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## RESEARCH ARTICLE

## Random point sets and their diffraction

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The diffraction of various random subsets of the integer lattice  $\mathbb{Z}^d$ , such as the coin tossing and related systems, are well understood. Here, we go one important step beyond and consider random point sets in  $\mathbb{R}^d$ . We present several systems with an effective stochastic interaction that still allow for explicit calculations of the autocorrelation and the diffraction measure. We concentrate on one-dimensional examples for illustrative purposes, and briefly indicate possible generalisations to higher dimensions.

In particular, we discuss the stationary Poisson process in  $\mathbb{R}^d$  and the renewal process on the line. The latter permits a unified approach to a rather large class of one-dimensional structures, including random tilings. Moreover, we present some stationary point processes that are derived from the classical random matrix ensembles as introduced in the pioneering work of Dyson and Ginibre. Their re-consideration from the diffraction point of view improves the intuition on systems with randomness and mixed spectra.

Keywords: diffraction spectra; stochastic point processes; random matrix ensembles.

#### Introduction 1.

Mathematical diffraction theory is an abstraction of kinematic diffraction [10] that is both mathematically rich and practically relevant. Its insight helps to explore the true setting and difficulty of the inverse problem of structure determination from (kinematic) diffraction data; compare [3, 5, 16] and references therein. Moreover, mathematical diffraction theory has several important connections with the theory of dynamical systems [6–9].

While this is well studied in the classic case of crystals and, more generally, pure point diffractive systems, much less is known about structures with continuous (or mixed) diffraction spectra. The Thue-Morse chain is a well-known example with singular continuous diffraction, but mixed dynamical spectrum; see [4, 17, 26] for more. Recently, some progress has also been made for point sets of stochastic origin; see [2] and references therein for a survey.

Nevertheless, the collection of fully worked out and understood examples is relatively meagre in comparison with the situation of pure point diffractive systems. Here, we summarise two important and versatile examples from [2] and augment them with two examples from the theory of random matrices. The latter essentially derive from old papers by Dyson [12] and Ginibre [15], which were later re-analysed by Mehta [21], though the results seem unknown in diffraction theory.

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 M. Baake and H. Kösters

Let us briefly recall the setting of mathematical diffraction theory; see [2, 18] and references therein for more. The underlying structure is modelled by an essentially translation bounded measure  $\omega$ , which may be signed or even complex; see [22] for background on measure theory. The corresponding *autocorrelation* measure  $\gamma$ , or autocorrelation for short, is defined as a volume-weighted limit,

$$\gamma = \lim_{R \to \infty} \frac{\omega_R * \widetilde{\omega_R}}{\operatorname{vol}(B_R)}, \tag{1}$$

where  $\omega_R$  denotes the restriction of  $\omega$  to the (open) ball of radius R around the origin. Moreover,  $\widetilde{\omega}$  is the 'flipped-over' measure defined by  $\widetilde{\omega}(g) = \overline{\omega(\widetilde{g})}$  for arbitrary continuous functions of compact support, with  $\widetilde{g}(x) = \overline{g(-x)}$ . We implicitly use the Riesz-Markov representation theorem that allows us to identify regular Borel measures with linear functionals on the space of continuous functions with compact support. In general, the limit in (1) need not exist, but we will only consider situations where it does, at least almost surely in the probabilistic sense.

By construction,  $\gamma$  is a positive definite measure, hence it is always Fourier transformable. Here, we follow the convention of [2], with the factor  $2\pi$  in the exponent (via  $e^{-2\pi ikx}$ ) rather than in front of the integral. The result is the diffraction  $\hat{\gamma}$ , which is a positive measure (by the Bochner-Schwartz theorem [22]) that describes, loosely speaking, how much intensity is scattered into any given volume of space; see [10, 18] for more. The diffraction measure has a unique decomposition

$$\widehat{\gamma} = (\widehat{\gamma})_{pp} + (\widehat{\gamma})_{sc} + (\widehat{\gamma})_{ac}$$
 (2)

into its *pure point* part (which is a countable sum of Dirac measures, known as Bragg peaks), its *absolutely continuous* part (which comprises everything that can be expressed by a locally integrable density relative to Lebesgue measure, known as diffuse scattering) and its *singular continuous* part (which is everything that remains, and is often disregarded in crystallography – but see [28]).

The focus of this paper is on systems with structural disorder, which means that we will see either purely absolutely continuous spectra or mixtures thereof with pure point spectra. We begin with a review of the Poisson process and the renewal process, where we follow [2] and adapt it to the concrete setting of crystallography. Then, we consider some point processes that can be extracted from random matrix theory and give rise to further examples that are explicitly computable.

## 2. Poisson process

The homogeneous Poisson process in  $\mathbb{R}^d$  is an ergodic point process that is often considered as a model for an ideal gas. If  $\rho$  denotes its (point) density, the process is characterised [2, 13, 14] by the two requirements that the number of points in a (measurable) set  $A \subset \mathbb{R}^d$  is Poisson distributed with parameter  $\rho\lambda(A)$ , where  $\lambda$  is Lebesgue measure, and that the number of points in sets  $A_1, A_2, \ldots, A_m$  are independent random variables, for any collection of pairwise disjoint, measurable subsets of  $\mathbb{R}^d$ . The Poisson process is a model for an ideal gas of pointlike particles.

Let us consider such a process, with density  $\rho$ . Due to ergodicity, almost every realisation of it possesses a natural autocorrelation, and the latter can be calculated via the Palm measure of the process [2, Thm. 3]. The result reads

$$\gamma_P = \rho \, \delta_0 + \rho^2 \lambda, \tag{3}$$

where  $\delta_0$  is the normalised Dirac measure at 0. With  $\hat{\delta_0} = \lambda$  and  $\hat{\lambda} = \delta_0$ , one obtains

 $\sim$  2s . . . . (4)

$$\widehat{\gamma_P} = \rho^2 \delta_0 + \rho \lambda, \tag{4}$$

which is the diffraction measure. We skip the proof, but mention that, in one dimension, the result can easily be derived from the renewal theorem discussed in Section 3, with an exponential waiting time distribution [2]. Apart from the trivial point measure at 0, the diffraction measure  $\widehat{\gamma}_P$  is absolutely continuous.

An interesting modification emerges from a marked Poisson process, where each point of a given realisation randomly gets the weight 1 or -1 with equal probability. This leads to the following modification of Eqs. (3) and (4).

**Theorem 2.1:** Consider a typical realisation of the homogeneous Poisson process of density  $\rho$  in  $\mathbb{R}^d$ , which is a simple point set  $\Lambda \subset \mathbb{R}^d$ . Let  $\omega = \sum_{x \in \Lambda} W_x \, \delta_x$  be a random Dirac comb where  $(W_x)_{x \in \Lambda}$  constitutes an i.i.d. family of random variables that take the values 1 and -1 with equal probability. Then, the corresponding autocorrelation and diffraction measures almost surely read

$$\gamma_{\omega} = \rho \, \delta_0 \quad and \quad \widehat{\gamma_{\omega}} = \rho \, \lambda.$$

**Proof:** This is the situation of the random weight model of [2, Ex. 7], applied to a stationary Poisson process, which is an ergodic and simple point process. The result now follows from [2, Thm. 4 and Cor. 1] by a small calculation.

When the density is  $\rho = 1$ , this is one of many examples with diffraction measure  $\lambda$ , which include the coin tossing sequence on the integer lattice and the Rudin-Shapiro sequence [5, 17], but also various dynamical systems of algebraic origin [9] such as Ledrappier's shift on  $\mathbb{Z}^2$ . This provides ample evidence that the inverse problem of structure determination becomes significantly more involved in the presence of diffuse scattering.

One limitation of the Poisson process for applications in physics is the missing uniform discreteness. This can be overcome by an additional hard-core condition, as in the classic Matérn process; see [24] and references therein for a formulation that matches our setting. Here, a realisation of a homogeneous Poisson process is randomly marked and then thinned out on the basis of a pairwise comparison up to a certain distance. This leads to a modified point set that is uniformly discrete (meaning that the minimum distance between any two points is a positive number). Despite this modification, autocorrelation and diffraction can still be calculated explicitly; see [2, 20] and references therein for more.

#### 3. Renewal process

The situation of random point sets is significantly simpler in one dimension, because a large class of processes can be characterised constructively as a renewal process. Here, one starts from a probability measure  $\mu$  on  $\mathbb{R}_+$  (the positive real line) and considers a machine that moves at constant speed along the real line and drops points on the line with a waiting time that is distributed according to  $\mu$ . Whenever this happens, the internal clock is reset and the process resumes. Let us (for simplicity) assume that both the velocity of the machine and the expectation value of  $\mu$  are 1, so that we end up with realisations that are, almost surely, point sets in  $\mathbb{R}$  of density 1 (after we let the starting point of the machine move to  $-\infty$ ).

Clearly, the process just described defines a stationary process. It can thus be analysed by considering all realisations which contain the point 0. Moreover, there

is a clear (distributional) symmetry around this point, so that we can determine the autocorrelation (in the sense of (1)) of almost all realisations from studying what happens to the right of 0. Indeed, if we want to know the frequency per unit length of the occurrence of two points at distance x (or the corresponding density), we need to sum the contributions that x is the first point after 0, the second point, the third, and so on. In other words, we almost surely obtain the autocorrelation

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

with  $\nu = \mu + \mu * \mu * \mu * \mu * \mu * \mu + \dots$  and  $\widetilde{\nu}$  as defined above, where the proper convergence of the sum of iterated convolutions follows from [2, Lemma 4]. Note that the point measure at 0 simply reflects that the almost sure density of the resulting point set is 1. Indeed,  $\nu$  is a translation bounded positive measure, and satisfies the renewal relations (see [14, Ch. XI.9] or [2, Prop. 1] for a proof)

$$\nu = \mu + \mu * \nu \quad \text{and} \quad (1 - \widehat{\mu}) \widehat{\nu} = \widehat{\mu},$$
 (6)

where  $\hat{\mu}$  is a uniformly continuous and bounded function on  $\mathbb{R}$ . Note that the second equation emerges from the first by Fourier transform, but has been rearranged to indicate why the set  $\{k \mid \widehat{\mu}(k) = 1\}$  will become important below. In this setting, the measure  $\gamma$  of (5) is both positive and positive definite.

Based on the structure of the support of the underlying probability measure  $\mu$ , one can now formulate the following result for the diffraction of the renewal process.

**Theorem 3.1:** Let  $\mu$  be a probability measure on  $\mathbb{R}_+$  with mean 1, and assume that a moment of  $\mu$  of order  $1+\varepsilon$  exists for some  $\varepsilon>0$ . Then, the point sets obtained from the stationary renewal process based on  $\mu$  almost surely have a diffraction measure of the form

$$\widehat{\gamma} = (\widehat{\gamma})_{pp} + (1-h)\lambda,$$

where h is a locally integrable function on  $\mathbb{R}$  that is continuous except for at most countably many points. It is given by

$$h(k) = \frac{2\left(|\widehat{\mu}(k)|^2 - \operatorname{Re}(\widehat{\mu}(k))\right)}{|1 - \widehat{\mu}(k)|^2}.$$

Moreover, the pure point part is given by

$$(\widehat{\gamma})_{\mathsf{pp}} = \begin{cases} \delta_0, & \text{if } \operatorname{supp}(\mu) \text{ is not a subset of a lattice}, \\ \delta_{\mathbb{Z}/b}, & \text{if } b\mathbb{Z} \text{ is the coarsest lattice that contains } \operatorname{supp}(\mu). \end{cases}$$

**Proof:** The process has a well-defined autocorrelation  $\gamma$  as outlined above and given in Eq. (5). Due to the ergodicity of the process, this means that almost every realisation of the process is a simple point set with this autocorrelation. Since  $\gamma$  is positive definite, it is Fourier transformable, with  $\hat{\gamma}$  being a positive measure on  $\mathbb{R}$ .

The point measure at 0 (which is always present) reflects the fact that the resulting point set almost surely has density 1; see [2, Thm. 1] and its proof for a detailed argument. The functional form of h can be calculated from the second renewal relation in (6) whenever  $\widehat{\mu}(k) \neq 1$ . Its local integrability everywhere is a consequence of the assumed moment condition, by an application of [25, Thm. 1.5.4].

The distinction via the nature of  $\operatorname{supp}(\mu)$  takes care of the set  $\{k \in \mathbb{R} \mid \widehat{\mu}(k) = 1\}$ , which is either  $\{0\}$  or countable. The result now follows from [2, Lemma 5 and Thm. 1] together with Remark 3 of the same paper.

Random point sets and their diffraction

The renewal process is a versatile method to produce point sets on the line. These include random tilings with finitely many intervals (which are Delone sets) as well as the homogeneous Poisson process on the line (where  $\mu$  is the exponential distribution with mean 1); see [2, Sec. 3] for explicit examples and applications.

## 4. Random matrix ensembles and random point sets on the line

The global eigenvalue distribution of random orthogonal, unitary or symplectic matrix ensembles is known to asymptotically follow the classic semi-circle law. More precisely, this law describes the eigenvalue distribution of the underlying ensembles of symmetric, Hermitian and symplectic matrices with Gaussian distributed entries. The corresponding random matrix ensembles are called GOE, GUE and GSE, with attached  $\beta$ -parameters 1, 2 and 4, respectively. They permit an interpretation as a Coulomb gas, where  $\beta$  is the power in the central potential; see [1, 21] for general background and [12] for the results that are relevant to our point of view.

For matrices of dimension N, the semi-circle has radius  $\sqrt{2N/\pi}$  and area N. Note that, in comparison to [21], we have rescaled the density by a factor  $1/\sqrt{\pi}$  here, so that we really have a semi-circle, and not a semi-ellipse. To study the local eigenvalue distribution with our application in mind, we rescale the central region (between  $\pm 1$ , say) by  $\sqrt{2N/\pi}$ . This leads, in the limit as  $N \to \infty$ , to a new ensemble of point sets on the line that can be interpreted as a stationary, ergodic point process of intensity 1; for  $\beta = 2$ , see [1, Ch. 4.2] or [23] and references therein for details. Since the process is simple (meaning that, almost surely, no point is occupied twice), almost all realisations are point sets of density 1.

It is possible to calculate the autocorrelation of these processes, on the basis of Dyson's correlation functions [12]. Though the latter originally apply to the circular ensembles, they have been adapted to the other ensembles by Mehta [21]. For all three ensembles mentioned above, this leads to an autocorrelation of the form

$$\gamma = \delta_0 + (1 - f(|x|))\lambda \tag{7}$$

where f is a locally integrable function that depends on  $\beta$ . Defining  $s(r) = \frac{\sin(\pi r)}{\pi r}$ , one obtains (with  $r \ge 0$ )

$$f(r) = \begin{cases} s(r)^2 + s'(r) \int_r^\infty s(t) \, dt, & \text{if } \beta = 1, \\ s(r)^2, & \text{if } \beta = 2, \\ s(2r)^2 - 2s'(2r) \int_0^r s(2t) \, dt, & \text{if } \beta = 4. \end{cases}$$
(8)

The diffraction measure is the Fourier transform of  $\gamma$ , which has also been calculated in [12, 21]. Observing  $\hat{\delta}_0 = \lambda$  and  $\hat{\lambda} = \delta_0$ , the result is always of the form

$$\widehat{\gamma} = \delta_0 + (1 - b(k))\lambda = \delta_0 + h(k)\lambda, \tag{9}$$

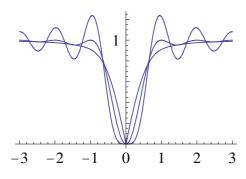
where  $b = \hat{f}$ . The Radon-Nikodym density h for  $\beta = 1$  reads

$$h_1(k) = \begin{cases} |k| (2 - \log(2|k| + 1)), & \text{if } |k| \le 1, \\ 2 - |k| \log \frac{2|k| + 1}{2|k| - 1}, & \text{if } |k| > 1, \end{cases}$$
 (10)

# Philosophical Magazine & Philosophical Magazine Letters

M. Baake and H. Kösters



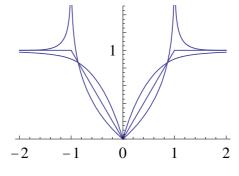


Figure 1. Absolutely continuous part of the autocorrelation (left) and the diffraction (right) for the three point set ensembles on the line, with  $\beta \in \{1,2,4\}$ . On the left, the oscillatory behaviour increases with  $\beta$ . On the right,  $\beta=2$  corresponds to the piecewise linear function with bends at 0 and  $\pm 1$ , while  $\beta=4$  shows a locally integrable singularity at  $\pm 1$ . The latter reflects the slowly decaying oscillations on the left.

where  $k \in \mathbb{R}$ . The result for  $\beta = 2$  is simpler and reads

$$h_2(k) = \begin{cases} |k|, & \text{if } |k| \le 1, \\ 1, & \text{if } |k| > 1, \end{cases}$$
 (11)

while  $\beta = 4$  leads to

$$h_4(k) = \begin{cases} \frac{1}{4} |k| (2 - \log|1 - |k||), & \text{if } |k| \le 2, \\ 1, & \text{if } |k| > 2. \end{cases}$$
 (12)

Figure 1 illustrates the three cases. To summarise:

**Theorem 4.1:** The eigenvalues of the Dyson random matrix ensembles for parameter  $\beta \in \{1, 2, 4\}$ , in the scaling of the local region around 0 as used above, almost surely give rise to point sets of density 1, with autocorrelation and diffraction measures as specified in Eqs. (7) and (9).

Note that  $h_4$  is smooth at  $k=\pm 2$ , but has integrable singularities at  $k=\pm 1$ . The latter are a consequence of the stronger oscillatory behaviour of the function  $f_4$  at integer values, as was already noticed in [12]. When extrapolating to other values of  $\beta$  (in particular to  $\beta > 4$ ), this is the onset of another Bragg peak.

It is well-known that the circular random matrix ensembles (COE, CUE, CSE) asymptotically give rise to the same local correlations [12, 21], and hence to the same autocorrelation and diffraction (after appropriate rescaling).

#### 5. Random matrix ensembles and random point sets in the plane

The above examples were derived from matrix ensembles with real eigenvalues, and thus lead to point processes in  $\mathbb{R}$ . There is also one ensemble, due to Ginibre [15] (see also [21]), of general complex matrices with Gaussian distributed entries that will give rise to a stationary point process in  $\mathbb{R}^2$ . Again, this emerges (by proper rescaling) from the eigenvalues (now seen as elements of the plane), which approach uniform distribution in a circle of radius  $\sqrt{N/\pi}$  (and hence area N) as  $N \to \infty$ .

As before, the system can be interpreted as a Coulomb gas, with a potential parameter  $\beta=2$ . Other matrix ensembles permit this interpretation, too, but do not seem to correspond to interesting stationary processes, wherefore we stick to Ginibre's example here.

# Philosophical Magazine & Philosophical Magazine Letters

Random point sets and their diffraction

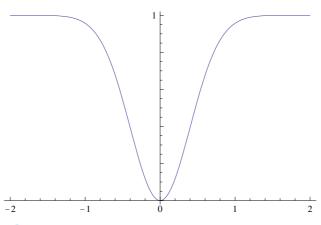


Figure 2. Radial dependence of the absolutely continuous part both of the autocorrelation and the diffraction measure for the planar point set ensemble, as derived from Ginibre's matrix ensemble.

Following the original approach of [15], the limit  $N \to \infty$  leads to a stationary and ergodic, simple point process of intensity 1, so that almost every realisation is a point set in the plane of density 1. Using complex variables  $z_i \in \mathbb{C} \simeq \mathbb{R}^2$ , the 2-point correlation function is of determinantal form,

$$\rho(z_1, z_2) = e^{-\pi(|z_1|^2 + |z_2|^2)} \begin{vmatrix} e^{\pi|z_1|^2} & e^{\pi z_1 \overline{z_2}} \\ e^{\pi \overline{z_1} z_2} & e^{\pi|z_2|^2} \end{vmatrix} = (1 - e^{-\pi|z_1 - z_2|^2}), \tag{13}$$

see [15] or [21] for a derivation. Note that, despite using complex coordinates here, the expression is calculated relative to the volume element of real coordinates (hence relative to Lebesgue measure, as in [21]). The result is translation invariant and only depends on the distance r between the two points.

As a consequence, the autocorrelation of a realisation almost surely reads

$$\gamma = \delta_0 + (1 - e^{-\pi r^2}) \lambda, \tag{14}$$

which is radially symmetric, with r as above. By a standard calculation, the Fourier transform of  $\gamma$  results in

$$\widehat{\gamma} = \delta_0 + \left(1 - e^{-\pi|k|^2}\right)\lambda,\tag{15}$$

so that we obtain a self-dual pair of measures under Fourier transform (as in the Poisson process of density 1). The radial dependence is illustrated in Figure 2.

**Theorem 5.1:** The Ginibre complex random matrix ensemble, in the scaling used above, almost surely results in point sets of density 1, with autocorrelation (14) and diffraction (15).

## Summary and Outlook

In this short communication, we have discussed several explicit examples of stochastic point sets with explicitly computable autocorrelation and diffraction measures. The viewpoint of point process theory provides a universal platform to do so, though our examples above also admit a direct approach. It would be interesting to extend this to a family of processes, with  $\beta$  as parameter in the spirit of [11, 19, 27], which then interpolates between the Poisson process of density 1 ( $\beta = 0$ ) and the integer lattice (which is approached as  $\beta \to \infty$ ).

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An interesting question concerns the connection with dynamical systems theory, in particular the general relation between diffraction and dynamical spectra. Recent progress suggests that such a connection might indeed exist, although it will certainly be more involved than in the pure point diffractive case.

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One fundamental shortcoming so far is the lack of understanding and explicit examples for randomness with interaction. A first step in that direction needs the inclusion of Gibbs measures for equilibrium states, though it is not clear at the moment to what extent one can derive explicit examples (such as the classic and well-known Ising lattice gas).

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