The Impact of Aperiodic Order on Mathematics

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Abstract

Mathematics has been strongly influenced by problems arising from physics. The existence of quasicrystals as strongly ordered structures which cannot be periodic has raised various mathematical questions that have stimulated developments in the areas of discrete geometry, harmonic analysis, group theory and ergodic theory. It seems that extra "internal dimensions" are useful in describing certain features of quasicrystal structure and their diffraction spectra. In particular N-dimensional crystalline symmetries can appear in the diffraction spectra of model sets. This paper describes recent work in discrete geometry suggested by the modelling of atomic positions in quasicrystals by Delone sets with restrictions on interpoint distances. It suggests one mechanism for the appearance and usefulness of "internal dimensions" in describing ordered aperiodic structures.

Keywords: Crystallographic group; Delone set; Ergodic theory; Matching rules; Aperiodicity

1. Introduction

Mathematics has been strongly influenced by problems arising from physics. David Hilbert included as the 18th problem on his famous list of 23 problems at the 1900 International Mathematical Congress the building up of space from congruent polyhedra, which contained as a subproblem proving that there are a finite number of crystallographic groups in N-dimensions, see [1]. Now N-dimensional problems may have seemed irrelevant to solid state physicists who consider three-dimensional structures, but the discovery of quasicrystals changed that. It seems that extra "internal dimensions" are useful in describing certain features of quasicrystal structure and their diffraction spectra. In particular N-dimensional crystalline symmetries can appear in the diffraction spectra of model sets. The existence of quasicrystals as strongly ordered structures which cannot be periodic has raised various mathematical questions that have stimulated developments in the areas of discrete geometry, harmonic analysis, group theory and ergodic theory.

It is impossible in a short space to indicate all the directions of interesting mathematics that have resulted, see [2], [3]. This paper considers three main themes : (1) A re-examination of what properties characterize a crystal, (2) A taxonomy of Delone sets which can represent quasicrystalline structure from the most strongly ordered ones to random tiling models, and (3) the problem of enforcing (weak) long range translational order using "local rules."

2. Tiling Models and Delone Set Models

The study of aperiodic structures with a strong form of ordering has been formalized in two different ways: tilings and Delone sets. In both cases the structure is considered to be composed of small pieces, which in one case are tiles and the other case are points.

Delone sets represent an idealized version of atomic structure for the solid state. They were introduced around 1930 by the Russian crystallographer and mathematician B. N. Delone [Delaunay] under the name (r, R)-set. A *Delone set* X is any (necessarily infinite) discrete set in $\mathbb{R}^n$ for which there are positive constants r and R such that each ball of radius r contains at most one point of X and each ball of radius R contains at least one point of X. The points of X represent atomic positions, and the conditions are equivalent to the set X having finite positive packing radius and covering radius by equal spheres.

Tiling models typically consider filling space using congruent copies of a possibily infinite number of different tile types (prototiles), but the case of most interest is that of a finite number of tile types. In some models the prototiles are moved by Euclidean motions, which we call tiling by isometries, and in others they are moved by translations only, which we call tiling by translations.

Tiling models and Delone set models are interconvertible in the following sense. Given a tiling, one can mark on each prototile a finite number of points, and the marks on all the tiles in a tiling then produce a Delone set associated to the tiling. In the opposite direction, to each Delone set is associated a tiling of space by the Voronoi cell associated to each of its points. (The *Voronoi cell* of a point $\mathbf{x}$in a discrete set X is the set of points in $\mathbb{R}^n$ closer to $\mathbf{x}$ than to any other point in X.) This correspondence of tilings and Delone sets is a rough one since it involves arbitrary choices, but the corresponding models have many properties in common, in the sense of dynamical systems discussed in §3.

Aperiodic tilings generated by local rules were first studied in mathematics in connection with a problem in mathematical logic. In 1961 Hao Wang raised the "domino problem": given a set of squares with colored edges which can tile the plane face-to-face with matching edge-colorings, must there always exist a periodic tiling using such prototiles. In 1966 Berger gave a negative answer, exhibiting a set of about 20000 different prototiles which tiled the plane, but only aperiodically. Berger showed that the problem of whether a partial tiling of the plane with such tiles could be extended to a full tiling was undecidable. In 1971 Raphael Robinson gave a much simpler construction, exhibiting 6 prototiles which tiled the plane, with only aperiodic tilings. Later in the decade came Roger Penrose's example of two prototiles which tiled the plane aperiodically (allowing rotations of the prototiles.) These last two constructions both reduced the number of prototiles using a symmetry principle: if prototiles can only be moved by translations, then Penrose's set consists of 20 prototiles.

Penrose tilings are a special case of a theory of aperiodic tilings with hierarchical properties, such as self-similarity. One question is: Can tilings with hierarchical properties be constructed by "local rules", i.e. can the prototiles be marked in various ways, with rules for how the marking of adjacent tiles match, so that the rules enforce the hierarchical structure? For Penrose tiles this was shown by de Bruijn in 1981. In general the answer is "yes," as shown by C. Goodman-Strauss [4].

This paper considers Delone set models. For nearly all tiling results there is a Delone set equivalent. Properties of self-similarity are most easily framed using tilings, but have been considered for exists a corresponding theory of substitution Delone sets, [5], [29].

3. Dynamical Systems and Diffractivity

A connection of tilings and dynamical systems was motivated in part by the problem of explaining symmetries in diffraction spectra by local properties. The symmetries observed on diffraction spectra are statistical symmetries, and "Bragg peaks" or point spectra indicate correlations between the interpoint distance vectors of a positive proportion of atoms in the sampled material. They do not require global symmetries to occur on the atomic level itself. On the mathematical side the dynamical systems connection appears in Mozes [9], and has been systematically studied by Radin [6]-[8].

The idea is to consider not a given Delone set X but the ensemble of all Delone sets that resemble it locally, i.e. can be approximated by translates of X in an arbitrarily large ball around the origin. A *patch* of radius R in a Delone set X is the intersection of the Delone set with a ball of radius R centered at a point of X. Two patches are considered to be the same if one is a translate of the other. Let $[[X]]$ denote the collection of all Delone sets Y such that every patch in Y, of whatever radius, is arbitrarily closely approximated by a translate of some patch in X. The set $[[X]]$ is closed under translations, meaning if Y is in X then so is $Y + \mathbf{t}$ for any $\mathbf{t} \in \mathbb{R}^n$. It forms a topological dynamical system under this action.

The simplest such systems are those that are *minimal*, i. e. every member Y has a dense orbit in $[[X]]$ under translations. For sets X that we later consider (Delone sets of finite type) this notion is equivalent to *repetitivity*, which asserts that for each radius R there is some larger radius R' such that any patch of radius R' in X contains a translate of every possible patch of radius R. Radin [7], [8] asserts that minimality can be viewed as ' a mathematical version of the "ground state" of a physical system.

One can now study symmetries of $[[X]]$. These symmetries leave the collection $[[X]]$ invariant but may move the individual members of $[[X]]$. In particular they may include crystallographically forbidden rotational symmetries. Going further, Radin [10] showed that an example, the pinwheel tiling, in which $[[X]]$ had the full orthogonal group $O(n, \mathbb{R})$ of point symmetries, although no member X can have such a symmetry group.

The notion of diffraction pattern is associated with metric dynamics. A set $[[X]]$ is uniquely ergodic if there is a unique translation-invariant (Borel) measure that can be defined on this set. For the sets we later consider (Delone sets of finite type) this notion is equivalent to every patch having a well-defined frequency of occurrence in larger and larger regions of X. Uniquely ergodic sets have a well-defined two-point correlation function, and the Fourier transform of this is a mathematical analogue of diffraction measure, see Hof [11]. This measure in general consists of a pure point component ("Bragg peaks"), a singular continuous component and an absolutely continuous component.

Two large classes of aperiodic sets have been found which have pure point diffraction spectra in this sense. The first are cut-and-project sets, which were essentially anticipated by Y. Meyer in 1972 under the name "model set." The second are certain kinds of substitution sets constructed by a hierarchical scheme. For details of such results, see Hof [11] and Gähler and Klitzing [12]. Cut-and-project constructions can produce sets whose diffraction pattern have noncrystalline symmetries, but in each dimension their point groups are of a restricted form, classified by Piunikhin, see [28, Theorem 2.1.1].

From the viewpoint of dynamical systems, Delone set models and tiling models are nearly equivalent. One can associate a topological dynamical system to each, and the rough procedure described in §2 generally gives equivalent dynamical systems. Different tilings give equivalent dynamical systems when they are "mutually locally derivable," see Baake et al [13].

4. Ideal Crystals

The simplest aperiodic sets should be those that most strongly resemble ideal crystals. An *ideal crystal* is a set X in $\mathbb{R}^n$ that is a finite number of translates of an n-dimensional lattice.

The discovery of quasicrystals led to a re-examination of those geometric properties of a set that are sufficient to force it to be an ideal crystal. We list several such properties.

(1) *Bounded Patch Counts.* The set X has the property that for each radius R, the number $N_R(X)$ of inequivalent patches of radius R under isometries in X is bounded by a constant c_1 independent of R (but which may depend on X.)

(2) *Discrete Pure Point Diffractivity.* The set X has a well-defined autocorrelation measure whose Fourier transform (diffraction measure) is a pure discrete measure which is supported on a Delone set.

(3) *Bounded Repetitivity.* There is a constant c_2 such that in each ball of radius c_2 in space contains a center point of a copy of each patch of radius R that occurs anywhere in X, irrespective of the value of R.

(4) *Integral Self-Similarity.* For each integer $m \geq 2$ the set X can be partitioned into a finite number of Delone sets X_j and each X_j can be partitioned into a finite union of translates of "inflated" copies $\{mX_k\}$ of the sets X_k, i.e. $X_j = \cup(mX_k + \mathbf{t}_{jk})$, where $\mathbf{t}_{jk}$ is a finite set of translations in $\mathbb{R}^n$.

Properties (1)- (3) each separately characterize ideal crystals. Property (1) is a "perfect local rules" property, and was established for regular point systems (a subclass of ideal crystals) by Delone et al. [14] in 1976. A general proof is given in Dolbilin et al [15]. That property (2) characterizes ideal crystals follows from a result of Cordoba [16]. Property (3) is discussed in Lagarias and Pleasants [17]. Property (4) holds for ideal crystals X, and it seems likely that it also characterizes ideal crystals.

5. Strongly Ordered Delone Sets

We now consider relaxations of the properties characterizing ideal crystals that include some aperiodic Delone sets, which form the "simplest" aperiodic sets according to these criteria.

(1′) *Volume-Bounded Patch Counts.* In $\mathbb{R}^n$ there is a constant c_3 such that the number of inequivalent patches of radius R under translations in X is at most c_3R^n.

(2′) *Pure Point Diffractivity.* The Delone set X has a well-defined autocorrelation measure whose Fourier transform is a pure discrete measure, but whose support may not be a discrete set.

(3′) *Linear Repetitivity.* There is a constant c_4 such that in each ball of radius $M_R(X) = c_4R$ in space there can be found in X a copy of each patch of radius R that occurs anywhere in X.

(4′) *Self-Similarity.* There is a constant $\alpha > 1$ such that the set X can be partitioned into a finite number of Delone subsets X_j and each X_j can be partitioned into by a finite number of translates of sets αX_k. (More generally, α can be replaced by an $n \times n$ nonnegative real matrix which is expanding, i.e. all of whose eigenvalues $|\lambda| > 1$.)

Each of conditions (1′)- (4′) treated by itself includes aperiodic sets, which are close to being crystalline in the appropriate sense. Properties (2′)- (4′) enforce some form of strong long-range order. Various self-similar sets are known to be linearly repetitive, and it is quite easy to show that linear repetitivity always implies (1′). There is no nice relation between (2′) and the other properties, but various explicit constructions of sets with properties (3′) or

(4′) also satisfy (2′). Concerning Property (1′) we have:

Conjecture *If X is an aperiodic Delone set in $\mathbb{R}^n$ then there is a positive constant c_3 depending on X such that X has at least $c_3 R^n$ translation-inequivalent patches of radius R, for each $R > 0$.*

This conjecture is raised in [17]. It is known bo be true in dimension $n = 1$, via [15, Theorem 1.3].

6. A Taxonomy for Delone Sets

We describe a taxonomy presented in [18] consisting of three classes of Delone sets specified by increasingly strong restrictions on their sets of interpoint vectors $X - X$, as follows.

Definition 6.1. Let X be a Delone set.

(i) X is a *finitely generated Delone set* if the additive group

$$[X - X] = \mathbb{Z}[\mathbf{x} - \mathbf{x}' : \mathbf{x}, \mathbf{x}' \in X] \qquad (1)$$

is finitely generated.

(ii) X is a *Delone set of finite type* if $X - X$ is a discrete closed subset of $\mathbb{R}^n$, i. e. the intersection of $X - X$ with any closed ball is a finite set.

(iii) X is a *Meyer set* if $X - X$ is a Delone subset of $\mathbb{R}^n$.

Note that in class (i) the additive group $[X - X]$ may be dense in $\mathbb{R}^n$. We show that class (i) includes class (ii), and class (ii) obviously includes class (iii). The class (iii) contains all cut-and-project sets as a subclass.

The class of finitely generated Delone sets seems too large to be interesting, but it is the largest class on which an "address map" can be defined.

Definition 6.2. Let X be a finitely generated Delone set in $\mathbb{R}^n$ with $rank(X) = s$, and choose a basis of $[X]$, say

$$[X] = \mathbb{Z}[\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_s] \ . \qquad (2)$$

The *address map* $\phi : [X] \to \mathbb{Z}^s$ associated to this basis is

$$\phi(\sum_{i=1}^{s} n_i \mathbf{v}_i) = (n_1, n_2, \ldots, n_s) \ . \qquad (3)$$

The address map provides a way to coordinatize the points of X viewed as embedded in a higher dimensional space $\mathbb{R}^s$, whose dimension is the rank of $[X]$.

Delone sets of finite type are those Delone sets which satisfy some set of "local rules" [18, Theorem 2.1].

Theorem 61. *A Delone set X is of finite type if and only if it has finitely many translation-equivalence classes of patches of radius $2R$, where R is its relative denseness constant. Any Delone set X of finite type is finitely generated.*

This "local rules" property motivates the name "finite type," as does an analogy with "finite type" systems in Mozes [9] and Radin [19, p. 38] Delone sets of finite type have the following characterization.

Theorem 62. *For a Delone set X in $\mathbb{R}^n$, the following properties are equivalent.*

(i) X is a Delone set of finite type, i.e. for each R there are only finitely many interpoint distance vectors in X of length at most R.

(ii) For each radius R, X has a finite number of translation-equivalence classes of R-patches.

(iii) The marked Voronoi tesselation of $\mathbb{R}^n$ induced by X has finitely many translation-inequivalent marked Voronoi domains.

(iv) X is finitely generated and for each address map $\phi : [X] \to \mathbb{Z}^s$ there is a constant C_0 such that

$$||\phi(\mathbf{x}) - \phi(\mathbf{x}')|| \le C_0 ||\mathbf{x} - \mathbf{x}'|| \ , \quad \textit{all } \mathbf{x}, \mathbf{x}' \in X \ .$$

Random tiling models of quasicrystalline structure when converted to Delone sets generally give Delone sets of finite type, analogously to (iii) above.

The class of Meyer sets was originally introduced by Meyer in terms of a property in harmonic analysis (relatively dense harmonious set). Meyer [20] showed that this definition was equivalent to property (ii) in the following theorem, and the equivalence of this to the definition of Meyer set given above was later-shown in [21].

Cut-and-project sets are a special subclass of Meyer sets. These sets were introduced by Meyer [22, p. 48] in 1972 under the name "model set."

Definition 6.3 Let Λ be a full rank lattice in $\mathbb{R}^d = \mathbb{R}^{n+m} = \mathbb{R}^n \times \mathbb{R}^m$, and let $\pi^{\|}$ and $\pi^{\perp}$ be orthogonal projections onto the factors $\mathbb{R}^n$ and $\mathbb{R}^m$, respectively. A *window* Ω is a bounded open subset of $\mathbb{R}^m$, and the *strip* $S(\Omega)$ in $\mathbb{R}^d$ associated to the window Ω is

$$S(\Omega) := \mathbb{R}^n \times \Omega = \{\mathbf{w} \in \mathbb{R}^d : \pi^{\perp}(\mathbf{w}) \in \Omega\} \ .$$

The *cut-and-project set* $X(\Lambda, \Omega)$ associated to the data (Λ, Ω) is

$$X(\Lambda, \Omega) = \pi^{\|}(\Lambda \cap S(\Omega)) \ . \qquad (4)$$

We call d the *dimension* of the data (Λ, Ω). A given cut-and-project set X may be constructed in many ways, using different pairs (Λ, Ω) and (Λ', Ω') of different dimensions.

Meyer sets have the following characterizations.

Theorem 63. *The following properties of a Delone set X in $\mathbb{R}^n$ are equivalent.*

(i) X is a Meyer set. That is, $X - X$ is a Delone set.

(ii) X is a Delone set and there is a finite set F such that $X - X \subseteq X + F$.

(iii) X is a finitely generated Delone set and every homomorphism $\psi : [X] \to \mathbb{R}^d$ for some $d \geq 1$ is an almost linear mapping on X, i.e. there is a linear map $\tilde{L} : \mathbb{R}^n \to \mathbb{R}^s$ and a constant C such that

$$||\phi(\mathbf{x}) - \tilde{L}(\mathbf{x})|| \leq C \ , \quad \textit{all} \ \ \mathbf{x} \in X \ .$$

(iv) X is a finitely generated Delone set and the address map $\phi : [X] \to \mathbb{Z}^s$ is an almost linear mapping on X.

(v) X is a finitely generated Delone set and there exists a nondegenerate cut-and-project set X' of dimension at most rank(X) such that

$$X \subseteq X' \ .$$

This result appears in [18, Theorem 3.1]. A thorough study of Meyer sets, with detailed proofs, appears in Moody [23]. The cut-and-project set X' containing X that appears in (v) is not necessarily irreducible.

In terms of the two constructions of sets with nice diffractivity properties, cut-and-project sets are always Meyer sets, while Delone sets constructed by the substitution method are always Delone sets of finite type, but not always Meyer sets. However, all known examples of substitution type Delone sets which have been proved to have pure point diffraction spectra are Meyer sets, see Solomyak [24] for analogous tiling results.

7. Local Rules Enforcing Translational Order

Delone sets of finite type have a weak form of translational order which is embodied in their lying in a finitely generated additive module in $\mathbb{R}^n$ (that is, a "quasilattice.") One can ask: "Can such weak translational order be enforced locally." To make this precise, we say that a set of *local rules* (under isometries) is a finite list $\mathcal{L}$ of possible patch types of a fixed radius R. Let $\Sigma_{\mathcal{E}}(\mathcal{L})$ denote the collection of all possible sets X each of whose R-patches is isometric to a patch in the list $\mathcal{L}$, i.e. these are the totality of sets that satisfy the local rules $\mathcal{L}$. The question then becomes, under what circumstances can one force all the sets in $\Sigma_{\mathcal{E}}(\mathcal{L})$ to be Delone sets of finite type, and to include a given Delone set X.

For ideal crystals the answer is "yes." More generally the answer is "yes" for any Delone set of finite type that is repetitive, which according to the criterion of §3 corresponds to a ground state, see [25, Theorem 1.1]

Theorem 71. *Let X be a Delone set of finite type X in $\mathbb{R}^n$ which is repetitive. Then there exists a set of local rules $\mathcal{L}$ under isometries such that X satisfies $\mathcal{L}$ and any other set Y that satisfies $\mathcal{L}$ is a Delone set of finite type.*

This result has the following interpretation. Local rules are restrictions on the local structure of a set. One can view them as being analogous to local minima of an energy function. In physical systems one often expects that the associated energy function is invariant under Euclidean motions. The theorem states that for any "ground state" X there are local rules which X satisfies which require that all Y satisfying them be Delone sets of finite type, so that $[Y]$ is a quasilattice. Thus the sets have a weak translational order describable using an address map, and this description uses a finite number of "internal dimensions." Thus minimization of a local energy function is a mechanism that could produce structures describable in this way. This mechanism does not necessarily account for the usefulness of "internal dimensions" in describing quasicrystalline structures, since electromagnetic forces are long range rather than local, but it is suggestive.

8. Perfect Local Rules

There are two natural notions of "perfectly ordered set" which apply to Delone sets of finite type, one coming from topological dynamics and the other coming from metric dynamics. The notion in topological dynamics is minimality, which here is equivalent to repetitivity, and the notion in metric dynamics is unique ergodicity, which here is equivalent to uniform patch frequencies. When can these conditions be enforced by local rules?

We say that $\mathcal{L}$ is a set of *perfect. local rules* when all sets that satisfy the rules are minimal (and in the same local isomorphism class.) There are two versions of this concept, depending on whether the local rules are enforced under translations or under isometries. The results of the last section allow one to show the following result [25, Section 5].

Theorem 81. *Let X be a Delone set of finite type in $\mathbb{R}^n$. Then X has perfect local rules under isometries, if and only if it has perfect local rules under translations.*

This result is useful insofar as perfect local rules under translations are much easier to check than perfect local rules under isometries. In the case of ideal crystals, for example, the existence of perfect local rules under translations is virtually immediate, taking the radius to be twice the diameter of a unit cell of the lattice. However the existence of perfect local rules under isometries is more subtle because the possible rotations of the patches have to be limited to a finite set.

The main source of examples of perfect local rules in the sense above comes from hierarchical constructions. In these examples the sets produced are not only repetitive, but are usually linearly repetitive in the sense of §5. The condition of linear repetitivity is so strong that it enforces "perfect ordering" in the sense of metric dynamics [17, Theorem 5.1].

Theorem 82. *If X is a Delone set of finite type in $\mathbb{R}^n$ which is linearly repetitive, then it has uniform patch frequencies, so is uniquely ergodic.*

In particular, this property guarantees that any such set X is diffractive. It has a well-defined diffraction measure, which however does not necessarily have any pure point spectrum.

Perfect local rules appear to be extremely rare. It is an open problem to characterize when they exist. Another question concerning them is which symmetry groups can occur in the diffraction spectrum of structures having perfect local rules under translations. The existing constructions show that certain non-crystalline symmetries can occur in two and three dimensions, and there is some evidence (but no mathematical proof I know of) that there are nontrivial restrictions on the symmetries.

When one considers perfect local rules under isometries, new phenomona appear. Radin [8], [19] has raised and studied the question of exactly which statistical symmetries can be enforced by perfect local rules under isometries and has found several different phenomona associated to group theory. The Conway-Radin pinwheel tiling yields an associated Delone set with perfect rules under isometries, which is not a Delone set of finite type, and a fortiori does not have perfect local rules under translations. Danzer [26] gives another example. There remain many open questions.

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