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A Comment on the Relation between Diffraction and Entropy

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Diffraction methods are used to detect atomic order in solids. While uniquely ergodic systems with pure point diffraction have zero entropy, the relation between diffraction and entropy is not as straightforward in general. In particular, there exist families of homometric systems, which are systems sharing the same diffraction, with varying entropy. We summarise the present state of understanding by several characteristic examples.

1 Introduction

Quantifying order or complexity in systems is a difficult task, as there are no universal measures of order or complexity. In the realm of solid state physics, atomic order is usually probed by diffraction experiments [17]. A pure point diffraction measure, which means a diffraction pattern comprising only Bragg peaks and no continuous component, is an indicator of atomic order. Crystalline solids are paradigms of pure point diffractive systems, and diffraction experiments are used to determine the symmetry and atomic structure of the crystal. More generally, perfect quasicrystals are also pure point diffractive, even though the diffraction peaks are located on a Fourier module that is dense in space. Nevertheless, at any experimental resolution, only finitely many diffraction peaks are resolved in any finite region of space, so the diffraction pattern appears discrete in practice. This is one commonly accepted model for real world quasicrystals [31].

Another measure of order versus complexity is the configurational entropy of a system [16]. In an ideal crystal, atomic positions are determined by those within a fundamental domain of the underlying lattice, and hence the configurational entropy is zero. This is also true for perfect quasicrystals, and pure point diffraction is indeed related to zero entropy, as shown in [9] for a large class of systems.

It is interesting to explore what happens with the relation between diffraction and entropy if one leaves the pure point regime; see [22] and references therein for examples. With increasing experimental resolution, continuous diffraction intensities are becoming more accessible (see [33] for a recent exposition), and it is important to understand their origin and the implications on the structure of the material under investigation. This is a first step in tackling the inverse problem of diffraction in the more general setting of mixed diffraction spectra.

In this short note, we aim to highlight the scope of the inverse problem, by presenting a variety of examples with continuous diffraction. These reveal that the picture is indeed rather complex. In particular, we recall a family of homometric (or isospectral) structures which cover a full available range of configurational entropy, from a (fully deterministic) case with zero entropy to a completely random case. In higher dimensions, a variety of possibilities exist, including lower rank entropy.

Most of the results below have appeared in original papers, but not in one source. We use this note to review some of the more recent attempts, and try to put them in a more systematic frame. After a brief recapitulation of mathematical diffraction theory, we proceed along this path mainly by way of characteristic examples.

2 Diffraction of weighted Dirac combs

Mathematical diffraction theory was pioneered by Hof in [20, 21], and should be considered as the rigorous mathematical counterpart of kinematic diffraction; compare [17] for background. For simplicity, we concentrate on the diffraction of weighted Dirac combs [11, 6]. A weighted Dirac comb of a general point set $S \subset \mathbb{R}^d$ is formally spelled out as

$$\omega \, = \sum_{x \in S} w(x)\, \delta_x \, = \, w\, \delta_S \, ,$$

where δ_x is the normalised point (or Dirac) measure at x, and $w(x)$ is a weight function (which may be complex). Here, $\delta_S := \sum_{x\in S} \delta_x$ is the Dirac comb of S. We assume that the set S and the weight function w are such that the corresponding weighted Dirac comb ω is a translation bounded measure, and that its natural *autocorrelation measure*

$$\gamma \, = \, \gamma_\omega \, = \, \omega \circledast \widetilde{\omega} \, := \lim_{R\to\infty} \frac{\omega|_R * \widetilde{\omega|_R}}{\mathrm{vol}(B_R)} \, , \tag{1}$$

exists. Here, B_R denotes the open ball of radius R around $0 \in \mathbb{R}^d$ and $\omega|_R$ the restriction of ω to B_R. For a measure μ, its 'flipped-over' version $\widetilde{\mu}$ is defined via $\widetilde{\mu}(g) = \overline{\mu(\widetilde{g})}$ for $g \in C_{\mathsf{c}}(\mathbb{R}^d)$, where $\widetilde{g}(x) = \overline{g(-x)}$. The volume-averaged (or Eberlein) convolution $\circledast$ is needed because ω itself generally is an unbounded measure, so the direct convolution is not defined. For instance, if λ denotes the standard Lebesgue measure (for volume), $\lambda * \lambda$ is not defined, while $\lambda \circledast \lambda = \lambda$. Note that different measures ω can share the same autocorrelation γ. This phenomenon is called *homometry*, and we shall see explicit examples later on.

The autocorrelation measure γ is *positive definite* (or of positive type) by construction, which means $\gamma(g * \widetilde{g}\,) \geq 0$ for all $g \in C_{\mathsf{c}}(\mathbb{R}^d)$. As a consequence, its Fourier transform $\widehat{\gamma}$ exists [15] and is a translation bounded, positive measure, called the *diffraction measure* of ω. It describes the outcome of kinematic diffraction of ω by quantifying how much scattering intensity reaches a given volume in d-space; see [20, 6, 7] for more details.

Relative to Lebesgue measure λ, we have the unique splitting

$$\widehat{\gamma} \, = \, \widehat{\gamma}_{\mathsf{pp}} + \widehat{\gamma}_{\mathsf{sc}} + \widehat{\gamma}_{\mathsf{ac}}$$

of $\widehat{\gamma}$ into its pure point part (the Bragg peaks, of which there are at most countably many), its absolutely continuous part (the diffuse scattering with locally integrable density relative to λ) and its singular continuous part (which is whatever remains). The last contribution, if present, is described by a measure that gives no weight to single points, but is still concentrated to an uncountable set of zero Lebesgue measure. Examples of such measures are provided by the Thue-Morse system and its generalisations; see [4, 3] and references therein.

3 Bernoullisation

The classic coin tossing process leads to the Dirac comb $\omega = \sum_{n\in\mathbb{Z}} X(n)\, \delta_n$, where the $(X(n))_{n\in\mathbb{Z}}$ form an i.i.d. family of random variables, each taking values 1 and -1 with probabilities p and $1-p$, respectively. By an application of the strong law of large numbers (SLLN), almost every realisation has the autocorrelation measure

$$\gamma \, = \, (2p-1)^2\, \delta_{\mathbb{Z}} + 4p(1-p)\, \delta_0 \, ,$$

and hence (via Fourier transform) the diffraction measure

$$\widehat{\gamma} \, = \, (2p-1)^2\, \delta_{\mathbb{Z}} + 4p(1-p)\, \lambda \, .$$

Here, we have used the classic Poisson summation formula $\widehat{\delta_{\mathbb{Z}}} = \delta_{\mathbb{Z}}$; compare [6] and references therein for a formulation in the diffraction context. When $p = \frac{1}{2}$, the diffraction boils down to

$\widehat{\gamma} = \lambda$. Here, the point part is extinct because the average scattering strength vanishes. For proofs, we refer to [10, 2].

The Bernoulli chain has (metric) entropy $H(p) = -p\log(p) - (1-p)\log(1-p)$, which is maximal for $p = \frac{1}{2}$, with $H(\frac{1}{2}) = \log(2)$. It vanishes for the deterministic limit cases $p \in \{0, 1\}$. For the latter, we have $\omega = \mp\delta_{\mathbb{Z}}$, and consequently obtain the diffraction measure $\widehat{\gamma} = \delta_{\mathbb{Z}}$, again via the Poisson summation formula.

In contrast, the (binary) Rudin-Shapiro chain is a deterministic system, with polynomial complexity function and thus zero entropy. The corresponding sequence of weights $(w(n))_{n\in\mathbb{Z}}$ with $w(n) \in \{\pm1\}$ can be defined recursively by the initial conditions $w(-1) = -1$, $w(0) = 1$, together with

$$w(4n + \ell) = \begin{cases} w(n), & \text{for } \ell \in \{0, 1\}, \\ (-1)^{n+\ell}\, w(n), & \text{for } \ell \in \{2, 3\}, \end{cases} \tag{2}$$

which determines $w(n)$ for all $n \in \mathbb{Z}$. Despite its deterministic nature, the autocorrelation measure is simply given by $\gamma_{\text{RS}} = \delta_0$, so that $\widehat{\gamma_{\text{RS}}} = \lambda$; see [5, 6] for further details and a simple proof. Alternatively, the result also follows from the exposition in [29, 28].

Now, the theory of random variables allows for an interpolation between the two cases as follows. Let us consider the random Dirac comb

$$\omega_p = \sum_{n\in\mathbb{Z}} w(n)\, X(n)\, \delta_n\,, \tag{3}$$

where $(X(n))_{n\in\mathbb{Z}}$ is, as above, an i.i.d. family of random variables with values in $\{\pm1\}$ and probabilities p and $1-p$. This 'Bernoullisation' of the Rudin-Shapiro comb can be viewed as a model of second thoughts, where the sign of the weight at position n is changed with probability $1-p$. By a (slightly more complicated) application of the SLLN, it can be shown [5] that the autocorrelation γ of the Dirac comb ω is almost surely given by

$$\gamma_p \;=\; (2p-1)^2\, \gamma_{\text{RS}} + 4p(1-p)\, \delta_0 \;=\; \delta_0\,,$$

irrespective of the value of the parameter $p \in [0, 1]$. This establishes the following result; see [5, 6] for details.

Theorem 1 *The family of random Dirac combs ω_p of Eq.* (3) *with $p \in [0, 1]$ are (almost surely) homometric (isospectral), with absolutely continuous diffraction measure $\widehat{\gamma_p} = \widehat{\gamma_{\text{RS}}} = \lambda$, irrespective of the value of p.*

This result shows that diffraction can be insensitive to entropy, because the family of Dirac combs ω_p of Eq. (3) continuously interpolates between the deterministic Rudin-Shapiro case with zero entropy and the completely random Bernoulli chain with maximal entropy $\log(2)$. Clearly, this example can be generalised to other sequences, and (by taking products) to higher dimensions.

4 Close-packed dimers

Another instructive example in one dimension was recently suggested by van Enter [14]. Partition $\mathbb{Z}$ into a close-packed arrangement of 'dimers' (pairs of neighbours), without gaps or overlaps. Clearly, there are two possibilities to do so. Next, decorate each pair randomly with either $(1, -1)$ or $(-1, 1)$, with equal probability. The set of all sequences defined in this way is given by

$$\mathbb{X} \;=\; \bigl\{ w \in \{\pm1\}^{\mathbb{Z}} \mid M(w) \subset 2\mathbb{Z} \text{ or } M(w) \subset 2\mathbb{Z}+1 \bigr\}\,,$$

where $M(w) := \{n \in \mathbb{Z} \mid w(n) = w(n+1)\}$. Note that $M(w)$ is empty precisely for the two periodic sequences $w(n) = \pm(-1)^n$.

Considering the corresponding signed Dirac comb on $\mathbb{Z}$ with weights $w(n) \in \{\pm1\}$, it can be shown that its autocorrelation almost surely exists and is given by [14]

$$\gamma \;=\; \delta_0 - \frac{1}{2}(\delta_1 + \delta_{-1})\,.$$

The corresponding diffraction measure is then

$$\widehat{\gamma} \, = \, \bigl(1 - \cos(2\pi k)\bigr)\lambda \, , \tag{4}$$

which is again a purely absolutely continuous diffraction measure. Here, the continuous density relative to λ is written as a function of k.

On first sight, the system looks disordered, with entropy of $\frac{1}{2}\log(2)$. This seems (qualitatively) reflected by the diffraction. However, the system also defines a dynamical system under the action of $\mathbb{Z}$, as generated by the shift $S\colon \mathbb{X} \longrightarrow \mathbb{X}$, with $(Sw)(n) := w(n+1)$. As such, it has a dynamical spectrum that does contain a pure point part, with eigenvalues 0 and $\frac{1}{2}$; we refer to [29] for general background on this concept, and to [14] for the actual calculation of the eigenfunctions. The extension to a dynamical system under the general translation action of $\mathbb{R}$ is a standard procedure known as suspension; see [16, Ch. 11.1] for an introduction, where the suspension is called a special flow.

This finding suggests that some degree of order must be present that is neither visible from the entropy calculation nor from the diffraction measure alone. Indeed, one can define a factor of the system by a continuous mapping $\phi\colon \mathbb{X} \longrightarrow \{\pm 1\}^{\mathbb{Z}}$ defined by $(\phi w)(n) = -w(n)w(n+1)$. It maps $\mathbb{X}$ globally 2:1 onto

$$\mathbb{Y} = \phi(\mathbb{X}) = \bigl\{ v \in \{\pm 1\}^{\mathbb{Z}} \mid v(n) = 1 \text{ for all } n \in 2\mathbb{Z} \text{ or all } n \in 2\mathbb{Z}+1 \bigr\}.$$

The autocorrelation and diffraction measure of the signed Dirac comb $v\delta_{\mathbb{Z}}$ for an element $v \in \mathbb{Y}$ are almost surely given by

$$\gamma \, = \, \frac{1}{2}\delta_0 + \frac{1}{2}\delta_{2\mathbb{Z}} \quad \text{and} \quad \widehat{\gamma} \, = \, \frac{1}{2}\lambda + \frac{1}{4}\delta_{\mathbb{Z}/2} \, .$$

The diffraction of the factor system $\mathbb{Y}$ uncovers the 'hidden' pure point part of the dynamical spectrum, which was absent in the purely absolutely continuous diffraction of the signed Dirac comb $w\delta_{\mathbb{Z}}$ with $w \in \mathbb{X}$. In summary, we have the following situation [14].

Theorem 2 *The diffraction measure of the close-packed dimer system $\mathbb{X}$ with balanced weights is purely absolutely continuous and given by Eq.* (4)*.*

The dynamical spectrum of the close-packed dimer system $\mathbb{X}$ under the translation action of $\mathbb{R}$ contains the pure point part $\mathbb{Z}/2$ together with a countable Lebesgue spectrum.

The non-trivial part $\mathbb{Z} + \frac{1}{2}$ of the dynamical point spectrum is not reflected by the diffraction spectrum of $\mathbb{X}$, but can be recovered via the diffraction spectrum of a suitable factor, such as $\mathbb{Y}$.

A similar observation can be made for the (generalised) Thue-Morse system; see [18, 3].

5 Ledrappier's model

For a long time, people had expected that higher dimensions are perhaps more difficult, but not substantially different. This turned out to be a false premise though, as can be seen from the now classic monograph [30].

In our present context, we pick one characteristic example, the system due to Ledrappier [24], to show one new phenomenon. Here, we consider a specific subset of the full shift space $\{\pm 1\}^{\mathbb{Z}^2}$, defined by

$$\mathbb{X}_{\mathrm{L}} \, = \, \bigl\{ w \in \{\pm 1\}^{\mathbb{Z}^2} \mid w(x)\, w(x+e_1)\, w(x+e_2) = 1 \;\text{ for all }\; x \in \mathbb{Z}^2 \bigr\}, \tag{5}$$

where e_1 and e_2 denote the standard Euclidean basis vectors in the plane. On top of being a closed subshift, $\mathbb{X}_{\mathrm{L}}$ is also an Abelian group (here written multiplicatively), which then comes with a unique, normalised Haar measure. The latter is also shift-invariant, and the most natural measure to be considered in our context.

The system is interesting because the number of patches of a given radius (up to translations) grows exponentially in the radius rather than in the area of the patch. This phenomenon is called *entropy of rank* 1, and indicates a new class of systems in higher dimensions. More precisely, along any lattice direction of $\mathbb{Z}^2$, the linear subsystems essentially behave like one-dimensional Bernoulli chains. It is thus not too surprising that the diffraction measure satisfies the following theorem, though its proof [13] has to take care of the special directions connected with the defining relations of $\mathbb{X}_{\mathrm{L}}$.

Theorem 3 *If w is an element of the Ledrappier subshift $\mathbb{X}_{\mathrm{L}}$ of Eq.* (5)*, the corresponding weighted Dirac comb $w\delta_{\mathbb{Z}^2}$ has diffraction measure λ, which holds almost surely relative to the Haar measure of $\mathbb{X}_{\mathrm{L}}$.*

So, the Ledrappier system is homometric to the full $\mathbb{Z}^2$-shift, which means that an element of either system almost surely has diffraction measure λ. As mentioned before, via a suitable product of two Rudin-Shapiro chains, also a deterministic system with diffraction λ exists. This clearly demonstrates the insensitivity of pair correlations to the (entropic) type of order or disorder in the underlying system.

Although correlation functions of higher order can resolve the situation in this case, one can consider other dynamical systems (such as the $(\times 2, \times 3)$-shift [13]) that share almost all correlation functions with the Bernoulli shift on $[0,1]^{\mathbb{Z}^2}$. This is a clear indication that our present understanding of 'order' is incomplete, and that we still lack a good set of tools for the detection of order.

6 Meyer sets with entropy

Meyer sets in Euclidean space are point sets $\varLambda \subset \mathbb{R}^d$ that are relatively dense in such a way that $\varLambda - \varLambda$ is still uniformly discrete. This innocently looking condition has deep consequences [25, 26, 23]. In particular, it is reasonable to consider Meyer sets as natural generalisations of lattices. They comprise perfect quasicrystals (as those obtained from the projection method), but are general enough to accommodate entropy as well.

As a simple example, start from the set $2\mathbb{Z}$ and add any subset of $2\mathbb{Z}+1$ to it, for instance a random selection of the latter. This is a Meyer set (it contains $2\mathbb{Z}$, so that it is relatively dense, while the Minkowski difference is a subset of $\mathbb{Z}$, hence uniformly discrete). Nevertheless, such a set has entropy. More generally, even though deterministic Meyer sets are the ones that have been studied in most detail so far, 'most' Meyer sets will have entropy, but still possess a high degree of intrinsic order. This is manifest from the following observation of Strungaru [32].

Theorem 4 *Let $S \subset \mathbb{R}^d$ be a Meyer set and $\omega := \delta_S$ the corresponding Dirac comb. If γ is any autocorrelation of ω, its Fourier transform $\widehat{\gamma}$ comprises a non-trivial pure point part. In particular, for any $\varepsilon > 0$, the set $\{k \in \mathbb{R}^d \mid \widehat{\gamma}(\{k\}) \geq (1-\varepsilon)\,\widehat{\gamma}(\{0\})\}$ is relatively dense.*

In this sense, long-range order in Meyer sets leaves a remarkable fingerprint. Considering subsets of a lattice, even without demanding their relative denseness, a related result was also proved in [1]. Let us take a closer look by means of a famous example from number theory.

7 Visible lattice points

The visible (or primitive) points of the square lattice are defined as

$$\mathcal{V} \, = \, \{(m,n) \in \mathbb{Z}^2 \mid \gcd(m,n) = 1\} \, .$$

$\mathcal{V}$ is clearly uniformly discrete, but contains holes of arbitrary size (as a consequence of the Chinese remainder theorem; see [12] for details). Consequently, $\mathcal{V}$ is neither a Meyer nor a Delone set. Nevertheless, the set $\mathcal{V}$ has a well-defined density ($6/\pi^2$), and positive topological entropy (of the same value, if using the logarithm to base 2). Moreover, one also has the following result.

Theorem 5 *The Dirac comb $\delta_{\mathcal{V}}$ has a pure point diffraction measure.*

The proof of this claim in [12] is constructive and also gives a closed (and computable) formula for the diffraction measure. In view of [9], it is somewhat astonishing that pure point diffraction and positive entropy go together like this. However, in a recent paper by Huck and Pleasants [27], it is shown that the natural *metric* entropy of $\mathcal{V}$ vanishes. The term 'natural' refers to the use of a nested sequence of growing discs as averaging sequence; see [12, Appendix] for details. The proof is again constructive, and explains the mechanism: The frequencies of arbitrary patches exist (though not uniformly so), which defines a natural invariant measure via suitable cylinder sets. Now, a small set of patches have large frequencies, while the majority sports small or tiny frequencies – and together this suffices to give metric entropy 0 (relative to this measure). The main point here is that the frequencies (for the measure) and the pair correlations (for the autocorrelation, and hence for the diffraction) are determined by means of the *same* averaging sequence, which clearly is the relevant pairing.

Note that other invariant measures exist (for instance via different averaging sequences), including examples with positive entropy. It is not known what the matching diffraction measure would be, but it is expected that they will show continuous components. A careful analysis of all invariant measures for this example seems an interesting open problem.

8 Concluding remarks

The examples above highlight different aspects of the quantification of order in terms of entropy and diffraction. While pure point diffractivity of uniquely ergodic systems [9] implies zero entropy, the general situation is complex, and there is no straightforward relation between entropy and diffraction; in fact, as the Bernoullisation example shows, diffraction can be completely insensitive to the (entropic) disorder of a system.

In the example of the closed-packed dimers, we referred to the dynamical spectrum (under the translation action). As this example together with the earlier observation in [18] shows, the diffraction and dynamical spectra are, in general, not the same, and can even have contributions of different spectral type. In the pure point case, the notions are equivalent (in the sense that the dynamical spectrum is pure point if and only if the diffraction spectrum is pure point [8]), but in general the dynamical spectrum contains additional information. It has been conjectured that the latter should correspond to the diffraction spectra of the system and all its factors.

Clearly, our understanding of 'order' is far from complete, and more work is required to arrive at a clearer picture of what 'order' means, and how to quantify it. Studying examples of the type discussed above is a first step in this direction, and a general frame is explained in [19, 2]. By mapping the range of possibilities, one gradually obtains a better understanding of the plethora of manifestations of order. This seems necessary in view of the hard inverse problem for systems with diffuse scattering.

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