (2), which applies to $k = 1$ in particular). With this, we can now rewrite our previous expression as

$$\zeta_{z,n}^{(\varOmega)} \; = \; \frac{\mathrm{card}\{x \in \varLambda_n \mid x - z \in \varLambda\}}{\mathrm{vol}(A_n)} \Big(\frac{N_n^{(1)}}{N_n^{(1)} + N_n^{(2)}} \frac{\sum^{(1)}}{N_n^{(1)}} + \frac{N_n^{(2)}}{N_n^{(1)} + N_n^{(2)}} \frac{\sum^{(2)}}{N_n^{(2)}} \Big),$$

where the term in brackets is the convex combination of two random measures. By (14), the factor in front of the bracket converges to $\eta(z)$. When this limit is non-zero, we know that $N_n^{(1)} \xrightarrow{n\to\infty} \infty$, so that

$$\frac{1}{N_n^{(1)}} \sum\nolimits^{(1)} \xrightarrow{\; n\to\infty \;} \mathbb{E}_Q(\varOmega) * \widetilde{\mathbb{E}_Q(\varOmega)} \qquad \text{(a.s.)} \tag{17}$$

by Lemma 4 and Eq. (15).

Now, since $\overline{A_n} \subset A_{n+1}$, we can see that the sequence $\bigl(N_n^{(2)}\bigr)_{n\in\mathbb{N}}$ is non-decreasing. Thus, either $N_n^{(2)}$ stays bounded (whence we can forget the contribution from $\sum^{(2)}/N_n^{(2)}$ because it stays a.s. bounded, while its prefactor converges to 0), or we also have $N_n^{(2)} \xrightarrow{n\to\infty} \infty$, in which case Lemma 4 gives us the almost sure convergence of the second random measure to the same limit as in (17). In this case, though we do not know whether the rational prefactors converge, we have a convex combination of two sequences that each almost surely converge to the same limit, which must then also be the limit of their convex combination. Put together, this gives

$$\zeta_{z,n}^{(\Omega)} \xrightarrow{n\to\infty} \eta(z) \cdot \mathbb{E}_Q(\Omega) * \widetilde{\mathbb{E}_Q(\Omega)} \qquad \text{(a.s.)}$$

for all $z \in \varLambda - \varLambda$ with $z \neq 0$.

Theorem 2. *Let $\varLambda \subset \mathbb{R}^d$ be an FLC point set, so that its Dirac comb $\delta_\varLambda$ possesses the autocorrelation measure $\gamma_\varLambda$ of* (12)*, relative to the fixed averaging sequence $\mathcal{A}$, and thus the diffraction measure $\widehat{\gamma}_\varLambda$. Let $(\Omega_x)_{x\in\varLambda}$ be a family of finite, integrable, complex i.i.d. random measures with common law Q and finite second moment measure, with Ω being any representative of this family, and consider the random measure $\delta_\varLambda^{(\Omega)} := \sum_{x\in\varLambda} \Omega_x * \delta_x$.*

Then, the sequence of approximating measures $\gamma_{\varLambda,n}^{(\Omega)}$ of (16) *almost surely converges, as $n \to \infty$, to the positive definite translation bounded autocorrelation measure*

$$\gamma_\varLambda^{(Q)} \;=\; \bigl(\mathbb{E}_Q(\Omega) * \widetilde{\mathbb{E}_Q(\Omega)}\bigr) * \gamma_\varLambda + \operatorname{dens}(\varLambda)\,\bigl(\mathbb{E}_Q(\Omega * \widetilde{\Omega}) - \mathbb{E}_Q(\Omega) * \widetilde{\mathbb{E}_Q(\Omega)}\bigr) * \delta_0 .$$

This measure has the Fourier transform

$$\widehat{\gamma}_\varLambda^{(Q)} \;=\; \bigl|\widehat{\mathbb{E}_Q(\Omega)}\bigr|^2 \cdot \widehat{\gamma}_\varLambda + \operatorname{dens}(\varLambda)\,\bigl(\mathbb{E}_Q(\Omega * \widetilde{\Omega}) - \mathbb{E}_Q(\Omega) * \widetilde{\mathbb{E}_Q(\Omega)}\bigr)^{\widehat{}} \cdot \lambda,$$

which is the almost sure diffraction measure of the random measure $\delta_\varLambda^{(\Omega)}$.

Proof. The previous calculations showed the individual almost sure convergence of the measures $\zeta_{z,n}^{(\Omega)}$. Since $\varLambda - \varLambda$ is locally finite and countable, this is sufficient for the almost sure convergence of the measures $\gamma_{\varLambda,n}^{(\Omega)}$ as well, because they are almost surely uniformly translation bounded by construction. The explicit formula for the autocorrelation measure $\gamma_\varLambda^{(Q)}$ now follows from elementary calculations.

The measure $\gamma_\varLambda^{(Q)}$ is positive definite, and its Fourier transform has the form claimed as a result of the convolution theorem [11, Ex. 4.18]. It is applicable here because all expectation measures involved are finite measures, so that their Fourier transforms are represented by uniformly continuous functions on $\mathbb{R}^d$. $\square$

Let us look at consequences of Theorem 2 in terms of some examples.

Example 6. Deterministic clusters. Let $S \subset \mathbb{R}^d$ be a finite point set, and consider $\Omega \equiv \delta_S = \sum_{x\in S} \delta_x$. Clearly, this completely deterministic case gives $\mathbb{E}_Q(|\Omega|) = \mathbb{E}_Q(\Omega) = \delta_S$ and $\mathbb{E}_Q(\Omega * \widetilde{\Omega}) = \delta_S * \widetilde{\delta_S}$, so that Theorem 2 results in $\gamma_\varLambda^{(\Omega)} = \bigl(\delta_S * \widetilde{\delta_S}\bigr) * \gamma_\varLambda$ and $\widehat{\gamma}_\varLambda^{(\Omega)} = |\widehat{\delta_S}|^2 \cdot \widehat{\gamma}_\varLambda$, which is always true in this case. A particularly simple instance of this emerges from $S = \{a\}$, which effectively means a global translation by a. This leads to the relations $\gamma_\varLambda^{(\Omega)} = \gamma_\varLambda$ and $\widehat{\gamma}_\varLambda^{(\Omega)} = \widehat{\gamma}_\varLambda$, as it must. $\Diamond$

Example 7. Random weight model. Here, we consider $\varOmega = H\delta_0$, where H is a complex-valued random variable with a law μ that satisfies $\mathbb{E}_\mu(|H|^2) < \infty$ (hence also $\mathbb{E}_\mu(|H|) < \infty$). Clearly, this gives $\mathbb{E}_Q(\varOmega) = \mathbb{E}_\mu(H)\,\delta_0$ and $\mathbb{E}_Q(\varOmega * \widetilde{\varOmega}) = \mathbb{E}_\mu(|H|^2)\,\delta_0$, so that Theorem 2 results in the following diffraction formula:

$$\widehat{\gamma}_\varLambda^{(\varOmega)} \;=\; |\mathbb{E}_\mu(H)|^2 \cdot \widehat{\gamma}_\varLambda + \mathrm{dens}(\varLambda)\left(\mathbb{E}_\mu(|H|^2) - |\mathbb{E}_\mu(H)|^2\right) \cdot \lambda \qquad \text{(a.s.)}.$$

The autocorrelation is clear from taking the inverse Fourier transform. ◊

Remark 7. A widely used special case of Example 7 is the random occupation model, or "$\varLambda$-gas". Here, $\varOmega$ may take the value δ_0 (with probability p, for "occupied") or 0 (with probability $1-p$, for "empty"). This almost surely gives the diffraction

$$\widehat{\gamma}_\varLambda^{(\varOmega)} \;=\; p^2 \cdot \widehat{\gamma}_\varLambda + \mathrm{dens}(\varLambda) \cdot p(1-p) \cdot \lambda,$$

which was derived in this setting in [7], and later generalised to Bernoulli and Markov systems [4] and significantly beyond [35, 36]. ◊

The results of Examples 6 and 7 can be extended in many ways, some of which will be met later on. One further possibility consists in replacing a point by a "profile", as described by an integrable function, or by a finite collection of such profiles, which could represent different types of atoms. The corresponding formulas for the autocorrelation and the diffraction are then easy analogues of the ones given so far.

Example 8. Random displacement model. Consider the random measure $\varOmega = \delta_X$, where X is an $\mathbb{R}^d$-valued random variable with law ν. So, ν is a probability measure on $\mathbb{R}^d$, assumed to have bounded mean. If $A \subset \mathbb{R}^d$ is a Borel set, one has

$$\mathbb{E}_Q(\varOmega)(A) \;=\; \int_{\mathbb{R}^d} \delta_x(A)\,\mathrm{d}\nu(x) \;=\; \int_{\mathbb{R}^d} \mathbf{1}_A(x)\,\mathrm{d}\nu(x) \;=\; \nu(A),$$

which shows that $\mathbb{E}_Q(\varOmega) = \nu$. Similarly, one finds $\mathbb{E}_Q(\varOmega * \widetilde{\varOmega}) = \nu(\mathbb{R}^d)\,\delta_0 = \delta_0$. Then, Theorem 2 results in the equations

$$\begin{aligned} \gamma_\varLambda^{(\varOmega)} &= (\nu * \widetilde{\nu}) * \gamma_\varLambda + \mathrm{dens}(\varLambda)\,(\delta_0 - \nu * \widetilde{\nu}) \qquad \text{(a.s.)},\\ \widehat{\gamma}_\varLambda^{(\varOmega)} &= |\widehat{\nu}|^2 \cdot \widehat{\gamma}_\varLambda \;+\; \mathrm{dens}(\varLambda)\,(1 - |\widehat{\nu}|^2) \cdot \lambda \qquad \text{(a.s.)}, \end{aligned}$$

which recovers Hof's result on the diffraction at high temperature [28]. ◊

In fact, Hof's approach, which also uses the SLLN, does not require the FLC property, though it then needs some ergodicity assumption on the underlying point set instead. Nevertheless, it is clear that the formulas of Theorem 2 should be robust, and also hold for other point sets, such as those coming from a homogeneous Poisson process. So, to complement our approach of this section, let us now consider ergodic point processes instead, meaning that also the set $\varLambda$ becomes part of the random structure.

5. Arbitrary dimensions: Point process approach

Here, we are interested in the diffraction of certain random subsets of $\mathbb{R}^d$, where we restrict ourselves to the situation that these subsets are self-averaging in a suitable way. This will be guaranteed by the ergodicity of the underlying stochastic process. It is convenient to start by putting ourselves in the context of random counting measures, which we now summarise in a way that is tailored to diffraction theory.

5.1. **Random measures and point processes.** Let $\mathcal{M}^+$ denote the set of all locally finite positive measures ϕ on $\mathbb{R}^d$ (where we mean to include the 0 measure). That ϕ is locally finite (some authors say ϕ is boundedly finite or that ϕ is a Radon measure) means that, for all bounded Borel sets A, $\phi(A) < \infty$. The space $\mathcal{M}^+$ is closed in the topology of vague convergence of measures (in fact, $\mathcal{M}^+$ is a complete separable metric space, see [16, A 2.6]). We let $\Sigma_{\mathcal{M}^+}$ denote the σ-algebra of Borel sets of $\mathcal{M}^+$. The latter can be described as the σ-algebra of subsets of $\mathcal{M}^+$ generated by the requirement that, for all Borel sets $A \subset \mathbb{R}^d$, the mapping $\phi \mapsto \phi(A)$ is measurable (compare [32, Chs. 1.1 and 1.2] for background).

A *random measure* on $\mathbb{R}^d$ is a random variable $\varPhi$ from a probability space $(\varTheta, \mathcal{F}, \pi)$ into $(\mathcal{M}^+, \Sigma_{\mathcal{M}^+})$. Let us write $\mathcal{P}(\mathcal{M}^+)$ for the convex set of probability measures on $\mathcal{M}^+$. The *distribution* of a random measure $\varPhi$ is the probability measure $P = P_{\varPhi} \in \mathcal{P}(\mathcal{M}^+)$, defined by $P = \pi \circ \varPhi^{-1}$. In other words, P is the *law* of $\varPhi$, written as $\mathcal{L}(\varPhi) = P$. Note that, as soon as P is given or determined, one can ignore the underlying probability space for most considerations.

For each $t \in \mathbb{R}^d$, let T_t denote the translation operator on $\mathbb{R}^d$, as defined by the mapping $x \mapsto t + x$. Clearly, one has $T_t T_s = T_{t+s}$, and the inverse of T_t is given by $T_t^{-1} = T_{-t}$. For functions f on $\mathbb{R}^d$, the corresponding translation action is defined via $T_t f = f \circ T_{-t}$, so that $T_t f(x) = f(x - t)$. Similarly, for $\phi \in \mathcal{M}^+$, let $T_x \phi := \phi \circ T_{-x}$ be the image measure under the translation, i.e., $(T_x \phi)(A) = \phi(T_{-x}(A)) = \phi(A - x)$ for any measurable subset $A \subset \mathbb{R}^d$, and $\int_{\mathbb{R}^d} f(y) \, \mathrm{d}(T_x \phi)(y) = \int_{\mathbb{R}^d} f(x + z) \, \mathrm{d}\phi(z)$ for functions. This means that there is a translation action of $\mathbb{R}^d$ on $\mathcal{M}^+$. Finally, we also have a translation action on $\mathcal{P}(\mathcal{M}^+)$, via $(T_x Q)(\phi) = Q(T_{-x} \phi)$.

Our primary interest is in random counting measures. A measure ϕ on $\mathbb{R}^d$ is called a *counting measure* if $\phi(A) \in \mathbb{N}_0$ for all bounded Borel sets A. These are positive integer-valued measures of the form $\phi = \sum_{i \in I} \delta_{x_i}$, where the index set I is (at most) countable and the support of ϕ is a locally finite subset of $\mathbb{R}^d$. The (positive) counting measures form a subset $\mathcal{N}^+ \subset \mathcal{M}^+$. We can repeat the above discussion of $\mathcal{M}^+$ by restricting everything to $\mathcal{N}^+$. The vague topology on $\mathcal{N}^+$ is the same as its topology inherited from $\mathcal{M}^+$, and its σ-algebra of Borel sets $\Sigma_{\mathcal{N}^+}$ consists of the intersections of the elements of $\Sigma_{\mathcal{M}^+}$ with $\mathcal{N}^+$. The concepts of the law of a random measure and the translation action by $\mathbb{R}^d$ carry over. In particular, for $x \in \operatorname{supp}(\phi)$ with $\phi \in \mathcal{N}^+$, $T_{-x}\phi$ corresponds to the counting measure obtained from ϕ by translating its support so that x is shifted to the origin.

A *point process* on $\mathbb{R}^d$ is a random variable $\varPhi$ from a probability space $(\varTheta, \mathcal{F}, \pi)$ into $(\mathcal{N}^+, \Sigma_{\mathcal{N}^+})$. Alternatively, a point process is a random measure for which π-almost all $\theta \in \varTheta$ are counting measures. Furthermore, it is called *simple* when, for π-almost all $\theta \in \varTheta$, the atoms of $\phi = \varPhi(\theta)$ have weight (or multiplicity) 1.

In the sequel, when we are dealing with point processes, we only use simple point processes, whence we feel free to identify point measures with their supports. In this case, the measures are Dirac combs of the form $\phi = \delta_S$ with $S \subset \mathbb{R}^d$ locally finite. Later on, we create compound processes in which an underlying point process is decorated with a random finite measure, and this will take us from $\mathcal{N}^+$ to $\mathcal{M}^+$, which is also the reason why we introduced random measures above.

A random measure (or a point process) $\varPhi$ is called *stationary* when its distribution P is translation invariant, i.e., when $T_t P = P \circ T_{-t} = P$ holds for all $t \in \mathbb{R}^d$. For $\varPhi$ with distribution P, the expectation measure $\mathbb{E}_P(\varPhi)$, defined by

$$\mathbb{E}_P(\varPhi)(A) \; = \; \mathbb{E}_P(\varPhi(A)) \; = \; \int_{\mathcal{N}^+} \phi(A) \, \mathrm{d}P(\phi), \quad \text{for } A \subset \mathbb{R}^d \text{ Borel}, \tag{18}$$

is a measure on $\mathbb{R}^d$ which gives the *expected* mass (or number of points) that $\varPhi$ has in A. In terms of the underlying probability space $(\varTheta, \mathcal{F}, \pi)$, one has

$$\mathbb{E}_P(\varPhi(A)) \; = \; \int_{\varTheta} \varPhi(\theta)(A) \, \mathrm{d}\pi(\theta) \; = \; \int_{\mathcal{N}^+} \varPhi(A) \, \mathrm{d}P(\varPhi),$$

where the latter expression is a slight abuse of notation, which we nevertheless adopt (as is common practice in the probability literature), because it suppresses the explicit dependence on $(\varTheta, \mathcal{F}, \pi)$.

Remark 8. If P is stationary, we have $T_t \mathbb{E}_P(\varPhi) = \mathbb{E}_P(\varPhi)$ for all $t \in \mathbb{R}^d$, whence $\mathbb{E}_P(\varPhi)$ must be a multiple of Lebesgue measure (the latter being Haar measure on $\mathbb{R}^d$). Consequently,

$$I_P(\varPhi) \; = \; \mathbb{E}_P(\varPhi) \; = \; \rho\lambda,$$

where $\rho \in [0, \infty]$ is usually called the *intensity* of P. In the setting of point processes, it also has the meaning of a point density, averaged over all realisations of the process. In the ergodic case (see below for a definition), it is then almost surely the density of a given realisation in the usual sense. We thus prefer to call ρ the *point density* of the simple point process or the *density* of the random measure. $\Diamond$

Let $\varPhi \colon (\varTheta, \mathcal{F}, \pi) \longrightarrow (\mathcal{X}, \varSigma_{\mathcal{X}})$ be a stationary random measure (where $\mathcal{X} = \mathcal{M}^+$) or point process ($\mathcal{X} = \mathcal{N}^+$), with law P. Then, $(\mathcal{X}, \varSigma_{\mathcal{X}}, P)$ is a probability space with translation invariant probability measure P. The random measure or point process $\varPhi$ is called *ergodic* when $(\mathcal{X}, \varSigma_{\mathcal{X}}, P)$ is ergodic, see below for more.

5.2. **Palm distribution and autocorrelation.** Let $P \in \mathcal{P}(\mathcal{N}^+)$ be stationary with finite point density $\rho < \infty$. Let $\mathbf{1}_{\mathcal{B}}$, as usual, denote the characteristic function of the set $\mathcal{B}$, and choose a Borel set $A \subset \mathbb{R}^d$ with $0 < \lambda(A) < \infty$. The *Palm distribution* P_0 is the probability measure on $\mathcal{N}^+$ that satisfies

$$P_0(\mathcal{B}) \; = \; \frac{1}{\mathbb{E}_P(\varPhi(A))} \int_{\mathcal{N}^+} \sum_{x \in A \cap \operatorname{supp}(\varPhi)} \varPhi(\{x\}) \, \mathbf{1}_{\mathcal{B}}\big(T_{-x}\varPhi\big) \, \mathrm{d}P(\varPhi) \tag{19}$$

for any $\mathcal{B} \in \varSigma_{\mathcal{N}^+}$, compare [48, Ch. 4.4] or [33, Ch. 3] for background. Due to stationarity, Remark 8 applies to $\mathbb{E}_P(\varPhi(A))$, whence the prefactor simplifies to $(\rho\lambda(A))^{-1}$. Note that the sum under the integral runs over at most countably many points. Moreover, the definition does *not* depend on the actual choice of A. Intuitively, P_0 describes the configuration $\varPhi$ as seen from a typical point in $\operatorname{supp}(\varPhi)$, with that point translated to the origin. Alternatively, in the case of simple random measures, one can think of P_0 as the distribution of $\varPhi$, conditioned on having a point measure at 0. This actually amounts to properly condition on an event of probability 0, which might need some further explanation.

The first point of view can be made precise, at least in the ergodic case, as a limit, via sampling points in $\varPhi$ over larger and larger balls, see [33, Thm. 3.6.6] or [16, Prop. 12.2.VI and Prop. 12.4.I] as well as Eq. (21) below. The second interpretation can be corroborated by conditioning $\varPhi$ to have a point in a small ball around 0 and then again taking a limit, see [16, Thm. 12.3.V]. In more precise terms, P_0 would be called the *Palm distribution with respect to* $0 \in \mathbb{R}^d$, compare [31, Ch. 10] or [16, Ch. 12.1]. Since we will mostly be dealing with the stationary scenario, we refrain from spelling out the full name.

There is an alternative approach to the Palm distribution, which also applies to the random measure case, compare [16, Chs. 12.1 and 12.2]. Let $\varPhi \colon (\varTheta, \mathcal{F}, \pi) \longrightarrow (\mathcal{M}^+, \varSigma_{\mathcal{M}^+})$ be a stationary random measure with law P and finite mean density $\rho < \infty$. Then, the *Palm measure* is the unique probability measure P_0 on $\mathcal{M}^+$ that satisfies

$$\mathbb{E}_P \left(\int_{\mathbb{R}^d} g(x, \varPhi) \, \mathrm{d}\varPhi(x) \right) \; = \; \rho \int_{\mathbb{R}^d} \int_{\mathcal{M}^+} g(x, T_x \psi) \, \mathrm{d}P_0(\psi) \, \mathrm{d}x \tag{20}$$

for all non-negative functions g on $\mathbb{R}^d \times \mathcal{M}^+$ for which $\int_{\mathbb{R}^d} \int_{\mathcal{M}^+} g(x, \phi) \, \mathrm{d}\phi(x) \, \mathrm{d}P(\phi)$ is finite. When dealing with point processes, all this reduces to $\mathcal{N}^+$ by simply replacing $\mathcal{M}^+$ with $\mathcal{N}^+$ throughout Eq. (20), compare [16, Ch. 2.2 and Eq. 12.2.3].

If $\varPhi$ is an ergodic stationary random measure, an application of the ergodic theorem implies that, almost surely,

$$\frac{1}{\lambda(B_n)} \int_{B_n} F(T_{-x} \varPhi) \, \mathrm{d}\varPhi(x) \; \xrightarrow{\, n \to \infty \,} \; \rho \int_{\mathcal{M}^+} F(\varPsi) \, \mathrm{d}P_0(\varPsi) \, , \tag{21}$$

for any non-negative measurable function $F \colon \mathcal{M}^+ \to \mathbb{R}$, see [16, Prop. 12.2.VI] or the proof of [33, Thm. 3.6.6]. Here and below, we write $\lambda(B_n)$ for $\mathrm{vol}(B_n(0))$.

In the literature, the probability measure P_0 is sometimes called the *Palm distribution* of P (with respect to 0), while the term 'Palm measure' is also in use for the unnormalised version ρP_0. The intensity measure of the latter coincides with the *autocorrelation measure* of the underlying process (a notion that we also adopt here) and is denoted by γ_P. This is motivated by the following result on the autocorrelation $\gamma_P^{(\varPhi)}$ of a given realisation, which is somewhat implicit in the literature. Its importance in our present context was first emphasised by Goueré in [23].

Theorem 3. *Let $\varPhi$ be a stationary and ergodic random measure with distribution P. Assume that P has finite density ρ, and that P has finite second moments in the sense that $\mathbb{E}_P(\varPhi(A)^2) < \infty$ for any bounded $A \subset \mathbb{R}^d$ (this follows for instance from the condition $\mathbb{E}_P(\varPhi(B_r(x))^2) < \infty$ for some open ball B_r). Let $\varPhi_n := \varPhi|_{B_n(0)}$ denote the restriction of $\varPhi$ to the ball of radius n around 0. Then, the* natural autocorrelation *$\gamma_P^{(\varPhi)}$ of $\varPhi$, which is defined via an averaging sequence of centred nested balls, almost surely exists and satisfies*

$$\gamma_P^{(\varPhi)} \; := \; \lim_{n \to \infty} \frac{\varPhi_n * \widetilde{\varPhi_n}}{\mathrm{vol}(B_n(0))} \; = \; \lim_{n \to \infty} \frac{\varPhi_n * \widetilde{\varPhi}}{\mathrm{vol}(B_n(0))} \; = \; \rho I_{P_0} \; = \; \gamma_P \, ,$$

where the limit refers to the vague topology on $\mathcal{M}^+$. Here, I_{P_0} is the first moment measure of the Palm distribution,

$$I_{P_0}(A) \; = \; \int_{\mathcal{M}^+} \varPsi(A) \, \mathrm{d}P_0(\varPsi), \qquad \textit{for } A \subset \mathbb{R}^d \textit{ Borel.}$$

Proof. Fix a test function, i.e., a bounded non-negative continuous function $g: \mathbb{R}^d \to [0,\infty)$ with compact support. Using Eq. (21) and $B_n^{\mathsf{c}} := \mathbb{R}^d \backslash B_n$, we have

$$\begin{aligned}\frac{1}{\lambda(B_n)} \int_{\mathbb{R}^d} g(x) \, \mathrm{d}\big(\varPhi_n * \widetilde{\varPhi_n}\big)(x) \; &= \; \frac{1}{\lambda(B_n)} \int_{B_n \times B_n} g(x-y) \, \mathrm{d}\varPhi(x) \, \mathrm{d}\varPhi(y) \\ &= \; \frac{1}{\lambda(B_n)} \int_{B_n} \Big(\int_{\mathbb{R}^d} g(x-y) \, \mathrm{d}\varPhi(y) \; - \int_{B_n^{\mathsf{c}}} g(x-y) \, \mathrm{d}\varPhi(y) \Big) \, \mathrm{d}\varPhi(x) \\ &= \; \frac{1}{\lambda(B_n)} \int_{B_n} F_g\big(T_{-x}\varPhi\big) \, \mathrm{d}\varPhi(x) \; - \; R_n(g)\end{aligned}$$

(note that both integrals inside the big brackets in the second line are finite because g has compact support), where $\phi \mapsto F_g(\phi) = \int_{\mathbb{R}^d} g(z) \, \mathrm{d}\phi(z)$ defines a measurable function, and the remainder is given by

$$R_n(g) \; = \; \frac{1}{\lambda(B_n)} \int_{B_n} \int_{B_n^{\mathsf{c}}} g(x-y) \, \mathrm{d}\varPhi(y) \, \mathrm{d}\varPhi(x) \, .$$

Note that R_n, which is a random measure, is precisely the difference between the elements of the two approximating sequences of random measures in the claim. In view of (21), it thus remains to show that $\lim_{n\to\infty} R_n = 0$ almost surely. Choose k so that $g(x) = 0$ for $|x| > k$, and fix some $\varepsilon > 0$. We then have, for $n > k/\varepsilon$,

$$R_n(g) \; \leq \; \frac{\|g\|_\infty}{\lambda(B_n)} \int_{B_n} \varPhi\big(B_n^{\mathsf{c}} \cap (x+B_k)\big) \, \mathrm{d}\varPhi(x) \; \leq \; \frac{\|g\|_\infty}{\lambda(B_n)} \int_{B_n \backslash B_{(1-\varepsilon)n}} \varPhi(x+B_k) \, \mathrm{d}\varPhi(x) \, ,$$

where $\phi \mapsto G(\phi) := \phi(B_k)$ is again measurable. Hence we obtain

$$\begin{aligned}R_n(g) \; &\leq \; \frac{\|g\|_\infty}{\lambda(B_n)} \int_{B_n} G\big(T_{-x}\varPhi\big) \, \mathrm{d}\varPhi(x) \; - \; \frac{\lambda(B_{(1-\varepsilon)n})}{\lambda(B_n)} \frac{\|g\|_\infty}{\lambda(B_{(1-\varepsilon)n})} \int_{B_{(1-\varepsilon)n}} G\big(T_{-y}\varPhi\big) \, \mathrm{d}\varPhi(y) \\ &\xrightarrow{n\to\infty} \; \big(1-(1-\varepsilon)^d\big) \, \|g\|_\infty \, \rho \int_{\mathcal{M}^+} G(\varPsi) \, \mathrm{d}P_0(\varPsi) \; = \; \big(1-(1-\varepsilon)^d\big) \, \|g\|_\infty \, \rho \, I_{P_0}(B_k)\end{aligned}$$

almost surely by (21). Now take $\varepsilon \searrow 0$ to conclude. □

Our assumption guarantees that the second moment measure $\mu^{(2)}$ of P, defined on cylinder sets $A \times A' \subset \mathbb{R}^d \times \mathbb{R}^d$ via $\mu^{(2)}(A \times A') = \int_{\mathcal{N}} \varPhi(A) \, \varPhi(A') \, \mathrm{d}P(\varPhi)$, is locally finite. This is necessary and sufficient for the existence of the intensity measure of the Palm distribution (as a locally finite measure). In fact, in the stationary scenario, the autocorrelation of the process, denoted by γ_P, satisfies $\gamma_P = \mu^{(2)}_{\mathrm{red}}$, where $\mu^{(2)}_{\mathrm{red}}$ is the so-called *reduced second moment measure* of P, and this, in turn, is the same as the intensity of the Palm measure. We offer a brief explanation of this (for more details, see [16, Prop. 12.2.V] or [48, Ch. 4.5]).

First, $\mu^{(2)}_{\mathrm{red}}$ is obtained from $\mu^{(2)}$ by disintegration, i.e., by factoring out the translation invariance. More precisely, following [16], $\mu^{(2)}_{\mathrm{red}}$ is the unique positive measure on $\mathbb{R}^d$ such that

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} h(x,y) \, \mathrm{d}\mu^{(2)}(x,y) \; = \; \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} h(u, u+v) \, \mathrm{d}\mu^{(2)}_{\mathrm{red}}(v) \, \mathrm{d}\lambda(u) \, , \qquad (22)$$

for all (real) functions $h \in C_{\mathsf{c}}(\mathbb{R}^d \times \mathbb{R}^d)$. In passing, we note that, when $h = f \otimes g$ is a product function (meaning that $h(x,y) := f(x)g(y)$), one finds

$$\mu^{(2)}(f \otimes g) \; = \; \mu^{(2)}_{\mathrm{red}}(\tilde{f} * g)$$

after an application of Fubini's theorem. Choosing $g = f$, it is clear that the measure $\mu^{(2)}_{\mathrm{red}}$ is positive definite. More generally, when dealing with complex-valued functions, one has to consider

$$\mu^{(2)}(\bar{f} \otimes g) \; = \; \mu^{(2)}_{\mathrm{red}}(\tilde{f} * g),$$

which leads to some technical complications later on. Since we consider real-valued component processes only, we can stick to the simpler case of real-valued functions.

The connection of the reduced second moment to the intensity measure of the Palm measure comes through applying (20) to a function on $\mathbb{R}^d \times \mathcal{M}^+$ defined by

$$(x, \phi) \; \mapsto \; g(x) \int_{\mathbb{R}^d} T_x h(y) \, \mathrm{d}\phi(y) \, , \tag{23}$$

where g, h are arbitrary but fixed non-negative measurable functions on $\mathbb{R}^d$. The left hand side of (20) then reads

$$\begin{aligned}\mathbb{E}_P \left(\int_{\mathbb{R}^d} g(x) \int_{\mathbb{R}^d} h(y-x) \, \mathrm{d}\varPhi(y) \, \mathrm{d}\varPhi(x) \right) \; &= \; \mathbb{E}_P \left(\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} g(x) h(y-x) \, \mathrm{d}\varPhi(y) \, \mathrm{d}\varPhi(x) \right) \\ &= \int_{\mathbb{R}^d \times \mathbb{R}^d} g(x) h(y-x) \, \mathrm{d}\mu^{(2)}(x,y) \; = \; \lambda(g) \cdot \mu^{(2)}_{\mathrm{red}}(h) \, ,\end{aligned}$$

where we employed Fubini's theorem and (22), while the right hand side reads

$$\begin{aligned}&\rho \int_{\mathbb{R}^d} \int_{\mathcal{M}^+} g(x) \int_{\mathbb{R}^d} (T_x h)(y) \, \mathrm{d}(T_x \phi)(y) \, \mathrm{d}P_0(\phi) \, \mathrm{d}\lambda(x) \\ &= \; \rho \int_{\mathbb{R}^d} \int_{\mathcal{M}^+} g(x) \int_{\mathbb{R}^d} h(y) \, \mathrm{d}\phi(y) \, \mathrm{d}P_0(\phi) \, \mathrm{d}\lambda(x) \; = \; \lambda(g) \cdot \rho I_{P_0}(h) \, .\end{aligned}$$

Here, we used the notation of the intensity of the Palm measure for its first moment. Comparing these two calculations gives

$$\mu^{(2)}_{\mathrm{red}} \; = \; \rho I_{P_0} \; = \; \gamma_P \, .$$

Remark 9. There are several different ways to define a reduced measure via disintegration. In particular, one could use $h(u, u \pm v)$ as well as $h(u \pm v, u)$ in Eq. (22). Using translation invariance of Lebesgue measure, this boils down to just two different possibilities, the one with $h(u, u+v)$ introduced above and the one with $h(u, u-v)$, which is used in [32, Prop. I.60]. Observing the relation

$$\widetilde{f * \tilde{g}} \; = \; \tilde{f} * g$$

together with $\widetilde{\mu^{(2)}} = \mu^{(2)}$, one can check that both versions define the same measure, as the process is restricted to positive (and thus real) random measures, so that no complex conjugation shows up in the $\widetilde{.}$-operation. Alternatively, one can use commutativity of the convolution together with the symmetry of $\mu^{(2)}$, which implies $\mu^{(2)}(f \otimes g) = \mu^{(2)}(g \otimes f)$. $\Diamond$

To formulate the standard Poisson process in this setting, let us start with an intuitive picture. Imagine independently putting single points on the sites of $\varepsilon\mathbb{Z}^d \subset \mathbb{R}^d$, each with probability $\rho\varepsilon^d$, and imagine a process that arises from this construction in the limit $\varepsilon \to 0$. For a rigorous construction, one can start from a tiling of $\mathbb{R}^d$ with translates of $[0,1)^d$ and then proceed, independently for each cell, as follows: Put a Poisson-(ρ) distributed number of points in the cell, with their locations independently and uniformly distributed over the given cell, see [48, Sec. 2.4.1] for details. Such a more elaborate approach is needed when $d > 1$ as there is no analogue of the renewal process we used for $d = 1$.

Example 9. Homogeneous Poisson process. This process on $\mathbb{R}^d$, with point density ρ (compare Remark 2), is a random counting measure $\varPhi$ (with distribution P) such that $\varPhi(A)$ is Poisson-$(\rho\lambda(A))$-distributed for any measurable $A \subset \mathbb{R}^d$ and that the random variables $\varPhi(A_1), \dots, \varPhi(A_m)$ are independent for any collection of pairwise disjoint $A_1, \dots, A_m \subset \mathbb{R}^d$. With this setting, the expectation measure of the process is given by $\mathbb{E}_P(\varPhi) = \rho\lambda$.

It is well-known that, under the Palm distribution, a Poisson process looks like the same Poisson process augmented by an additional point at 0, so that

$$P_0(\mathcal{B}) \; = \; \int \mathbf{1}_{\mathcal{B}}(\varPhi + \delta_0) \, \mathrm{d}P(\varPhi), \qquad \text{for } \mathcal{B} \subset \mathcal{N} \tag{24}$$

(alternatively, write $\mathcal{L}(\varPhi + \delta_0) = P_0$, or $P * \delta_{\delta_0} = P_0$), by a theorem of Slivnyak, compare [48, Example 4.3]. This is intuitively obvious from the approximation via independent coin flips on $\varepsilon\mathbb{Z}^d$ and the idea of obtaining the Palm distribution via conditioning on the presence of a point at 0. In our particular case, this results in $I_{P_0} = \delta_0 + I_P = \delta_0 + \rho\lambda$. Since homogeneous Poisson processes are stationary and ergodic with respect to the translation action of $\mathbb{R}^d$, we can now apply Theorem 3.

Consequently, for almost all realisations $\varPhi$ of a homogeneous Poisson process with point density ρ, the autocorrelation measure and the diffraction measure are given by

$$\gamma_P \; = \; \rho \, \delta_0 + \rho^2 \lambda \qquad \text{and} \qquad \widehat{\gamma}_P \; = \; \rho^2 \, \delta_0 + \rho \, \lambda \, , \tag{25}$$

by an application of Eq. (4). This also extends Example 1 to arbitrary finite values of the intensity ρ. $\Diamond$

5.3. **Compound processes.** Let us now go one step further by adding random clusters to the picture. To this end, let a stationary ergodic point process $\varPhi$ be given, with law P, point density ρ, and locally finite expectation measure $\mathbb{E}_P(\varPhi)$. This is called the *centre process* from now on. Moreover, let $\varPsi \in \mathcal{M}^+$ be a positive random measure with law Q, subject to the condition that both its expected total number of points, $m := \mathbb{E}_Q\bigl(\varPsi(\mathbb{R}^d)\bigr) > 0$, and the second moment, $\mathbb{E}_Q\bigl(\bigl(\varPsi(\mathbb{R}^d)\bigr)^2\bigr)$, are finite. This is the *component process*. We will also consider signed component processes $\varPsi$ with values in $\mathcal{M}$, in which case we will assume that the second moment of the total variation measure is finite; see the appendix for some details on the required notions and modifications for signed measures.

A combined cluster process, or *cluster process* for short, is a combination of a centre process and a component process of cluster type, and is obtained by replacing each point $x \in \operatorname{supp}(\varPhi)$ by an independent copy of $\varPsi$, translated to that point x. We denote such a process by the pair $(\varPhi_P, \varPsi_Q)$. As before, we restrict ourselves to finite clusters here. Formally, let $\varPsi_1, \varPsi_2, \dots$ be independent copies of $\varPsi$ (these are the individual *clusters*). When $\varPhi = \sum_i \delta_{X_i}$, we put

$$\varPhi_{\mathsf{cl}} \; := \; \sum_i T_{X_i} \varPsi_i \; = \; \sum_i \delta_{X_i} * \varPsi_i \, ,$$

and denote its distribution by P_{cl}. Note that, when $\varPsi \equiv \delta_0$ is deterministic and concentrated to one point, we simply obtain $\mathcal{L}(\varPhi_P, \varPsi_Q) = \mathcal{L}(\varPhi)$, and the cluster process coincides with the centre process.

If Ψ is a counting measure, the cluster process (Φ_P, Ψ_Q) is again stationary and ergodic, and its expected point density is given by $m\rho$, by [16, Prop. 10.3.IX]. This property actually holds in larger generality, which we need later on.

Proposition 2. *Let Φ be a stationary and ergodic point process with law P, finite point density ρ and locally finite second moments. Let Ψ be a random measure with law Q, finite mean and finite second moment. Then, the combined cluster process, which is a random measure, is again ergodic.*

Proof. If the component process is a (positive) point process as well, this result is stated and proved in [16]. The necessary modifications for an extension to a (possibly signed) random measure as component process, which seem to be well-known but which we could not explicitly trace in the literature, are sketched in the appendix. □

The second moment measures of the three processes are connected in a way that permits an explicit calculation of the autocorrelation $\gamma_{P_{\mathsf{cl}}}$ in terms of γ_P and various expectation measures of the component process governed by Q. To make use of this powerful connection, we recall another disintegration formula, this time for any random variable Ξ of the cluster process:

$$\mathbb{E}_{P_{\mathsf{cl}}}(\Xi) \; = \; \mathbb{E}_P\big(\mathbb{E}_Q(\Xi \mid \text{given the centres})\big), \tag{26}$$

which follows from the standard theorems on conditional expectation.

We are now in the position to use Eq. (22) in conjunction with Theorem 3 and Eq. (26) to calculate $\mu_{\mathsf{cl}}^{(2)}$, and thus the autocorrelation of almost all realisations of the cluster process, where we first concentrate on positive random measures. The extension to signed measures follows in Section 5.4.

Given a measure $\mu \in \mathcal{M}^+$ and a μ-measurable function g on $\mathbb{R}^d$ (possibly complex-valued), we define a new function g_μ on $\mathbb{R}^d$ via

$$g_\mu(x) \; := \; (T_x\mu)(g)\,, \tag{27}$$

which is again measurable. It is easy to check that g_μ satisfies

$$\widetilde{g_\mu} \; = \; \tilde{g}_{\tilde{\mu}}\,. \tag{28}$$

Lemma 5. *Let $\mu \in \mathcal{M}^+$ and let γ be a positive translation bounded measure on $\mathbb{R}^d$. Then, one has the identity*

$$\big(\mu * \tilde{\mu} * \gamma\big)(f * \tilde{g}) \; = \; \gamma(f_\mu * \widetilde{g_\mu})\,.$$

This identity also holds when both μ and γ are signed measures.

Proof. Let f and g be μ-measurable real-valued functions such that $f * \tilde{g}$ is a continuous function with compact support. One then finds

$$\begin{aligned}
\big(\mu * \tilde{\mu} * \gamma\big)(f * \tilde{g}) \; &= \; \int\!\!\int \Big(\int f(x+z+\xi)\,\mathrm{d}\mu(x)\Big)\Big(\int \tilde{g}(y-\xi)\,\mathrm{d}\tilde{\mu}(y)\Big)\,\mathrm{d}\lambda(\xi)\,\mathrm{d}\gamma(z)\\
&= \; \int\!\!\int \big(T_{z+\xi}\mu\big)(f)\,\big(T_{-\xi}\tilde{\mu}\big)(\tilde{g})\,\mathrm{d}\lambda(\xi)\,\mathrm{d}\gamma(z)\\
&= \; \int\!\!\int f_\mu(z+\xi)\,\tilde{g}_{\tilde{\mu}}(-\xi)\,\mathrm{d}\lambda(\xi)\,\mathrm{d}\gamma(z) \; = \; \gamma(f_\mu * \widetilde{g_\mu})\,,
\end{aligned}$$

where all integrals are over $\mathbb{R}^d$ and (28) was used in the last step. □

Lemma 6. *Let λ be Lebesgue measure on $\mathbb{R}^d$, as before, and μ a finite Borel measure. Then, one has $\mu * \lambda = c\lambda$ with $c = \mu(\mathbb{R}^d)$.*

Proof. Let g be a continuous function on $\mathbb{R}^d$ with compact support and observe that, for all $x \in \mathbb{R}^d$, $\lambda(T_{-x}g) = (T_x\lambda)(g) = \lambda(g)$ due to translation invariance of λ. The convolution $\mu * \lambda$ is well-defined as μ is finite while λ is translation bounded [11, Prop. 1.13]. One thus has

$$\begin{aligned}\big(\mu * \lambda\big)(g) \;&=\; \int_{\mathbb{R}^d\times\mathbb{R}^d} g(x+y)\,\mathrm{d}\lambda(y)\,\mathrm{d}\mu(x) \;=\; \int_{\mathbb{R}^d} \lambda(T_{-x}g)\,\mathrm{d}\mu(x)\\ &=\; \int_{\mathbb{R}^d} \lambda(g)\,\mathrm{d}\mu(x) \;=\; \mu(\mathbb{R}^d)\,\lambda(g).\end{aligned}$$

Since g was arbitrary, the claim follows. □

Lemma 7. *Under the general assumptions on the component process, one has*

$$\begin{aligned}\mathbb{E}_Q\big(\varPsi * \widetilde{\varPsi}\big)(f*\tilde{g}) \;&=\; \lambda\big(\mathbb{E}_Q(f_{\varPsi}\,\overline{g_{\varPsi}})\big) \quad \textit{and}\\ \big(\mathbb{E}_Q(\varPsi) * \widetilde{\mathbb{E}_Q(\varPsi)}\big)(f*\tilde{g}) \;&=\; \lambda\big(f_{\mathbb{E}_Q(\varPsi)}\,\overline{g_{\mathbb{E}_Q(\varPsi)}}\big),\end{aligned}$$

where f and g are possibly complex-valued.

Proof. Let f and g be chosen as in the previous proofs, with complex-valued functions permitted. The two claims can now be established by the following calculations. For the first one, observe

$$\begin{aligned}\mathbb{E}_Q\big(\varPsi * \widetilde{\varPsi}\big)(f*\tilde{g}) \;&=\; \mathbb{E}_Q\Big(\int_{\mathbb{R}^d}\Big(\int_{\mathbb{R}^d} f(x-\xi)\,\mathrm{d}\varPsi(x)\Big)\Big(\int_{\mathbb{R}^d}\tilde{g}(y+\xi)\,\mathrm{d}\widetilde{\varPsi}(y)\Big)\,\mathrm{d}\lambda(\xi)\Big)\\ &=\; \mathbb{E}_Q\Big(\int_{\mathbb{R}^d}\big(T_{-\xi}\varPsi(f)\big)\,\big(T_{\xi}\widetilde{\varPsi}(\tilde{g})\big)\,\mathrm{d}\lambda(\xi)\Big)\\ &=\; \int_{\mathbb{R}^d}\mathbb{E}_Q\,\Big(\big(T_s\varPsi(f)\big)\,\big(T_{-s}\widetilde{\varPsi}(\tilde{g})\big)\Big)\,\mathrm{d}\lambda(s) \;=\; \lambda\big(\mathbb{E}_Q(f_{\varPsi}\,\overline{g_{\varPsi}})\big),\end{aligned}$$

where we have used the fact that $\tilde{g}_{\widetilde{\varPsi}} = \widetilde{g_{\varPsi}}$ in the last equality. The second claim follows from

$$\begin{aligned}\big(\mathbb{E}_Q(\varPsi) * \widetilde{\mathbb{E}_Q(\varPsi)}\big)(f*\tilde{g}) \;&=\; \int_{\mathbb{R}^d}\big(T_s\mathbb{E}_Q\varPsi(f)\big)\,\overline{\big(T_s\mathbb{E}_Q\varPsi(g)\big)}\,\mathrm{d}\lambda(s)\\ &=\; \int_{\mathbb{R}^d} f_{\mathbb{E}_Q(\varPsi)}(s)\,\overline{g_{\mathbb{E}_Q(\varPsi)}(s)}\,\mathrm{d}\lambda(s) \;=\; \lambda\big(f_{\mathbb{E}_Q(\varPsi)}\,\overline{g_{\mathbb{E}_Q(\varPsi)}}\big),\end{aligned}$$

where intermediate steps for the first equality here, which are similar to those of the previous calculation, have not been repeated. □

Recall that the covariance of two real-valued random variables X and Y related to the law Q is defined as

$$\operatorname{cov}_Q(X,Y) \;:=\; \mathbb{E}_Q(X\,Y) - \mathbb{E}_Q(X)\,\mathbb{E}_Q(Y)\,. \tag{29}$$

Proposition 3. *Let $(\varXi, P_{\mathsf{cl}})$ be a combined cluster process with stationary centre point process $(\varPhi, P)$ and real component process $(\varPsi, Q)$, both with the usual assumptions on means and second moments as used above. Then, one has the reduction formula*

$$\mu^{(2)}_{P_{\mathsf{cl}}}(f\otimes g) \;=\; \mu^{(2)}_{P}\big(f_{\mathbb{E}_Q(\varPsi)}\otimes g_{\mathbb{E}_Q(\varPsi)}\big) + \rho\,\lambda\big(\operatorname{cov}_Q(f_{\varPsi}, g_{\varPsi})\big),$$

where ρ is the point density of the centre process and the covariance is defined as in (29)*.*

Proof. By assumption and the disintegration formula (26), one finds

$$\begin{aligned}\mu^{(2)}_{P_{\mathsf{cl}}}(f\otimes g) &= \int_{\mathcal{M}^+} \varXi(f)\,\varXi(g)\,\mathrm{d}P_{\mathsf{cl}}(\varXi)\\ &= \int_{\mathcal{N}^+} \mathbb{E}_Q\Big(\sum_{x,y\in\operatorname{supp}(\varPhi)} \varPsi_x(T_{-x}f)\,\varPsi_y(T_{-y}g)\Big)\,\mathrm{d}P(\varPhi)\,,\end{aligned}$$

where $\varPsi_x$ denotes the random measure at centre x. Since $\varPsi_x$ and $\varPsi_y$ are independent for $x\neq y$, the double sum over the support is split into a sum over the diagonal ($x=y$) and a sum over all remaining terms ($x\neq y$). Using the linearity of the expectation operator, the integrand can now be rewritten as a sum over two contributions, namely

$$\sum_{x,y} \mathbb{E}_Q\big(\varPsi(T_{-x}f)\big)\,\mathbb{E}_Q\big(\varPsi(T_{-y}g)\big) \quad \text{and}$$

$$\sum_{x} \Big(\mathbb{E}_Q\big(\varPsi(T_{-x}f)\,\varPsi(T_{-x}g)\big) - \mathbb{E}_Q\big(\varPsi(T_{-x}f)\big)\,\mathbb{E}_Q\big(\varPsi(T_{-x}g)\big)\Big).$$

Inserting the first term into the previous calculation leads to the contribution

$$\mu^{(2)}_P\big(\mathbb{E}_Q(f_\varPsi)\otimes\mathbb{E}_Q(g_\varPsi)\big) \;=\; \mu^{(2)}_P\big(f_{\mathbb{E}_Q(\varPsi)}\otimes g_{\mathbb{E}_Q(\varPsi)}\big)$$

while the second results in

$$\mathbb{E}_P(\varPhi)\big(\operatorname{cov}_Q(f_\varPsi,g_\varPsi)\big) \;=\; \rho\,\lambda\big(\operatorname{cov}_Q(f_\varPsi,g_\varPsi)\big),$$

where the last step follows from the stationarity of $(\varPhi,P)$. □

Theorem 4. *Let $\varPhi$ be a stationary and ergodic point process with law P, finite point density ρ and locally finite second moments. Let $\varPsi$ be a random measure with law Q, finite expectation measure and finite second moments. If $(\varXi,R)$ denotes the combined cluster process built from the centre process $(\varPhi,P)$ and the component process $(\varPsi,Q)$, it is also stationary and ergodic.*

Moreover, the autocorrelation of the combined process satisfies

$$\gamma^{(R)} \;=\; \big(\mathbb{E}_Q(\varPsi) * \widetilde{\mathbb{E}_Q(\varPsi)}\big) * \gamma_P + \rho\,\big(\mathbb{E}_Q(\varPsi * \widetilde{\varPsi}) - \mathbb{E}_Q(\varPsi) * \widetilde{\mathbb{E}_Q(\varPsi)}\big),$$

and this is almost surely the natural autocorrelation of a given realisation of the cluster process.

Proof. Choose two measurable functions f and g such that $f*\tilde g$ exists and is a continuous function with compact support. Then, one finds

$$\begin{aligned}\gamma_{P_{\mathsf{cl}}}(f*\tilde g) \;=\; \mu^{(2)}_{P_{\mathsf{cl}}}(f\otimes g) &\;=\; \mu^{(2)}_P\big(f_{\mathbb{E}_Q(\varPsi)}\otimes g_{\mathbb{E}_Q(\varPsi)}\big) + \rho\,\lambda\big(\operatorname{cov}_Q(f_\varPsi,g_\varPsi)\big)\\ &= \gamma_P\big(f_{\mathbb{E}_Q(\varPsi)} * \widetilde{g_{\mathbb{E}_Q(\varPsi)}}\big) + \rho\,\big(\mathbb{E}_Q(\varPsi*\widetilde{\varPsi}) - \mathbb{E}_Q(\varPsi)*\widetilde{\mathbb{E}_Q(\varPsi)}\big)(f*\tilde g)\,,\end{aligned}$$

where $\mathbb{E}_P(\varPhi)=\rho\lambda$ due to stationarity of $(\varPhi,P)$. The second step makes use of Lemma 7.

The formula for the autocorrelation now follows from the observation that

$$\gamma_P\big(f_{\mathbb{E}_Q(\varPsi)} * \widetilde{g_{\mathbb{E}_Q(\varPsi)}}\big) \;=\; \big(\mathbb{E}_Q(\varPsi)*\widetilde{\mathbb{E}_Q(\varPsi)}*\gamma_P\big)(f*\tilde g),$$

which is an application of Lemma 5. The remaining claims are clear due to the assumed ergodicity, via an application of Proposition 2. □

An application of the convolution theorem gives the following consequence, where also the identity $\widehat{\mathbb{E}_Q(\varPsi)} = \mathbb{E}_Q(\widehat{\varPsi})$ was used to highlight the structure of the result.

Corollary 1. *Under the assumption of Theorem 4, the diffraction measure of the combined cluster process is given by*

$$\widehat{\gamma}_R \;=\; \big|\mathbb{E}_Q(\widehat{\varPsi})\big|^2 \cdot \widehat{\gamma}_P + \rho \left(\mathbb{E}_Q(|\widehat{\varPsi}|^2) - |\mathbb{E}_Q(\widehat{\varPsi})|^2\right) \lambda$$

which is then almost surely also the diffraction measure of a given realisation. □

The result resembles our previous formulas, as was to be expected. Before we discuss possible generalisations beyond the case of positive random measures, let us look at some examples.

Example 10. Poisson cluster process. An important special case emerges when the centre process is the homogeneous Poisson process of Example 9, with point density ρ. Let γ_P and $\widehat{\gamma}_P$ be the corresponding measures. If we couple a cluster component process $\varPsi$ to it, with law Q and $m := \mathbb{E}_Q(\varPsi)(\mathbb{R}^d)$ its expected number of points, our general formula for the compound process $(\varPhi_P, \varPsi_Q)$ applies. With Lemma 6, the convolution formula can be simplified, and the result reads as follows.

For almost all realisations of a Poisson cluster process $(\varPhi_P, \varPsi_Q)$, the natural autocorrelation measure exists and is given by

$$\gamma_P^{(Q)} \;=\; (m\rho)^2 \lambda + \rho \, \mathbb{E}_Q(\varPsi * \widetilde{\varPsi}) \, ,$$

where $\mathbb{E}_Q(\varPsi * \widetilde{\varPsi})$ is a finite positive measure (of expected total mass $\geq m^2$), due to our general assumption that $\mathbb{E}_Q\big((\varPsi(\mathbb{R}^d))^2\big)$ is finite. Consequently, the diffraction measure is almost surely given by

$$\widehat{\gamma}_P^{(Q)} \;=\; (m\rho)^2 \delta_0 + \rho \left(\mathbb{E}_Q(\varPsi * \widetilde{\varPsi})\right)^{\widehat{}} \cdot \lambda,$$

where $\left(\mathbb{E}_Q(\varPsi * \widetilde{\varPsi})\right)^{\widehat{}}$ is a uniformly continuous Radon-Nikodym density for Lebesgue measure. These formulas include the case of deterministic clusters, compare Example 6. ◊

Remark 10. An interesting pair of processes is the combination of the homogeneous Poisson process from Example 9 with Hof's random displacement model from Example 8. A simple calculation shows that $\gamma_P^{(\nu)} = \gamma_P$ and $\widehat{\gamma}_P^{(\nu)} = \widehat{\gamma}_P$ in this case (and, in fact, P_{cl} and P have the same law here). From a physical point of view, this is in line with the behaviour of an ideal gas at high temperatures. When the Poisson process is a good model for the gas, and random displacement one for the disorder due to high temperature, compare the discussion in [28], the combination should still be an ideal gas – and this is precisely what happens, and is reflected by the two identities. ◊

Example 11. Neyman-Scott processes. Let K be a non-negative random integer with law $\mathcal{L}(K) = \mu$, mean $m := \mathbb{E}_\mu(K)$ and finite second moment, $\mathbb{E}_\mu(K^2) < \infty$. Now, let $Y_1, Y_2, \ldots$ be a family of $\mathbb{R}^d$-valued i.i.d. random variables with common distribution ν, and independent of K. Define the cluster distribution via

$$\varPsi \;:=\; \sum_{j=1}^{K} \delta_{Y_j} \, ,$$

i.e., a cluster has a random size K, while the positions of its atoms are independently drawn from the probability distribution ν. The induced distribution for Ψ is again called Q. With a calculation similar to the one in Example 8, one finds

$$\mathbb{E}_Q(\Psi)(A) \;=\; \mathbb{E}_Q\Big(\sum_{i=1}^{K} \mathbf{1}_A(X_i)\Big) \;=\; \mathbb{E}_\mu\Big(\sum_{i=1}^{K} \int_{\mathbb{R}^d} \mathbf{1}_A(X_i)\,\mathrm{d}\nu(X_i)\Big) \;=\; \mathbb{E}_\mu\big(K\cdot\nu(A)\big) \;=\; m\nu(A)$$

for $A \subset \mathbb{R}^d$ Borel, so that $\mathbb{E}_Q(\Psi) = m\nu$ and $\mathbb{E}_Q(\Psi) * \mathbb{E}_Q(\widetilde{\Psi}) = m^2(\nu * \widetilde{\nu})$. Moreover, one has

$$\mathbb{E}_Q(\Psi * \widetilde{\Psi})(A) \;=\; \mathbb{E}_Q\Big(\sum_{k,\ell=1}^{K} \mathbf{1}_A(X_k - X_\ell)\Big) \;=\; m\,\delta_0(A) + \mathbb{E}_\mu\big(K(K-1)\big)(\nu * \widetilde{\nu})(A),$$

which gives $\mathbb{E}_Q(\Psi * \widetilde{\Psi}) = m\,\delta_0 + \mathbb{E}_\mu\big(K(K-1)\big)(\nu * \widetilde{\nu})$, so that the general formulas from Theorem 2 can now again be applied. Note that $\mathbb{E}_\mu\big(K(K-1)\big) = \mathbb{E}_\mu(K^2) - m$.

If the centre process is once more the homogeneous Poisson process with mean point density ρ, Lemma 6 gives similar simplifications as in Example 10. Consequently, the autocorrelation is almost surely given by

$$\gamma_P^{(Q)} \;=\; (m\rho)^2\,\lambda + m\rho\delta_0 + \rho\big(\mathbb{E}_\mu(K^2) - m\big)\,(\nu * \widetilde{\nu})\,,$$

whence the corresponding diffraction measure is given by

$$\widehat{\gamma}_P^{(Q)} \;=\; (m\rho)^2\,\delta_0 + \rho\big(m + (\mathbb{E}_\mu(K^2) - m)|\widehat{\nu}|^2\big)\,\lambda\,,$$

which is an interesting extension of the Poisson process. $\Diamond$

5.4. **Autocorrelation for signed (ergodic) processes.** It is intuitively clear that the results of this section are not really restricted to point processes or positive measures for the clusters. Here, we sketch how they can be adapted to the situation of signed random measures. Consider a stationary, possibly signed, random measure Ψ (with law Q and "finite second moments", meaning that $\mathbb{E}_Q\big(|\Psi(A)|^2\big) < \infty$ holds for any bounded $A \subset \mathbb{R}^d$), with second moment measure $\mu^{(2)}$, defined as before via

$$\int_{\mathbb{R}^d\times\mathbb{R}^d} f(x,y)\,\mathrm{d}\mu^{(2)}(x,y) \;=\; \mathbb{E}_Q\Big(\int_{\mathcal{M}}\int_{\mathcal{M}} f(x,y)\,\mathrm{d}\Psi(x)\,\mathrm{d}\Psi(y)\Big),$$

say for bounded f with compact support. The reduced second moment measure $\mu^{(2)}_{\mathrm{red}}$ on $\mathbb{R}^d$ with the property

$$\mu^{(2)}_{\mathrm{red}}(f * \tilde{g}) \;=\; \mu^{(2)}(f \otimes g) \tag{30}$$

is defined in complete analogy to the positive case. The analogue of Theorem 3 is:

Theorem 5. *Let Φ be a stationary and ergodic random signed measure with distribution P. Assume that Φ has finite second moments in the sense that $\mathbb{E}_P\big(|\Phi(A)|^2\big) < \infty$ for any bounded measurable set $A \subset \mathbb{R}^d$ (which follows for example from $\mathbb{E}_P\big(|\Phi(B_r(x))|^2\big) < \infty$ for some open ball B_r). Let $\Phi_n := \Phi|_{B_n}$ denote the restriction of Φ to the ball of radius n around 0. Then, the natural autocorrelation of Φ, which is defined with an averaging sequence of nested balls, almost surely exists and satisfies*

$$\gamma^{(P)} \;:=\; \lim_{n\to\infty} \frac{\Phi_n * \widetilde{\Phi_n}}{\lambda(B_n)} \;=\; \lim_{n\to\infty} \frac{\Phi_n * \widetilde{\Phi}}{\lambda(B_n)} \;=\; \mu^{(2)}_{\mathrm{red}}\,,$$

where the limit refers to the vague topology on $\mathcal{N}$. Here, $\mu^{(2)}_{\mathrm{red}}$ is the reduced second moment measure of P according to (30)*.*

Proof. The proof is a variation of the proof of Theorem 3. Fix a continuous function $h : \mathbb{R}^d \to \mathbb{R}$ with compact support. We have to check that

$$\frac{1}{\lambda(B_n)}\big(\varPhi_n * \widetilde{\varPhi_n}\big)(h) \longrightarrow \mu^{(2)}_{\mathrm{red}}(h) \qquad \text{almost surely as } n \to \infty. \tag{31}$$

Let $\varPhi$ be an ergodic random signed measure as above and F an ergodic random function on $\mathbb{R}^d$, the latter with the property that

$$\mathbb{E}_P\Big(\int_A |F(x)|\,\mathrm{d}|\varPhi|(x)\Big) \;<\; \infty \tag{32}$$

for any bounded measurable $A \subset \mathbb{R}^d$. We can then define an additive covariant spatial process X_A in the sense of [38], indexed by bounded measurable subsets A via

$$X_A \;:=\; \int_A F(x)\,\mathrm{d}\varPhi(x).$$

Note that ergodicity of $\varPhi$ and F implies that (X_A) is again ergodic, meaning that the shift-invariant σ-field is trivial. Now, [38, Cor. 4.9] yields

$$\lim_{n\to\infty} \frac{1}{\lambda(B_n)} X_{B_n} \;=\; \mathbb{E}_P\Big(\frac{1}{\lambda(B_1)} X_{B_1}\Big) \qquad \text{(a.s.)}$$

Applying this to $\varPhi$ as in the theorem and together with $F(x) := \int_{\mathbb{R}^d} h(x-y)\,\mathrm{d}\varPhi(y)$ yields

$$\begin{aligned}
\lim_{n\to\infty}\frac{1}{\lambda(B_n)}\int_{B_n} F(x)\,\mathrm{d}\varPhi(x) \;&=\; \lim_{n\to\infty}\frac{1}{\lambda(B_n)}\big(\varPhi_n * \widetilde{\varPhi}\big)(h)\\
&= \mathbb{E}_P\Big(\frac{1}{\lambda(B_1)}\int_{B_1}\int_{\mathbb{R}^d} h(x-y)\,\mathrm{d}\varPhi(y)\,\mathrm{d}\varPhi(x)\Big)\\
&= \frac{1}{\lambda(B_1)}\int_{\mathbb{R}^d\times\mathbb{R}^d} \mathbf{1}_{B_1}(x)\,h(x-y)\,\mathrm{d}\mu^{(2)}(x,y)\\
&= \frac{1}{\lambda(B_1)}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \mathbf{1}_{B_1}(x)\,h(z)\,\mathrm{d}\mu^{(2)}_{\mathrm{red}}(z)\,\mathrm{d}x \;=\; \int_{\mathbb{R}^d} h\,\mathrm{d}\mu^{(2)}_{\mathrm{red}}
\end{aligned}$$

almost surely, which is almost the claim. The difference between $\varPhi_n * \widetilde{\varPhi}$ and $\varPhi_n * \widetilde{\varPhi_n}$ can be treated as in the proof of Theorem 3. $\square$

Combining Proposition 4 and Theorem 5, and observing that the calculations in the proof of Proposition 3 carry over literally to the signed case, we obtain

Corollary 2. *The statements of Theorem* 4 *and Corollary* 1 *remain true for cluster processes with signed clusters.* $\square$

5.5. **Equilibria of critical branching Brownian motions in $d \geq 3$.** Consider a system of particles performing independent Brownian motions in $\mathbb{R}^d$, $d \geq 3$ (for ease of comparison with the cited literature, we assume that the variance parameter is $\sigma^2 = 2$).

Additionally, each particle, after an exponentially distributed lifetime with parameter V, either doubles or dies, where each possibility occurs with probability 1/2. In the situation of a birth event, the daughter particles appear at the position of the mother. Note that if we start with a finite number of particles, the expected number of particles is preserved for all time, as the expected number of offspring equals 1. This is what “critical” in the name refers to. Imagine we start such a system from a homogeneous Poisson process with point density ρ, denote by $\varPhi_t$ the random configuration observed at time $t \geq 0$, and its distribution by P_t. P_t is stationary with point density ρ, see [26] and the references given there for background.

It follows from [26, Thm. 2.3] that the intensity measure of the Palm distribution of P_t is given by

$$I_{(P_t)_0} \;=\; \delta_0 + (\rho + f_t)\lambda\,, \tag{33}$$

where

$$f_t(x) \;=\; V \int_0^t \int_{\mathbb{R}^d} p_s(0,y)\, p_s(y,x)\,\mathrm{d}y\,\mathrm{d}s = \frac{V}{2}\int_0^{2t} p_u(0,x)\,\mathrm{d}u\,,$$

with $p_t(x,y) = (4\pi t)^{-d/2} \exp\bigl(-|x-y|^2/(4t)\bigr)$ the d-dimensional Brownian transition density (with variance parameter 2). As explained in [26], there is a genealogical interpretation behind (33): In view of the interpretation of the Palm distribution as the configuration around a typical individual, δ_0 is the contribution of this individual, $f_t\,\lambda$ that from its relatives in the family decomposition of the branching process, and $\rho\lambda$ is the contribution from unrelated individuals.

Furthermore, by [26, Thm. 2.2], P_t converges (vaguely) towards P_∞, which is the unique ergodic equilibrium distribution with point density ρ (cf [13] for uniqueness), and the limit $t \to \infty$ can be taken in (33) to obtain

$$I_{(P_\infty)_0} \;=\; \delta_0 + (\rho + f_\infty)\lambda\,,$$

where

$$f_\infty(x) \;=\; \frac{V}{2}\int_0^\infty p_u(0,x)\,\mathrm{d}u \;=\; \frac{V}{2}\,\frac{\Gamma\bigl(\frac{d-2}{2}\bigr)}{4\pi^{d/2}}\,\frac{1}{|x|^{d-2}}$$

is (up to the prefactor $V/2$) the Green function of Brownian motion. Thus, using Lemma 1, we have

Corollary 3. *Let $\varPhi_\infty$ be a realisation of the critical branching Brownian motion, from the equilibrium distribution P_∞. The autocorrelation is then almost surely given by*

$$\gamma \;=\; \rho\delta_0 + \rho(\rho + f_\infty)\lambda\,,$$

while the corresponding diffraction measure is then

$$\widehat{\gamma} \;=\; \rho^2\delta_0 + \rho\Bigl(1 + \frac{V}{2}\,\frac{1}{4\pi^2|k|^2}\Bigr)\,\lambda\,.$$

Remark 11. One can also consider the scenario where, instead of Brownian motion, particles move during their lifetime according to a symmetric stable process of index $\alpha \in (0,2]$ in $\mathbb{R}^d$ ($\alpha = 2$ corresponds to Brownian motion). Such processes have discontinuous paths, and their transition density $p_t^{(\alpha)}(x,y) = p_t^{(\alpha)}(0,y-x)$ satisfies

$$\int_{\mathbb{R}^d} e^{ik\cdot x} p_t^{(\alpha)}(0,x)\,\mathrm{d}x \;=\; \exp(-t|k|^\alpha)$$

(in general, no explicit form of $p_t^{(\alpha)}$ is known). By [26, Thm. 2.2], non-trivial equilibria exist if the spatial dimension d satisfies $d > \alpha$. In this case, a reasoning analogous to that above yields the following: The autocorrelation of a realisation $\varPhi_\infty^{(\alpha)}$ of the equilibrium of a system of critical branching symmetric α-stable processes (with density ρ) is almost surely given by

$$\gamma \;=\; \delta_0 + (\rho + f_\infty^{(\alpha)})\lambda\,,$$

where

$$f_\infty^{(\alpha)}(x) \;=\; \frac{V}{2}\int_0^\infty p_u^{(\alpha)}(0,x)\,\mathrm{d}u \;=\; \frac{V}{2}\,\frac{\Gamma((d-\alpha)/2)}{2^\alpha \pi^{d/2}\Gamma(\alpha/2)}\,\frac{1}{|x|^{d-\alpha}}$$

(for the form of the Green function of the symmetric α-stable process, see [12, Ex. 1.7]). Hence, the diffraction measure is almost surely given by

$$\widehat{\gamma} \;=\; \rho^2\delta_0 + \rho\Big(1 + \frac{V}{2}\frac{1}{(2\pi)^\alpha |k|^\alpha}\Big)\lambda\,,$$

by another application of Lemma 1. $\Diamond$

Note that, due to the independence properties of the branching mechanism, these equilibria can also be considered as Poisson cluster processes. In contrast to the scenario considered above, clusters in $\varPhi_\infty$ are infinite, and the spatial correlation decays only algebraically (without being integrable).

6. Outlook

This article demonstrates that various aspects of mathematical diffraction theory for random point sets and measures can be approached systematically with methods from point process theory, as was originally suggested in [23]. At the same time, the approach is sufficiently concrete to allow for many explicitly computable examples, several of which were presented above. They comprise many formulas from the somewhat scattered literature on this subject in a unified setting. There are, of course, many more examples, but we hope that the probabilistic platform advertised here will prove useful for them as well.

The next step in this development needs to consider point processes and random measures with interactions, such as those governed by Gibbs measures. First steps are contained in [28, 4, 23, 35, 36, 9, 17, 10] and indicate that both qualitative and quantitative results are possible, though some further development of the theory is needed.

A continuation along this path would also make the results more suitable for real applications in physics and crystallography, though it is largely unclear at the moment what surprises the corresponding inverse problem might have to offer here.

Appendix: Ergodicity for cluster processes with signed random measures

Let $\mathcal{M} = \mathcal{M}(\mathbb{R}^d)$ be the space of (locally finite) real or signed measures on $\mathbb{R}^d$, equipped with the topology of vague convergence, with $\mathcal{M}^+ = \mathcal{M}^+(\mathbb{R}^d)$ denoting the subspace of positive measures. Let $\varSigma_{\mathcal{M}}$ denote the Borel-σ-algebra of $\mathbb{R}^d$. Note that the latter is also generated by the mappings $\mathcal{M} \ni \mu \mapsto \mu(A)$, for bounded and measurable sets $A \subset \mathbb{R}^d$. Recall that any $\mu \in \mathcal{M}$ admits a unique Hahn-Jordan decomposition

$$\mu \;=\; \mu_+ - \mu_- \quad \text{with } \mu_+,\, \mu_- \in \mathcal{M}^+ \text{ mutually singular.}$$

The mappings $\mu \mapsto \mu_+$, $\mu \mapsto \mu_-$ are $\varSigma_{\mathcal{M}}$-measurable. We write $|\mu| := \mu_+ + \mu_- \in \mathcal{M}^+$ for the total variation measure of μ. A *random signed measure* $\varPhi$ is a random variable with values in $(\mathcal{M}, \Sigma_{\mathcal{M}})$. In the context of signed random measures, it is convenient to work with the *characteristic functional*

$$\varphi_{\Phi}(h) := \mathbb{E}\Big[\exp\big(i \textstyle\int h \, \mathrm{d}\Phi\big)\Big], \tag{34}$$

which is defined for any $h : \mathbb{R}^d \to \mathbb{R}$ bounded measurable with compact support. In analogy to the Laplace functional for positive random measures, the distribution of Φ is determined by φ_{Φ}.

Here, we are interested in signed cluster processes: Let Φ be a stationary counting process with finite intensity ρ, and Ψ_j, $j = 1, 2, \ldots$ independent (and independent from Φ), identically distributed random signed measures such that $\mathbb{E}\big[|\Psi_1|\big]$ is a *finite* measure. Then, given a realisation $\Phi = \sum_j \delta_{X_j}$, where X_j are the positions of the atoms of Φ (in some enumeration), the cluster process is defined as

$$\Xi := \sum_j T_{X_j} \Psi_j \, . \tag{35}$$

Note that for any bounded $B \subset \mathbb{R}^d$,

$$\mathbb{E}\big[|\Xi(B)|\big] \le \mathbb{E}\Big[\sum_j |\Psi_j|(B - X_j)\Big] = \rho \int_{\mathbb{R}^d} \int_{B-x} \mathrm{d}\mathbb{E}\big[|\Psi_1|\big] \, \mathrm{d}x = \rho\big(\mathbb{E}\big[|\Psi_1|\big] * \lambda\big)(B) < \infty \, ,$$

so that (35) is indeed well-defined.

Let B_n be the (closed) ball of radius n around $0 \in \mathbb{R}^d$.

Lemma 8. *Let Ψ be a signed random measure on $\mathbb{R}^d$. The following are equivalent:*

(1) *Ψ is ergodic.*
(2) *For any $U, V \in \Sigma_{\mathcal{M}}$,,*

$$\lim_{n\to\infty} \frac{1}{\lambda(B_n)} \int_{B_n} \big(\mathbb{P}\big(\Psi \in U \cap T_x V\big) - \mathbb{P}(\Psi \in U)\, \mathbb{P}(\Psi \in V)\big) \, \mathrm{d}x = 0 \, .$$

(3) *For any $g, h \colon \mathbb{R}^d \to \mathbb{R}$ measurable with compact support,*

$$\lim_{n\to\infty} \frac{1}{\lambda(B_n)} \int_{B_n} \big(\varphi_{\Psi}(g + T_x h) - \varphi_{\Psi}(g)\, \varphi_{\Psi}(h)\big) \, \mathrm{d}x = 0 \, .$$

Furthermore, it suffices to restict to U, V to a semiring which generates $\Sigma_{\mathcal{M}}$ in (2), and it suffices to restrict to continuous g, h with compact support in (3).

Proof. This is a straightforward adaptation of the proofs of Propositions 10.3.III and 10.3.VI and Lemma 10.3.II of [16] to the signed case. □

The following result is an analogue [16, Prop. 10.3.IX] for the signed measure case. Since we have not been able to find a proof in the literature, we provide a sketch.

Proposition 4. *Let Φ, Ψ_j, and $\Xi := \sum_j T_{X_j} \Psi_j$ be as above. If Φ is ergodic, then Ξ is ergodic as well.*

Sketch of proof. We will verify condition (3) from Lemma 8. Observe that for any $f : \mathbb{R}^d \to \mathbb{R}$ with compact support and any $\varepsilon > 0$, we can find $R < \infty$ such that

$$\mathbb{P}\Bigg(\sum_{j\,:\,|X_j| \ge R} \bigg| \int f \,\mathrm{d}(T_{X_j}\Psi_j) \bigg| \ge \varepsilon \Bigg) \le \varepsilon\,. \tag{36}$$

To check (36), let R' be large enough so that $\mathrm{supp}(f) \subset [-R', R']^d$, and note that for $R > R'$, the lefthand side of (36) is bounded by

$$\mathbb{P}\Bigg(\sum_{j\,:\,||X_j||_\infty \ge R} |\Psi_j|\big([-R', R']^d + X_j\big) \ge \frac{\varepsilon}{||f||_\infty} \Bigg) \le \frac{||f||_\infty}{\varepsilon}\,\mathbb{E}\Bigg[\sum_{j\,:\,||X_j||_\infty \ge R} |T_{X_j}\Psi_j|\big([-R', R']^d\big) \Bigg].$$

The expectation on the righthand side above equals

$$\begin{aligned}\rho \int\limits_{\mathbb{R}^d \setminus [-R,R]^d} \int\limits_{\mathbb{R}^d} &\mathbf{1}_{[-R',R']^d}(x-y)\,\mathrm{d}\mathbb{E}\big[|\Psi_1|\big](y)\,\mathrm{d}x \\ &\le \rho(2R')^d\,\mathbb{E}\big[|\Psi_1|\big]\big(\mathbb{R}^d \setminus [-(R-R'), (R-R')]^d\big),\end{aligned}$$

which converges to 0 as $R \to \infty$ because $\mathbb{E}\big[|\Psi_1|\big]$ is a finite measure.

Let $g, h\colon \mathbb{R}^d \to \mathbb{R}$ continuous with compact support and define

$$G(\Phi) := \mathbb{E}\Big[\exp\big(i\textstyle\int g\,\mathrm{d}\Xi\big)\,\Big|\,\Phi\Big], \quad H(\Phi) := \mathbb{E}\Big[\exp\big(i\textstyle\int h\,\mathrm{d}\Xi\big)\,\Big|\,\Phi\Big].$$

Decompose

$$\begin{aligned}\int (g + T_x h)\,\mathrm{d}\Xi \;=\; &\sum_{j\,:\,X_j \in [-R,R]^d} \int T_{X_j} g\,\mathrm{d}\Psi_j \;+ \sum_{j\,:\,X_j \notin [-R,R]^d} \int T_{X_j} g\,\mathrm{d}\Psi_j \\ &+ \sum_{j\,:\,X_j \in [-R,R]^d - x} \int T_{X_j + x} h\,\mathrm{d}\Psi_j \;+ \sum_{j\,:\,X_j \notin [-R,R]^d - x} \int T_{X_j + x} h\,\mathrm{d}\Psi_j\,,\end{aligned}$$

and choose R so large that (36) is fulfilled for $f = g$ and $f = h$. Recall that for any real-valued random variables X, Y with $\mathbb{P}(|Y| \ge \varepsilon) \le \varepsilon$, we have

$$\Big|\mathbb{E}\,e^{i(X+Y)} - \mathbb{E}\,e^{iX}\Big| \le \mathbb{E}\,\Big|e^{i(X+Y)} - e^{iX}\Big| \le \mathbb{E}\Big[\big|e^{iX}\big|\,\big|e^{iY} - 1\big|\Big] \le \varepsilon + \mathbb{P}(|Y| \ge \varepsilon) \le 2\varepsilon.$$

For $A \subset \mathbb{R}^d$, write $\Xi_A := \sum_{j\,:\,X_j \in A} T_{X_j}\Psi_j$ for the random measure which consists of clusters with centres in A. For $x \in \mathbb{R}^d \setminus [-2R, 2R]^d$, we then have

$$\begin{aligned}&\Big|\mathbb{E}\left[\exp\left(i\textstyle\int (g + T_x h)\,\mathrm{d}\Xi\right)\right] - \mathbb{E}\left[G(\Phi)H(T_x\Phi)\right]\Big| \\ &\le\; \Big|\mathbb{E}\left[\exp\left(i\textstyle\int (g + T_x h)\,\mathrm{d}\Xi\right)\right] - \mathbb{E}\left[\exp\left(i\textstyle\int g\,\mathrm{d}\Xi_{[-R,R]^d} + i\textstyle\int T_x h\,\mathrm{d}\Xi_{[-R,R]^d - x}\right)\right]\Big| \\ &\quad + \Big|\mathbb{E}\left[\mathbb{E}\left[\exp\left(i\textstyle\int g\,\mathrm{d}\Xi_{[-R,R]^d} + i\textstyle\int T_x h\,\mathrm{d}\Xi_{[-R,R]^d - x}\right)\Big|\,\Phi\right]\right] - \mathbb{E}\left[G(\Phi)H(T_x\Phi)\right]\Big|.\end{aligned}$$

The first term on the righthand side is bounded by 2ε. Observing that the conditional expectation in the second term is in fact a product because clusters with centres in disjoint regions are (conditionally) independent, we can bound the second term from above by

$$\begin{aligned}
&\Big|\mathbb{E}\Big[\mathbb{E}\Big[\exp\Big(i\!\int g \,\mathrm{d}\Xi_{[-R,R]^d}\Big)\Big|\,\Phi\Big]\Big(\mathbb{E}\Big[\exp\Big(i\!\int T_x h \,\mathrm{d}\Xi_{[-R,R]^d-x}\Big)\Big|\,\Phi\Big]-H(T_x\Phi)\Big)\Big]\Big|\\
&\qquad+\Big|\mathbb{E}\Big[\Big(\mathbb{E}\Big[\exp\Big(i\!\int g\,\mathrm{d}\Xi_{[-R,R]^d}\Big)\Big|\,\Phi\Big]-G(\Phi)\Big)H(T_x\Phi)\Big]\Big|\\
&\quad\le\ \mathbb{E}\Big|\exp\Big(i\!\int T_x h\,\mathrm{d}\Xi_{[-R,R]^d-x}\Big)-\exp\big(i\!\int T_x h\,\mathrm{d}\Xi\big)\Big|\\
&\qquad+\mathbb{E}\Big|\exp\Big(i\!\int g\,\mathrm{d}\Xi_{[-R,R]^d}\Big)-\exp\big(i\!\int g\,\mathrm{d}\Xi\big)\Big|,
\end{aligned}$$

which is not more than 2ε.

Thus, using the relations $\mathbb{E}\big[\mathbb{E}\big[\exp\big(i\int(g+T_x h)\,\mathrm{d}\Xi\big)\,\big|\,\Phi\big]\big] = \varphi_{\Xi}(g+T_x h)$, $\mathbb{E}\,G(\Phi) = \varphi_{\Xi}(g)$, and $\mathbb{E}\,H(\Phi)=\mathbb{E}\,H(T_x\Phi)=\varphi_{\Xi}(h)$, we obtain
(37)

$$\begin{aligned}
&\limsup_{n\to\infty}\frac{1}{\lambda(B_n)}\Big|\int_{B_n}\big(\varphi_{\Psi}(g+T_x h)-\varphi_{\Psi}(g)\,\varphi_{\Psi}(h)\big)\,\mathrm{d}x\Big|\\
&\qquad\le\ \limsup_{n\to\infty}\frac{1}{\lambda(B_n)}\Big|\int_{B_n}\big(\mathbb{E}\big[G(\Phi)H(T_x\Phi)\big]-\mathbb{E}\big[G(\Phi)\big]\mathbb{E}\big[H(\Phi)\big]\big)\,\mathrm{d}x\Big|+4\varepsilon\ =\ 4\varepsilon
\end{aligned}$$

by ergodicity of Φ (in order to deduce this literally from statement (2) in Lemma 8, one can for instance discretise the support of g and h and approximate $G(\Phi)$, $H(\Phi)$ with functions depending only on the random vector $(\Phi(c_i))_{1\le i\le N}$, where $\{c_i \mid 1\le i\le N\}$ is a collection of disjoint (small) cubes). Finally, take $\varepsilon\to 0$ to conclude. □

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References

[1] Y. Ataman, On positive definite measures, *Monatsh. Math.* **79** (1975) 265–272.
[2] M. Baake, Diffraction of weighted lattice subsets, *Can. Math. Bulletin* **45** (2002) 483–498; `arXiv:math.MG/0106111`.
[3] M. Baake, D. Frettlöh and U. Grimm, A radial analogue of Poisson's summation formula with applications to powder diffraction and pinwheel patterns, *J. Geom. Phys.* **57** (2007) 1331–1343; `arXiv:math.SP/0610408`.
[4] M. Baake and M. Höffe, Diffraction of random tilings: Some rigorous results, *J. Stat. Phys.* **99** (2000) 219–261; `arXiv:math-ph/9904005`.
[5] M. Baake and D. Lenz, Deformation of Delone dynamical systems and pure point diffraction, *J. Fourier Anal. Appl.* **11** (2005) 125–150; `arXiv:math.DS/0404155`.
[6] M. Baake, D. Lenz and R.V. Moody, Characterisation of models sets by dynamical systems, *Ergodic Th. & Dynam. Syst.* **27** (2007) 341–382; `arXiv:math.DS/0511648`.
[7] M. Baake and R.V. Moody, Diffractive point sets with entropy, *J. Phys. A: Math. Gen.* **31** (1998) 9023–9038; `arXiv:math-ph/9809002`.
[8] M. Baake and R.V. Moody, Weighted Dirac combs with pure point diffraction, *J. reine angew. Math. (Crelle)* **573** (2004) 61–94; `arXiv:math.MG/0203030`.
[9] M. Baake and B. Sing, Diffraction spectrum of lattice gas models above T_c, *Lett. Math. Phys.* **68** (2004) 165–173; `arXiv:math-ph/0405064`.

[10] M. Baake and N. Zint, Absence of singular continuous diffraction for discrete multi-component particle models, *J. Stat. Phys.* **129** (2007), in press; `arXiv:0709.2061`.

[11] C. Berg and G. Forst, *Potential Theory on Locally Compact Abelian Groups*, Springer, Berlin (1975).

[12] R.M. Blumenthal and R.K. Getoor, *Markov Processes and Potential Theory*, Academic Press, New York (1968).

[13] M. Bramson, J.T. Cox and A. Greven, Invariant measures of critical spatial branching processes in high dimensions, *Ann. Probab.* **25** (1997) 56–70.

[14] A. Córdoba, Dirac combs, *Lett. Math. Phys.* **17** (1989) 191–196.

[15] J.M. Cowley, *Diffraction Physics*, 3rd ed., North-Holland, Amsterdam (1995).

[16] D.D. Daley and D. Vere-Jones, *An Introduction to the Theory of Point Processes*, Springer, New York (1988).

[17] X. Deng and R.V. Moody, Dworkin's argument revisited: point processes, dynamics, diffraction, and correlations, *J. Geom. Phys.*, in press; `arXiv:0712.3287 (math.DS)`.

[18] A.C.D. van Enter and J. Miękisz, How should one define a (weak) crystal?, *J. Stat. Phys.* **66** (1992) 1147–1153.

[19] N. Etemadi, An elementary proof of the strong law of large numbers, *Z. Wahrsch. verw. Gebiete* **55** (1981) 119–122.

[20] W. Feller, *An Introduction to Probability Theory and Its Applications*, vol. II, 2nd ed., Wiley, New York (1972).

[21] J. Gil de Lamadrid and L.N. Argabright, *Almost Periodic Measures*, Memoirs AMS, vol. **65**, no. 428, AMS, Providence, RI (1990).

[22] B.V. Gnedenko, *Theory of Probability*, 6th ed., CRC press, Amsterdam (1998).

[23] J.-B. Gouéré, Diffraction and Palm measure of point processes, *Comptes Rendus Acad. Sci. (Paris)* **342** (2003) 141–146. `arXiv:math.PR/0208064`.

[24] J.-B. Gouéré, Quasicrystals and almost periodicity, *Commun. Math. Phys.* **255** (2005) 655–681; `arXiv:math-ph/0212012`.

[25] A. Guinier, *X-Ray Diffraction in Crystals, Imperfect Crystals and Amorphous Bodies*, reprint, Dover, New York (1994).

[26] L.G. Gorostiza and A. Wakolbinger, Persistence criteria for a class of branching particle systems in continuous time, *Ann. Probab.* **19** (1991) 266–288.

[27] A. Hof, On diffraction by aperiodic structures, *Commun. Math. Phys.* **169** (1995) 25–43.

[28] A. Hof, Diffraction by aperiodic structures at high temperatures, *J. Phys. A: Math. Gen.* **28** (1995) 57–62.

[29] M. Höffe, Diffraction of the dart-rhombus random tiling, *Mat. Science Eng.* **294–296** (2000) 373–376; `arXiv:math-ph/9911014`.

[30] M. Höffe and M. Baake, Surprises in diffuse scattering, *Z. Kristallogr.* **215** (2000) 441–444; `arXiv:math-ph/0004022`.

[31] O. Kallenberg, *Random Measures*, 3rd ed., Akademie-Verlag, Berlin (1983).

[32] A.F. Karr, *Point Processes and Their Statistical Inference*, 2nd ed., Dekker, New York (1991).

[33] J. Kerstan, K. Matthes and J. Mecke, *Unbegrenzt teilbare Punktprozesse*, Akademie-Verlag, Berlin (1974).

[34] P. Kramer and R. Neri, On periodic and non-periodic space fillings of $\mathbb{E}^m$ obtained by projection, *Acta Cryst.* **A40** (1984) 580–587.

[35] C. Külske, Universal bounds on the selfaveraging of random diffraction measures, *Probab. Th. Rel. Fields* **126** (2003) 29–50; `arXiv:math-ph/0109005`.

[36] C. Külske, Concentration inequalities for functions of Gibbs fields with application to diffraction and random Gibbs measures, *Commun. Math. Phys.* **239** (2003) 29–51.

[37] R.V. Moody, 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`.

[38] X.X. Nguyen and H. Zessin, Ergodic theorems for spatial processes, *Z. Wahrsch. verw. Geb.* **48** (1979) 133–158.

[39] R. Penrose, The role of aesthetics in pure and applied mathematical research, *Bull. Inst. Math. Appl.* **10** (1974) 266–271.

[40] M.A. Pinsky, *Introduction to Fourier Analysis and Wavelets*, Brooks/Cole, Pacific Grove, CA (2002).

[41] C. Radin, Aperiodic tilings, ergodic theory, and rotations, in: *The Mathematics of Long-Range Aperiodic Order*, ed. R.V. Moody, NATO-ASI Series C 489, Kluwer, Dordrecht (1997), pp. 499–519.

[42] M. Reed and B. Simon, *Methods of Modern Mathematical Physics I: Functional Analysis*, 2nd ed., Academic Press, San Diego (1980).

[43] W. Rudin, *Fourier Analysis on Groups*, reprint, Wiley, New York (1990).

[44] D. Shechtman, I. Blech, D. Gratias and J.W. Cahn, Metallic phase with long-range orientational order and no translational symmetry, *Phys. Rev. Lett.* **53** (1984) 183–185.

[45] M. Schlottmann, 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.

[46] M. Schlottmann, 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.

[47] W. Steurer et al., What is a crystal? *Z. Kristallographie* **222** (2007), 308–319.

[48] D. Stoyan, W.S. Kendall and J. Mecke, *Stochastic Geometry and its Applications*, Akademie-Verlag, Berlin (1987).

[49] K. Urban and M. Feuerbacher, Structurally complex alloy phases, *J. Non-Cryst. Solids* **334 & 335** (2004) 143–150.

[50] N.G. Ushakov, *Selected Topics in Characteristic Functions*, Brill Academic Publishers, Utrecht (1999).

[51] T.R. Welberry, *Diffuse X-Ray Scattering and Models of Disorder*, Clarendon Press, Oxford (2004).