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Quasicrystals / Quasicristaux

Quasicrystals, model sets, and automatic sequences

Quasicristaux, ensembles modèles et suites automatiques

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ABSTRACT

We survey mathematical properties of quasicrystals, first from the point of view of harmonic analysis, then from the point of view of morphic and automatic sequences.

RÉSUMÉ

Nous proposons un tour d'horizon des propriétés mathématiques des quasicristaux, d'abord du point de vue de l'analyse harmonique, ensuite du point de vue des suites morphiques et automatiques.

1. Roots

In the late sixties, the second author introduced some point sets $\Lambda \subset \mathbb{R}^n$ that generalize lattices [1–4]. *Meyer sets* and *model sets* are defined in the next section. Roger Penrose discovered in 1974 his famous pavings with the pentagonal symmetry. In 1981, N.G. de Bruijn proved that the set Λ of vertices of the Penrose paving is a *model set* (de Bruijn was unaware of the definition of *model sets* and rediscovered it). Then the diffraction pattern of Λ could be computed as in [2]. In 1982, D. Shechtman discovered quasicrystals. D. Shechtman was unaware of what was achieved previously. Denis Gratias and Robert Moody unveiled the connections between *model sets*, *Meyer sets*, and quasicrystals.

After defining *model sets* and *Meyer sets*, we present some recent discoveries where model sets are playing a seminal role (Sections 3, 4, and 5).

Another approach to quasicrystals involves sequences generated by morphisms of the free monoid, in particular the (binary) Fibonacci sequence. Surveying works starting from two seminal papers one by Kohmoto, Kadanoff, and Tang [5], the other by Östlund, Pandit, Rand, Schellnhuber, and Siggia [6], we will describe in passing Sturmian sequences and automatic sequences. A last section will describe attempts to find links between the model set theory approach and the approach through morphic and/or automatic sequences.

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2. Model sets

Definition 2.1. A collection of points $\Lambda \subset \mathbb{R}^n$ is a Delone set if there exist two radii $R_2 > R_1 > 0$ such that:

(a) every ball with radius R_1, whatever be its location, cannot contain more than one point in Λ;
(b) every ball with radius R_2, whatever be its location, shall contain at least one point in Λ.

Definition 2.2. A *Meyer set* is a subset Λ of $\mathbb{R}^n$ fulfilling the following two conditions:

(a) Λ is a Delone set;
(b) there exists a finite set $F \subset \mathbb{R}^n$ such that

$$\Lambda - \Lambda \subset \Lambda + F$$

If $F = \{0\}$, then Λ is a lattice.

J.-C. Lagarias proved in [7] that (b) can be replaced by the weaker condition that $\Lambda - \Lambda$ is a Delone set.

We now define "model sets" and unveil the connection between model sets and *Meyer sets*. The following definition can be found in [2].

Let $\Gamma \subset \mathbb{R}^n \times \mathbb{R}^m = \mathbb{R}^N$ be a lattice. If $(x, t) \in \mathbb{R}^n \times \mathbb{R}^m$, we write $p_1(x, t) = x$, $p_2(x, t) = t$. We assume that p_1 once restricted to Γ is an injective mapping onto $\Gamma_1 = p_1(\Gamma)$. We make the same assumption on p_2. We furthermore assume that $p_1(\Gamma)$ is dense in $\mathbb{R}^n$ and $p_2(\Gamma)$ is dense in $\mathbb{R}^m$.

Definition 2.3. Let $Q \subset \mathbb{R}^m$ be a compact set. Then the model set $\Lambda_Q \subset \mathbb{R}^n$ is defined by:

$$\Lambda_Q = \left\{p_1(\gamma);\ \gamma \in \Gamma, p_2(\gamma) \in Q\right\} \tag{1}$$

A model set is simple if $m = 1$ and $Q = I$ is an interval.

Theorem 2.4. *A model set is a Meyer set. Conversely, if Λ is a Meyer set, there exists a model set M (or a lattice M) and a finite set F such that $\Lambda \subset M + F$.*

3. Almost periodic patterns

Definition 3.1. A real valued function f defined on $\mathbb{R}^n$ is a generalized almost periodic (g-a-p) function if it is a Borel function and if for every positive ϵ there exist two almost periodic functions g_ϵ and h_ϵ such that:

$$g_\epsilon \leqslant f \leqslant h_\epsilon \tag{2}$$

and, $\mathcal{M}$ denoting the mean value,

$$\mathcal{M}(h_\epsilon - g_\epsilon) \leqslant \epsilon \tag{3}$$

A Borel measure μ on $\mathbb{R}^n$ is a g-a-p measure if for every compactly supported continuous function g, the convolution product $\mu * g$ is a g-a-p function.

Definition 3.2. A set $\Lambda \subset \mathbb{R}^n$ is an almost periodic pattern if the associated sum of Dirac masses $\sigma_\Lambda = \sum_{\lambda\in\Lambda} \delta_\lambda$ is a g-a-p measure.

Theorem 3.3. *Let us assume that the compact set Q in Definition 2.3 is Riemann integrable. Then the corresponding model set Λ_Q is an almost periodic pattern.*

This is not an empty statement since almost periodic patterns have a rigid arithmetic structure as the following theorem shows:

Theorem 3.4. *Let Λ_θ, $\theta > 2$, be the set of all finite sums $\sum_{k\geqslant 0} \epsilon_k \theta^k$ with $\epsilon_k \in \{0, 1\}$. Then Λ_θ is an almost periodic pattern if and only if θ is a Pisot–Vijayaraghavan number.*

These two theorems are proved in [2].

4. Beyond Shannon

The Fourier transform of $f \in L^1(\mathbb{R}^n)$ will be defined by:

$$\hat{f}(\xi) = \int_{\mathbb{R}^n} \exp(-2\pi i \xi \cdot x) f(x)\,\mathrm{d}x, \quad \xi \in \mathbb{R}^n \tag{4}$$

Let $K \subset \mathbb{R}^n$ be a compact set and $E_K \subset L^2(\mathbb{R}^n)$ be the translation invariant subspace of $L^2(\mathbb{R}^n)$ consisting of all $f \in L^2(\mathbb{R}^n)$ whose Fourier transform $\hat{f}(\xi) = \int \mathrm{e}^{-2\pi \mathrm{i} x \cdot \xi} f(x)\,\mathrm{d}x$ vanishes on $\mathbb{R}^n \setminus K$. We now follow H.J. Landau.

Definition 4.1. A set $\Lambda \subset \mathbb{R}^n$ is a set of stable sampling for E_K if there exists a constant C such that:

$$f \in E_K \quad \Rightarrow \quad \|f\|_2^2 \leqslant C \sum_{\lambda \in \Lambda} \left| f(\lambda) \right|^2 \tag{5}$$

Then we have [4,8].

Theorem 4.2. *Let $K \subset \mathbb{R}^n$. Then simple model sets Λ are sets of stable sampling for E_K whenever the density of Λ is larger than the measure of K.*

This theorem does not cover the limiting case where the density of Λ equals the measure of K. In one dimension and in the periodic case, an outstanding theorem by G. Kozma and N. Lev gives an answer. The integral part $[x]$ of a real number x is the largest integer $k \in \mathbb{Z}$ such that $k \leqslant x$. Let $\theta > 1$ be a real number and let us define $\Lambda_\theta \subset \mathbb{Z}$ by $\Lambda_\theta = \{[k\theta], k \in \mathbb{Z}\}$. With these notations, we have [9].

Theorem 4.3. *Let us assume that $\theta > 1$ is irrational. Let $S \subset \mathbb{T}$ be a finite union of intervals J_m, $1 \leqslant m \leqslant M$. We assume that the sum of the lengths of these intervals equals the density θ^{-1} of Λ_θ and that the length of each J_m belongs to $\theta^{-1}\mathbb{Z} + \mathbb{Z}$.*

Then any square summable function f defined on S can be uniquely written as a generalized Fourier series:

$$f(x) = \sum_{\lambda \in \Lambda_\theta} c_\lambda \exp(2\pi \mathrm{i} \lambda x) \tag{6}$$

where the frequencies λ belong to Λ_θ and the coefficients c_λ belong to $l^2(\Lambda_\theta)$. This series converges on f in $L^2(S)$.

This properties would not hold if Λ were replaced by an ordinary lattice. Aliasing then occurs.

5. Quasicrystals and 1-dimensional sequences

In quasicrystalline materials, the atoms are disposed in a way that is neither periodic, as in crystals, nor randomly disordered, as in glasses. Rather atoms follow intermediate patterns. Furthermore, the first quasicrystals described in [10] have a structure similar to the (2-dimensional) Penrose tiling, which is essentially determined by a one-dimensional binary sequence beginning in 0 1 0 0 1 0 1 0 ... and known as the (binary) Fibonacci sequence. It was thus tempting to try and introduce "one-dimensional" quasicrystals as sequences taking their values in a finite set, "similar" to the binary Fibonacci sequence. See Fig. 1.

The first papers with this approach seem to be the paper by Kohmoto, Kadanoff, and Tang [5] and the paper of Östlund, Pandit, Rand, Schellnhuber, Siggia [6]. In these two papers, the authors study a tight-binding Hamiltonian occurring in the discrete Schrödinger equation where the potentials are given by a "quasiperiodic" sequence, i.e., a sequence with "some order in it" (think of a linear chain of masses and springs, where all springs are identical and where the masses are distributed according to some "ordered" sequence). The sequence considered in these two papers was the binary Fibonacci sequence. It happens that this sequence belongs to two distinct families of sequences, making both families interesting in this context: the Sturmian sequences on the one hand, the morphic sequences on the other one. The reader wanting to know more about discrete Schrödinger operators with "quasiperiodic potentials", in particular in the case of Sturmian or morphic—also called *substitutional*—potentials, can begin with the survey paper of Sütő, with its rich list of Refs. [11].

5.1. Sturmian sequences

Sturmian sequences were introduced by Morse and Hedlund in 1940 [12]. They can be defined either as cutting sequences or by an explicit formula (see Definition 5.1 below). Cutting the square grid $\mathbb{Z}^2$ by a straight line with irrational slope gives a sequence of points: define a binary sequence by choosing 0 or 1 according to the nth intersection being on a horizontal line or on a vertical line (we omit technicalities for when the intersection is both on a horizontal line and on a vertical line, which can happen only once since the slope of the straight line is irrational). Of course, cutting the square

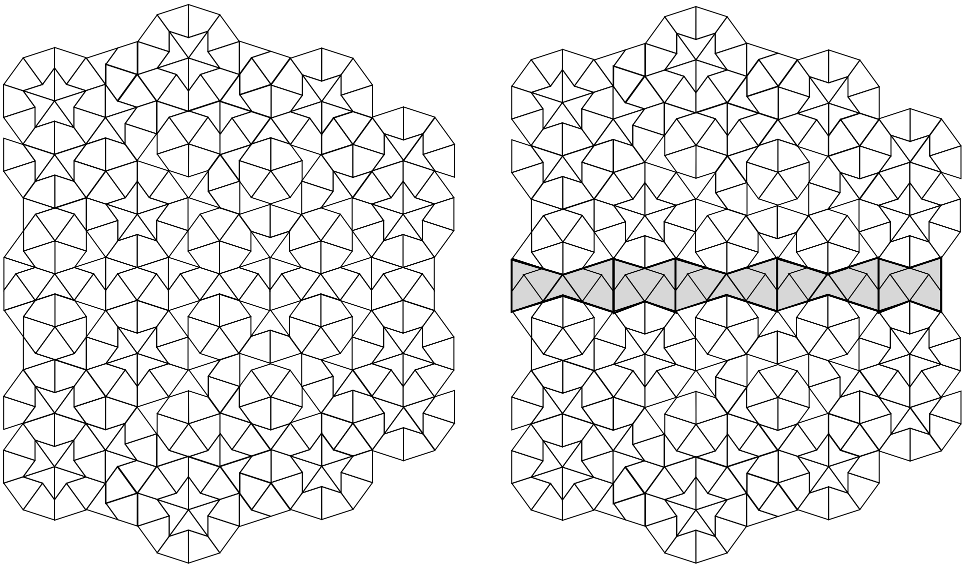

Fig. 1. Representing on this fragment of Penrose tiling the two types of bow ties shaded on the right (long and short) by 0 and 1, one recognizes the beginning of the binary Fibonacci sequence.

grid by a straight line is the same as playing billiard on a square and coding the itinerary of the ball by 0's or 1's if it bounces on a horizontal or on a vertical side of the square (think of folding the grid on its elementary square). These definitions can easily be proven equivalent to the explicit definition below. The reader interested in Sturmian sequences can consult the second chapter of Lothaire's book [13].

Definition 5.1. A sequence $(u_n)_{n\geqslant 0}$ is called *Sturmian* if there exist an irrational number α in $(0,1)$ and a real number ρ such that:

- either for all $n \geqslant 0$, $u_n = \lfloor \alpha(n+1)+\rho \rfloor - \lfloor \alpha n+\rho \rfloor$,
- or for all $n \geqslant 0$, $u_n = \lceil \alpha(n+1)+\rho \rceil - \lceil \alpha n+\rho \rceil$

where $\lfloor x \rfloor$ and $\lceil x \rceil$ stand for the lower integer part (or floor) and the upper integer part (or ceiling) of the real number x.

Taking $\alpha = \rho = (\sqrt{5}-1)/2$ the golden ratio, one obtains the sequence $0\,1\,0\,0\,1\,0\,1\,0\ldots$ known as the (binary) Fibonacci sequence.

Remark 1. Note that, by their definition, Sturmian sequences are binary sequences taking only the values 0 and 1.

What is remarkable is that Sturmian sequences are in some sense the "simplest" nonperiodic sequences. Namely let us define, after Morse and Hedlund [14], the (block-)complexity of a sequence.

Definition 5.2. Let $\mathbf{u} = (u_n)_{n\geqslant 0}$ be a sequence taking finitely many values. The (*block-*)*complexity* of sequence $\mathbf{u}$, denoted by $p_{\mathbf{u}}$, is the function defined on $\mathbb{N}\setminus\{0\}$ by: $p_{\mathbf{u}}(k)$ is the number of distinct blocks of length k occurring in $\mathbf{u}$.

Remark 2. If $\mathbf{u}$ takes r values, then for all $k \geqslant 1$, one has $1 \leqslant p_{\mathbf{u}}(k) \leqslant r^k$. In particular, if $\mathbf{u}$ is "random", one should expect that all possible blocks occur in $\mathbf{u}$, thus the complexity of $\mathbf{u}$ is maximal and equal to r^k. On the other hand, it is not very difficult to prove (see [14]) that a sequence $\mathbf{u}$ such that there exists some $k \geqslant 1$ with $p_{\mathbf{u}}(k) \leqslant k$ **must** be periodic from some index on. In other words, any nonperiodic sequence $\mathbf{u}$ must have $p_{\mathbf{u}}(k) \geqslant k+1$ for all $k \geqslant 1$.

Thus the nonperiodic sequences with minimal complexity would be the sequences for which $p_{\mathbf{u}}(k) = k+1$ for all $k \geqslant 1$, if such sequences exist. Note that these sequences must be binary sequences because $p_{\mathbf{u}}(1) = 2$. The result obtained by Morse and Hedlund [12] and by Coven and Hedlund [15] is that the sequences satisfying $p_{\mathbf{u}}(k) = k+1$ for all $k \geqslant 1$ are *exactly the Sturmian sequences*.

5.2. Morphic sequences; automatic sequences

Another property of the Fibonacci sequence is that it can be generated as follows. Start from 0 and replace repeatedly each 0 by 0 1, and each 1 by 0. This gives

0
0 1
0 1 0
0 1 0 0 1
0 1 0 0 1 0 1 0
0 1 0 0 1 0 1 0 0 1 0 0 1
...

this sequence of "words" on the "alphabet" $\{0, 1\}$ converges to an infinite sequence of 0's and 1's which is exactly the binary Fibonacci sequence. We give some formal definitions.

Definition 5.3. Given a finite set A (also called *alphabet*), the free monoid generated by A, denoted by A^* is the set of all finite sequences (also called *words*)—including the empty sequence—with values in A. The operation that makes A^* a monoid is the *concatenation* of words: it is clearly associative, and the empty word is the unit.

Given two finite sets A and B, a *morphism* σ from A^* to B^* is a homomorphism of monoids from A^* to B^*. It is clearly defined by its values on A. If the words $\sigma(a)$ all have the same length d (i.e., the same number of letters), the morphism σ is said to be *uniform* or more precisely *d-uniform*.

Definition 5.4. Let A be a finite set. Let σ be a morphism from A^* to A^*. Suppose that there exists some $a \in A$ and some word $w \in A^*$ such that $\sigma(a) = aw$ and $\sigma(w) \neq \emptyset$. Then the sequence of words $\sigma^j(a)$ converges to an infinite word denoted by $\sigma^\infty(a)$, which is said to be *an iterative fixed point* of σ.

Remark 3. The topology in Definition 5.4 is the topology of simple convergence, i.e., the product topology on $A^{\mathbb{N}}$, where each copy of A is equipped with the discrete topology. Also σ can be extended by continuity to $A^{\mathbb{N}}$, which shows that $\sigma(\sigma^\infty(a)) = \sigma^\infty(a)$, i.e., that $\sigma^\infty(a)$ is indeed a fixed point of (the extension of) σ.

Example 1. We give two classical examples.

- The Fibonacci sequence: take $A = \{0, 1\}$ and define σ by $\sigma(0) = 0\,1$, $\sigma(1) = 0$. Then it can be proven that the sequence $\sigma^\infty(0) = 0\,1\,0\,0\,1\,0\,1\,0\ldots$ is equal to the Fibonacci sequence (Definition 5.1).
- The Thue–Morse sequence: take $A = \{0, 1\}$ and define σ by $\sigma(0) = 0\,1$, $\sigma(1) = 10$. Then $\sigma^\infty(0) = 0\,1\,1\,0\,1\,0\,0\,1\,1\ldots$ which is called the Thue–Morse (or Prouhet–Thue–Morse) sequence (see, e.g. [16] for a survey of numerous properties of this sequence).

Definition 5.5. Let A and B be two finite sets. Let σ be a morphism from A^* to A^*. Suppose that there exist some $a \in A$ and some word $w \in A^*$ such that $\sigma(a) = aw$ and $\sigma(w) \neq \emptyset$. Let φ be a map from A to B. This map φ can be extended (pointwise) to a map from $A^* \cup A^{\mathbb{N}}$ to $B^* \cup B^{\mathbb{N}}$. The sequence $\varphi(\sigma^\infty(a))$ is said to be *morphic*. If furthermore the morphism σ is d-uniform, the sequence $\varphi(\sigma^\infty(a))$ is said to be *automatic* or more precisely *d-automatic*.

Example 2. The Fibonacci sequence and the Thue–Morse sequence are both morphic (see Example 1, and take $B = A$ and $\varphi = id$). Furthermore the Thue–Morse sequence is 2-automatic.

Note that automatic sequences are, in some sense, easier to deal with than general morphic sequences. The reason is that the nth term of a d-automatic sequence involves the expansion of the integer n in base d. This is also reflected in the number-theoretic properties of automatic sequences. A seminal result in this direction is a theorem due to Christol [17] and Christol, Kamae, Mendès France, and Rauzy [18], which states that a sequence $(a_n)_{n\geqslant 0}$ with values in a finite field $\mathbb{F}_q$ is q-automatic if and only if the formal power series $\sum a_n X^n$ is algebraic over the field $\mathbb{F}_q(X)$. For more about automatic sequences see [19], see also [20].

5.3. Sturmian iterative fixed points of morphisms

In view of the fact that the Fibonacci sequence, playing the role of a toy-model for quasicrystals, is both Sturmian and iterative fixed point of some morphism, one can ask for all sequences having this property. Interestingly enough, the question was answered without reference to or motivation from the theory of quasicrystals. The main result is the following theorem.

Theorem 5.6. *(See [21].) Let $\alpha \in (0, 1)$ and $\rho \in [0, 1)$. Define $\mathbf{u} = (u_n)_{n\geqslant 0}$, with $u_n = \lfloor (n+1)\alpha + \rho \rfloor - \lfloor n\alpha + \rho \rfloor$. Then, the Sturmian sequence $\mathbf{u}$ is an iterative fixed point of a morphism if and only if*

- *α is quadratic, ρ belongs to $\mathbb{Q}(\alpha)$;*

- $\alpha' > 1$, $1 - \alpha' \leqslant \rho' \leqslant \alpha'$ *or* $\alpha' < 0$, $\alpha' \leqslant \rho' \leqslant 1 - \alpha'$

where α' (*resp.* ρ') *stands for the conjugate of* α (*resp.* ρ)*, when these numbers are quadratic.*

Remark 4. A large literature addresses the question of characterizing the iterated fixed points of morphisms that are Sturmian. Yasutomi gave the first complete answer in [21]. Other proofs were given afterwards: let us cite in particular the proof given in [22] that uses *Rauzy fractals* (these fractals with a flavor of number theory are a generalization of a fractal studied by G. Rauzy in [23]).

6. Model sets and morphic sequences

A natural question after having seen quasicrystals as model sets, and having in mind the morphic and automatic sequences as possible toy-models for quasicrystals, is to study model sets that are morphic or automatic. A first idea is to demand that sequences modelling quasicrystals be *repetitive* or even *linearly repetitive*. Note that these terms correspond in the literature of symbolic dynamics to what is called *uniformly recurrent* resp. *linearly uniformly recurrent* sequences. Recall that a sequence is said to be repetitive if for each $k > 0$, there exists an integer $M(k)$ such that any block of length $M(k)$ of the sequence contains at least one copy of every block of length k occurring in the sequence. The sequence is called linearly repetitive if furthermore one can choose $M(k) = O(k)$. These notions are extended to two dimensions in the nice paper by Lagarias and Pleasants [24].

Another idea is, since automatic sequences are easier to generalize to several dimensions than morphic sequences, to try to characterize 2-dimensional model sets that are automatic. Not many papers were devoted to this study. We cite one article by Barbé and von Haeseler [25] giving a necessary and sufficient condition for a 2-dimensional automatic sequence to be Delone. The condition is too technical to be given here. We just note that a 2-dimensional generalization of the Thue–Morse sequence is Delone, while the authors give other examples of automatic sequences that are or are not Delone.

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