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Topological Bragg Peaks and How They Characterise Point Sets

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The positions of the Bragg peaks in point set diffraction show up as eigenvalues of a dynamical system. Topological Bragg peaks arise from topological eigenvalues and determine the torus parametrisation of the point set. We will discuss how qualitative properties of the torus parametrisation characterise the point set.

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1. Introduction

The position $\boldsymbol{k}$ of a Bragg peak in the X-ray diffraction picture of a material can be mathematically described as a point for which $\hat{\gamma}(\{\boldsymbol{k}\}) > 0$ [1, 2]. Here $\hat{\gamma}$ is the Fourier transform of the autocorrelation of the material which is considered in an approximation in which the material is modeled by a point set neglecting any kind of thermal fluctuations or other time evolution. The approach to point sets based on dynamical systems theory allows to give a more catchy way of saying which points may be the position of a Bragg peak: *$\boldsymbol{k}$ may be the position of a Bragg peak if the plane wave* $\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}$ *with wave vector $\boldsymbol{k}$ is in phase with the material.* It roughly means that the phase of the wave ought to be, up to a small error, the same at $\boldsymbol{x}$ and at $\boldsymbol{y}$ provided the local configurations around $\boldsymbol{x}$ and $\boldsymbol{y}$ are the same. A more precise formulation of this phrase needs a little effort and will be made below in a *topological* context (Def. 1).

In mathematical terms it means that $\boldsymbol{k}$ is a *topological eigenvalue* and we call a Bragg peak *topological* if its position corresponds to such an eigenvalue. Our intent is to show how this topological aspect of diffraction can be used to characterise point patterns.

Leaving details to later let us illustrate such a characterisation by comparing the famous Fibonacci tiling with its "scrambled" version. The Fibonacci tiling arises from a cut and project pattern which looks similar on different scales. Its diffraction may be considered to be topological in the sense that all its Bragg peaks are topological. The technique of fusion [3] allows to construct modifications of the Fibonacci tiling by scrambling it slightly up on each scale.† The scrambling is so rare that it is statistically irrelevant and therefore does not modify the diffraction. It affects however the topology. Depending on the choice of tile lengths, the Bragg peaks of the scrambled version are either never topological‡, or only some of them are topological.

Now our results can be phrased loosely in the following way: the more topological Bragg peaks there are, the more regular is the structure in a geometric sense. The original Fibonacci tiling is perfectly regular as it comes from a cut and project pattern. The scrambled version which has still some topological Bragg peaks satisfies the Meyer property, which means a strong constraint on the set of difference vectors between points. The scrambled version which does not have any topological Bragg peaks does not satisfy the Meyer property and its geometry is not yet well understood.

It would be interesting to find out whether this topological aspect of diffraction can be measured in an experiment. While diffraction experiments are of statistical nature, and therefore insensitive to scrambling, the Schrödinger equation is not and so scrambling might affect the electronic properties.

Many aspects of the material presented here will be explained in more detail in [4].

2. Topological Bragg peaks

In this section we explain more clearly what we mean by a topological Bragg peak. The concept originates from the study of point sets through their associated topological dynamical systems. This approach to study point sets is extremely useful catching also many aspects of diffraction, see [5] for more information. The recent monograph on aperiodic order [6] contains a detailed discussion of the mathematical theory of diffraction.

2.1. Point patterns

In this article we consider a particular class of point sets to which we simply refer to as point patterns. Let $B(\boldsymbol{0}, R) = \{\boldsymbol{y} \in \mathbb{R}^n \| \|\boldsymbol{x}\| \le R\}$ be the ball of radius R centered at the origin and, for a point set Λ, by $\Lambda - \boldsymbol{x}$ the point set shifted by $\boldsymbol{x}$, $\Lambda - \boldsymbol{x} = \{\boldsymbol{y} - \boldsymbol{x} | \boldsymbol{y} \in \Lambda\}$. A *point pattern* $\Lambda \subset \mathbb{R}^n$ is a point set in $\mathbb{R}^n$ which satisfies the following conditions:

(1) Λ is *uniformly discrete*, i.e. there is a minimal distance between points;

(2) Λ is *relatively dense*, i.e. there is $R > 0$ so that any ball of radius R contains a point of Λ. Points appear with bounded gaps;

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†See also the contribution of Frank for more details.

‡When saying that we exclude the Bragg peak at $\mathbf{0}$ from our consideration as it is always topological.

(3) Λ has *finite local complexity*, i.e., up to translation, one finds only finitely many local configurations of a given size. More precisely the collection of so-called R-patches $\{B(\mathbf{0},R)\cap(\Lambda-\boldsymbol{x}),\boldsymbol{x}\in\Lambda\}$ is finite, and this for any choice of R;

(4) Λ is *repetitive*, i.e. local configuration repeats inside Λ with bounded gaps.

Are these conditions realistic for describing atomic positions of materials? Condition 1 certainly is. Condition 2 says that the material should not have arbitrarily large holes. Condition 3 is the strongest restriction and represents an idealisation which one can find in cut and project sets used to describe ideal quasicrystals, but it would not allow for small random variations. Having required condition 3, the last condition seems a reasonable one to describe homogeneous materials. Let us add that from a mathematical point of view, condition 3 is so far indispensible in order to obtain the kind of rigidity results we describe below.

Among the point patterns are some Meyer sets and cut and project sets.

2.1.1. Meyer sets

A point set $\Lambda\subset\mathbb{R}^n$ is a *Meyer set* if it is relatively dense and the set of difference vectors $\Delta=\{\boldsymbol{x}-\boldsymbol{y}:\boldsymbol{x},\boldsymbol{y}\in\Lambda\}$ is uniformly discrete. This is a very elementary geometric condition. Interestingly, the latter is equivalent to an analytic condition, namely that for all choices of $\epsilon>0$ the set $\Lambda^\epsilon=\{\boldsymbol{k}\in\hat{\mathbb{R}}^n:|\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}-1|\le\epsilon,\forall\boldsymbol{x}\in\Lambda\}$ is relatively dense. This says that the set of wave vectors for which the phase of the plane wave is, up to an error of ϵ, equal to 1 on all points of Λ, is relatively dense. There are quite a few more equivalent conditions to the above (see [7]) of which we mention one more: A set is a Meyer set if it is a relatively dense subset of a cut and project set.

An example of a Meyer set which is not a cut and project set can be derived from the famous Thue–Morse substitution $0\mapsto 0110, 1\mapsto 1001$. Iterating this substitution yields

0110100110010110100101100110100110010110011010010110100110

which should be thought of as a finite part of a bi-infinite sequence. Now the subset $\Lambda\subset\mathbb{Z}$ given by the positions of the digit 1 yields a Meyer set in $\mathbb{R}$, since difference vectors are integer multiples of the unit vector in $\mathbb{R}$.

Any Meyer set is uniformly discrete, relatively dense and has finite local complexity. So repetitive Meyer sets are point patterns.

2.1.2. Cut and project sets

We assume that the reader is familiar with the concept of a cut and project set, as it has been used since the early days of the discovery of quasicrystals for their description. We use the name *cut and project set* synonymously for what is called *model set* in the mathematics literature allowing the internal space of the construction to be more general than a vector space, namely to be a (locally compact) Abelian group (see [7]). If the acceptance domain (or atomic surface) has a boundary whose measure is 0 (this rules out many acceptance domains with fractal boundary) then the cut and project set is called *regular.* Any cut and project set is a Meyer set. Ignoring a little somewhat annoying detail we may say that a cut and project set is repetitive.

2.2. Pattern equivariant functions

Given a point pattern $\Lambda\subset\mathbb{R}^n$ and a function $f:\mathbb{R}^n\to\mathbb{C}$ we want to make precise what it means for f to depend only on the local configurations in the pattern. We have in mind a generalisation of the concept of a periodic function to which it specialised if Λ were a periodic set.

We say that $f:\mathbb{R}^n\to\mathbb{C}$ is *pattern equivariant*[§] for Λ if for all $\epsilon>0$ there exists $R>0$ such that whenever the R-patches at $\boldsymbol{x}$ and at $\boldsymbol{y}$ are the same, then $|f(\boldsymbol{x})-f(\boldsymbol{y})|<\epsilon$. Here we mean that the R-patches at $\boldsymbol{x}$ and at $\boldsymbol{y}$ are the same if $B(\mathbf{0},R)\cap(\Lambda-\boldsymbol{x})=B(\mathbf{0},R)\cap(\Lambda-\boldsymbol{y})$, that is, the local configuration of size R at $\boldsymbol{x}$ is the same as the one at $\boldsymbol{y}$ when they both have been shifted to the origin. The example of a pattern equivariant function which the reader should have in mind is a potential energy function for a particle in a material whose atomic positions are given by Λ each atom contributing to the potential energy with its local potential.

Definition 1. *Let $\mathcal{B}_{\mathrm{top}}$ denote the set of vectors $\boldsymbol{k}$ for which the plane wave $f_{\boldsymbol{k}}(\boldsymbol{x})=\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}$ is pattern equivariant for Λ. A Bragg peak is called topological if its position $\boldsymbol{k}$ belongs to $\mathcal{B}_{\mathrm{top}}$.*

Thus $\boldsymbol{k}\in\mathcal{B}_{\mathrm{top}}$ if the phase of the plane wave at a point $\boldsymbol{x}$ is determined with more and more precision by the local configuration surrounding $\boldsymbol{x}$; the larger the size of the configuration the more precise the phase is determined. Any $\boldsymbol{k}\in\mathcal{B}_{\mathrm{top}}$ corresponds to a Bragg peak, although perhaps an extinct one, that is, a Bragg peak whose intensity is 0 [8]. In this sense $\mathcal{B}_{\mathrm{top}}$ *is the set of positions of topological Bragg peaks for Λ.* Taking into account extinct Bragg peaks may appear somewhat artificial but we gain the benefit that $\mathcal{B}_{\mathrm{top}}$ forms a group. Definition 1 does not involve a statistical ingredient but rests on continuity properties, which is why we call the Bragg peak topological.

2.3. The dynamical system of a point pattern

It is most useful to study the dynamical system associated with a point pattern. There are several versions of it which all more or less contain the same information. We present here the algebra version and the version based on a space: the continuous hull of Λ.

2.3.1. Algebra version

Consider the set A_Λ of *continuous* functions $f:\mathbb{R}^n\to\mathbb{C}$ which are *pattern equivariant* for the point pattern Λ. A_Λ is a commutative (C^*-) algebra under pointwise addition and multiplication. Moreover, the group of translations $\mathbb{R}^n$ acts on A_Λ, that is, each vector of translation

[§] In the literature one finds also the terminology *weakly pattern equivariant* for this.

$\boldsymbol{x} \in \mathbb{R}^n$ gives rise to a map $\alpha_{\boldsymbol{x}} : A_\Lambda \to A_\Lambda$, namely

$$\alpha_{\boldsymbol{x}}(f)(\boldsymbol{y}) = f(\boldsymbol{y} - \boldsymbol{x}). \tag{1}$$

This comes about as translation preserves the properties of a function to be continuous and pattern equivariant. The triple $(A_\Lambda, \mathbb{R}^n, \alpha)$ is called the (algebraic) topological dynamical system associated with Λ. The name 'dynamical system' has nothing to do with a time evolution but is simply used by mathematicians for the action of a group on an algebra or a space (the group is in our case is $\mathbb{R}^n$, the group of space translations, and the action is α).

Definition 2. *An eigenvalue of the dynamical system $(A_\Lambda, \mathbb{R}^n, \alpha)$ is a vector $\boldsymbol{k} \in \mathbb{R}^n$ for which there exists a non-zero element $f \in A_\Lambda$ (its eigenfunction) such that*

$$\alpha_{\boldsymbol{x}}(f) = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} f. \tag{2}$$

It follows that f must be a multiple of the plane wave, $f = cf_{\boldsymbol{k}}$ with $c = f(\mathbf{0})$. Thus *a position of a topological Bragg peak is an eigenvalue of the dynamical system $(A_\Lambda, \mathbb{R}^n, \alpha)$.*

We now let $A_\Lambda^{\mathrm{eigen}}$ be the algebra generated by the eigenfunctions to eigenvalues of the system $(A_\Lambda, \mathbb{R}^n, \alpha)$. The property of being an eigenfunction is preserved under translation and so we have a subsystem $(A_\Lambda^{\mathrm{eigen}}, \mathbb{R}^n, \alpha)$ of the system $(A_\Lambda, \mathbb{R}^n, \alpha)$. All what we will have to say depends on the relation between $A_\Lambda^{\mathrm{eigen}}$ and A_Λ.

2.3.2. Torus parametrisation

To each commutative C^*-algebra corresponds a topological space in such a way that the algebra can be seen as the algebra of continuous functions over the space. This space is called the Gelfand spectrum of the algebra. The *continuous hull* Ω_Λ of Λ is the Gelfand spectrum of A_Λ, that is, $A_\Lambda \cong C(\Omega_\Lambda)$. It has been the subject of intensive study. Its elements are the point patterns which are locally indistinguishable from Λ, because they have the same local configurations. From a physical point of view, any element of Ω_Λ is as good as Λ to describe the material.

Now the action on A_Λ becomes an action on Ω_Λ: $\alpha_{\boldsymbol{x}}(\Lambda') = \Lambda' - \boldsymbol{x}$. The triple $(\Omega_\Lambda, \mathbb{R}^n, \alpha)$ is the space version of the dynamical system associated with Λ.

The Gelfand spectrum of $A_\Lambda^{\mathrm{eigen}}$ turns out to be a group $\mathbb{T}_\Lambda$, in fact it is the (Pontrayagin) dual group of $\mathcal{B}_{\mathrm{top}}$. $\mathbb{T}_\Lambda$ is a torus, or a limit of tori. The inclusion of $A_\Lambda^{\mathrm{eigen}}$ in A_Λ as a subalgebra gives rise to a surjective map $\pi : \Omega_\Lambda \to \mathbb{T}_\Lambda$ which commutes with the actions. This map π is called the *torus parametrisation.* In the mathematical literature one calls $\mathbb{T}_\Lambda$ also the maximal equicontinuous factor of Ω_Λ. Our results below are based on the study of $\pi : \Omega_\Lambda \to \mathbb{T}_\Lambda$ and in particular, how close it is to a bijection.

2.3.3. Topological conjugacy

We say that two point patterns Λ and Λ' are *topologically conjugate* if their associated dynamical systems are topologically conjugate, that is, there exists a homeomorphism $\phi : \Omega_\Lambda \to \Omega_{\Lambda'}$ which commutes with the actions. If moreover $\phi(\Lambda) = \Lambda'$ then the topological conjugacy is called pointed.

A well known example of a topological conjugacy is a local derivation which goes both ways, one says that Λ and Λ' are *mutually locally derivable* in this case. Topologically equivalent point patterns have the same dynamical properties, in particular they have the same positions of topological Bragg peaks and the same torus parameterization.

2.3.4. Diffraction and the dynamical system

We explain roughly how diffraction is related to the eigenvalues of the dynamical system. More can be found in the concise review [2] which includes also a list of references to the original articles. There is an ergodic probability measure μ on Ω_Λ which has to do with the physical phase in which the material is and brings in the statistical aspect of diffraction. We may then look for solutions to (2) which have eigenfunctions which do not necessarily belong to A_Λ, or equivalently to $C(\Omega_\Lambda)$, but to the larger space $L^2(\Omega_\Lambda, \mu)$ of functions on Ω_Λ which are square integrable with respect to (w.r.t.) μ. We may therefore have more solutions and a larger group of eigenvalues $\mathcal{B}$. To distinguish the two concepts of eigenvalues one calls the former *topological eigenvalues* and the more general ones *L^2-eigenvalues*¶ as their eigenfunction is square integrable but not necessarily continuous. The main result says the following: *The position of a diffraction Bragg peak is an L^2-eigenvalue.* Not every L^2-eigenvalue needs to come from a diffraction Bragg peak but the group $\mathcal{B}$ is generated by the positions of the Bragg peaks. The elements of $\mathcal{B}$ which do not come from a diffraction Bragg peak are interpreted as extinct (invisible) Bragg peaks [8]. The positions of topological Bragg peaks generate $\mathcal{B}_{\mathrm{top}}$ which is a subgroup of $\mathcal{B}$. In this work, only $\mathcal{B}_{\mathrm{top}}$, that is, topological Bragg peaks play a role.

3. Results

We will present two kinds of results. For the first kind we assume that we have a repetitive Meyer set and obtain a characterisation depending on how close the torus parametrisation $\pi : \Omega_\Lambda \to \mathbb{T}_\Lambda$ is to a bijective map. For the second kind we assume only that we have a point pattern obtaining a partial classification of point patterns up to topological conjugacy. Recall that the torus parametrisation is always surjective.

3.1. Characterisation of repetitive Meyer sets

Theorem 1. *Let $\Lambda \subset \mathbb{R}^n$ be a repetitive Meyer set. Then $\mathcal{B}_{\mathrm{top}}$ contains n linearly independent vectors [9]. In other words, $\mathbb{T}_\Lambda$ is at least as large as an n-torus $\mathbb{T}^n$. Furthermore:*

(1) *The torus parametrisation π is injective on at least one point if and only if Λ is a cut and project set [10].*

¶The expression measurable eigenvalue is also used.

(2) *The torus parametrisation π is almost everywhere injective*[‖] *if and only if Λ is a regular cut and project set [11].*

(3) *π is bijective if and only if Λ is a periodic set (has n independent periods) [11, 12].*

3.2. Classification of point patterns up to topological conjugacy

Theorem 2 ([9]). *Let $\Lambda \subset \mathbb{R}^n$ be a point pattern. Λ is topologically conjugate to a repetitive Meyer set if and only if $\mathcal{B}_{\mathrm{top}}$ contains n linearly independent vectors.*

Corollary 1. *Let $\Lambda \subset \mathbb{R}^n$ be a point pattern.*

(1) *The torus parametrisation π is injective on at least one point if and only if Λ is topologically conjugate to a cut and project set.*

(2) *The torus parametrisation π is almost everywhere injective if and only if Λ is topologically conjugate to a regular cut and project set.*

(3) *π is bijective if and only if Λ is a periodic set (has n independent periods).*

3.3. Beyond cut and project sets

In order to treat also cases in which there is no point on which π is injective we consider three numbers which measure how close Ω_Λ sits above $\mathbb{T}_\Lambda$. The first two are the maximal rank Mr, and the minimal rank mr, which are the largest, respectively smallest, number of elements the pre-image $\pi^{-1}(t)$ of t can have when varying over $t \in \mathbb{T}_\Lambda$. The really interesting third rank is the so-called coincidence rank. To define it we first introduce the relation that two elements $\Lambda_1, \Lambda_2 \in \Omega_\Lambda$ are proximal ($\Lambda_1 \sim \Lambda_2$) if there exists a sequence $(\boldsymbol{x}_k)_{k\in\mathbb{N}} \subset \mathbb{R}^n$ so that $\Lambda_1 - \boldsymbol{x}_k$, and $\Lambda_2 - \boldsymbol{x}_k$ coincide on the patch of radius k up to a translation of size smaller than $\frac{1}{k}$. This notion is more intuitive for the Meyer sets: two Meyer sets $\Lambda_1, \Lambda_2 \in \Omega_\Lambda$ are proximal if and only if Λ_1 and Λ_2 agree on larger and larger balls. Now the *coincidence rank* cr is defined to be the largest possible cardinality m of a collection of elements $\Lambda_1, \ldots, \Lambda_m \in \pi^{-1}(t)$ which satisfy $\Lambda_i \not\sim \Lambda_j$ $(i \neq j)$. This number turns out not to depend on t.

Note that $cr \leq mr \leq Mr$ and that the case $mr = 1$ corresponds to cut and project sets. Furthermore $cr = mr$ whenever Ω_Λ contains an element which is not proximal to any other element. Primitive Meyer substitution tilings yield examples for which $cr = mr \leq Mr < \infty$ [13]. The Thue–Morse substitution has $cr = 2$.

Theorem 3 ([4]). *Let Λ be a non-periodic point pattern. If cr is finite then Λ is topologically conjugate to a Meyer set and $\mathcal{B}_{\mathrm{top}} \subset \mathbb{R}^n$ is dense.*

[‖]This means that there exists a subset $\mathbb{T}^0_\Lambda \subset \mathbb{T}_\Lambda$ of measure 1 such that each point of $\mathbb{T}^0_\Lambda$ has a unique pre-image.

3.4. How far does $(\Omega_\Lambda, \mathbb{R}^n)$ characterize Λ?

The above classification of point patterns is up to topological conjugacy. We therefore need to understand to which extent topological conjugacy preserves the properties of a point set, like for instance the Meyer property. The first result in this direction is the following:

Theorem 4 ([9]). *Let $\Lambda \subset \mathbb{R}^n$ be a point pattern. Λ and Λ' are pointed topologically conjugate whenever for all $\epsilon > 0$ exists a point pattern Λ_ϵ such that Λ and Λ_ϵ are mutually locally derivable and Λ_ϵ and Λ' are shape conjugate. Moreover, within ϵ of each point of Λ_ϵ is a point of Λ' and vice versa.*

Here, a *shape conjugation* is a deformation of the pattern which preserves finite local complexity and induces a topological conjugacy. This notion may be formulated in the context of pattern equivariant cohomology [14, 15]. In fact, the shape conjugations of Λ are classified by a subgroup of the first cohomology group of Λ. First investigations show that this group is rather small and so there are few shape conjugations. Whereas shape conjugations of cut and project sets with convex polyhedral acceptance domain yield again cut and project sets, we also found examples of more general cut and project sets which allow for shape conjugations yielding point patterns which are not even Meyer sets [16].

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