Quasicrystals: algebraic, combinatorial and geometrical aspects

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Abstract. The paper presents mathematical models of quasicrystals with particular attention given to cut-and-project sets. We summarize the properties of higher-dimensional quasicrystal models and then focus on the one-dimensional ones. For the description of their properties we use the methods of combinatorics on words.

Keywords. Quasicrystals, cut-and-project set, infinite word, palindrome, substitution

1. Introduction

Crystals have been admired by people since long ago. Their geometrical shape distinguished them from other solids. Rigorous study of crystalline structures started in years 1830–1850 and was crowned around 1890 by famous list of Fedorov and Schoenflies which contained 32 classes of crystals. Their classification was based purely on geometry and algebra. The simplest arrangement, arrangement found in natural crystals, is a simple repetition of a single motive. In mathematics, it is described by the lattice theory, in physics, the subject is studied by crystallography. Repetition of a single motive means periodicity. Another remarkable property, characteristic for crystals, is their rotational symmetry, i.e. invariance under orthogonal linear transformations.

Important consequence of the lattice theory is that neither planar nor space (three-dimensional) periodic structures can reveal rotational symmetry of order 5 or higher than 6, see [27].

The discovery made by Max von Laue in 1912 enabled the study of the atomic structure of crystals via X-ray diffraction patterns and, in fact, justified the theoretical work developed by crystallography before. In case of periodic structures, the type of rotational symmetry of the crystal corresponds to the type of rotational symmetry of the diffraction diagram.

The discovery that rapidly solidified aluminium-manganese alloys has a three-dimensional icosahedral symmetry, made by Shechtmann et al. [28] in 1982, was therefore an enormous surprise for the crystallographic society. The diffraction diagram of

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this alloy revealed five-fold rotational symmetry. Materials with this and other crystallographically forbidden symmetries were later fabricated also by other laboratories by different technologies. They started to be called quasicrystals.

Schechtman’s discovery shows that periodicity is not synonymous with long-range order. The definition of long-range order is however not clear. By this term crystallographers usually understand ordering of atoms in the material necessary to produce a diffraction pattern with sharp bright spots. This is also used in the general definition of crystal adopted by Crystallographic Union at its meeting in 1992.

The only clear requirement agreed upon by all scientists is that the set modeling quasicrystal, i.e. positions of atoms in the material, should be a Delone set. Roughly speaking, this property says that atoms in the quasicrystal should be ’uniformly’ distributed in the space occupied by the material. Formally, the set $\Sigma \subseteq \mathbb{R}^d$ is called Delone if

(i) (uniform discreteness): there exists $r_1 > 0$ such that each ball of radius $r_1$ contains at most one element of $\Sigma$;

(ii) (relative density): there exists $r_2 > 0$ such that each ball of radius $r_2$ contains at least one element of $\Sigma$.

The requirement of the Delone property is however not sufficient, for, also positions of atoms in an amorphous matter form (a section of) a Delone set. Therefore Delone sets modeling quasicrystals must satisfy other properties. According to the type of these additional requirements there exist several approaches to quasicrystal definitions [21, 22]: The concept of Bohr (Besicovich) almost periodic set, is based on Fourier analysis. The second concept of Patterson sets is based on a mathematical analogue of X-ray diffraction, developed by Hof. The third concept, developed by Yves Meyer, is based on restriction on the set $\Sigma - \Sigma$ of interatomic distances. It is elegant and of purely geometric nature: A Meyer set $\Sigma \subseteq \mathbb{R}^d$ is a Delone set having the property that there exists a finite set $F$ such that

$$\Sigma - \Sigma \subseteq \Sigma + F.$$ 

In [21], Lagarias has proven that a Meyer set can equivalently be defined as a Delone set $\Sigma$ such that $\Sigma - \Sigma$ is also Delone.

There exists a general family of sets $\Sigma$ that are known to have quasicrystalline properties: the so-called cut and project sets, here abbreviated to $C&P$ sets. Various subclasses of these sets appear to satisfy all three above quoted definitions of quasicrystals.

The paper is organized as follows: The construction of quasicrystal models by cut and projection is introduced in Section 2 and illustrated on an example of cut-and-project set with 5-fold symmetry in Section 3. The remaining part of the paper focuses on the properties of one-dimensional cut-and-project sets. Section 4 provides their definition Sections 5-7 provide their diverse properties, both geometric and combinatorial.

2. Cut-and-project Sets

The construction of a cut-and-project set ($C&P$ sets) starts with a choice of a full rank lattice: let $x_1, x_2, \ldots, x_d \in \mathbb{R}^d$ be linearly independent vectors over $\mathbb{R}$, the set
is called a lattice. It is obvious that a lattice is a Delone set. Mathematical model for ideal crystal (or perfect crystal) in \( \mathbb{R}^d \) is a set \( \Lambda \), which is formed by a finite number of shifted copies of a single lattice \( L \). Formally, \( \Lambda \) is a perfect crystal if \( \Lambda = L + S \), where \( S \) is a finite set of translations.

Since lattices satisfy \( L - L \subset L \) and a perfect crystal satisfies \( \Lambda - \Lambda \subset \Lambda - S \), they are both Meyer sets. The Meyer concept of quasicrystals thus generalizes the classical definition of crystals. Perfect crystal is however a periodic set, i.e. \( \Lambda + x \subset \Lambda \) for any \( x \in L \), and therefore it is not a suitable model for quasicrystalline materials, which reveal rotational symmetries incompatible with periodicity. We shall now describe a large class of Meyer sets which are not invariant under translation.

Let \( L \) be a full rank lattice in \( \mathbb{R}^d \) and let \( \mathbb{R}^d \) be written as a direct sum \( V_1 \oplus V_2 \) of two subspaces. One of the subspaces, say \( V_1 \), plays the role of the space onto which the lattice \( L \) is projected, we call \( V_1 \) the physical space, the other subspace, \( V_2 \), determines the direction of the projection map. \( V_2 \) is called the inner space. Let us denote by \( \pi_1 \) the projection map on \( V_1 \) along \( V_2 \), and analogically for \( \pi_2 \).

We further require that the full rank lattice is in general position, it means that \( \pi_1 \) is one-to-one when restricted to \( L \), and that the image of the lattice \( L \) under the projection \( \pi_2 \) is a set dense in \( V_2 \). The situation can be diagrammed as follows:

\[
\begin{array}{ccc}
V_1 & \xrightarrow{\pi_1} & \mathbb{R}^d & \xrightarrow{\pi_2} & V_2 \\
\cup & & L & & \\
\end{array}
\]

For the definition of \( C&\)P sets we need also a bounded set \( \Omega \in V_2 \), called acceptance window, which realizes the "cut". The \( C&\)P set is then defined as

\[
\Sigma(\Omega) := \{ \pi_1(x) \mid x \in L \text{ and } \pi_2(x) \in \Omega \}.
\]

A cut-and-project set \( \Sigma(\Omega) \) with acceptance window \( \Omega \) is formed by lattice points projected on \( V_1 \), but only those whose projection on \( V_2 \) belongs to \( \Omega \), i.e. by projections of lattice points found in the cartesian product \( V_1 \times \Omega \).

Figure 1 shows the construction of a \( C&\)P set with one-dimensional physical and one-dimensional inner space. The acceptance window here is an interval in \( V_2 \). And the cylinder \( V_1 \times \Omega \) is a strip in the plane.

Let us list several important properties of \( C&\)P sets:

- \( \Sigma(\Omega) + t \not\subset \Sigma(\Omega) \) for any \( t \in V_1 \), i.e. \( \Sigma(\Omega) \) is not an ideal crystal.
- If the interior \( \Omega^\circ \) of the acceptance window is not empty, then \( \Sigma(\Omega) \) is a Meyer set.
- If \( \Sigma \) is a Meyer set, then there exists a \( C&\)P set \( \Sigma(\Omega) \) with \( \Omega^\circ \neq \emptyset \) and a finite set \( F \) such that \( \Sigma \subset \Sigma(\Omega) + F \).

First two properties can be derived directly from the definition of a \( C&\)P set; the third one has been shown in [22].

The aim of physicists is to find a mechanism which forces atoms in the quasicrystalline matter to occupy given positions. All physical approaches for describing crystals are based on minimum energy argument. If one wants at least to have a chance to find a
physical explanation why a given Delone set is a suitable model for a quasicrystal then the number of various neighborhoods of atoms (of points) in the Delone set must be finite. This requirement is formalized in the notion of finite local complexity: We say that a Delone set $\Sigma$ is of finite local complexity if for any fixed radius $r$ all balls of this radius $r$ contain only finitely many different configurations of points of $\Sigma$ up to translation.

It follows from their definition, that Meyer sets have finite local complexity. Therefore the condition $\Omega^c \neq \emptyset$ ensures that a $C&P$ set $\Sigma(\Omega)$ has finite local complexity.

Another physically reasonable requirement on the model of quasicrystal is that every configuration of points are found in the modeling set infinitely many times. This property may be for example ensured by the requirement that the boundary of the acceptance window has an empty intersection with the image of the lattice by the projection, i.e. $\partial \Omega \cap \pi_2(L) = \emptyset$.

### 3. Cut-and-project Sets with Rotational Symmetry

Recalling the motivation for introducing the notion of quasicrystals, one should ask about conditions ensuring existence of a crystallographically forbidden symmetry. For this, conditions on the acceptance window alone are not sufficient. The construction of a two-dimensional $C&P$ set with 5-fold symmetry has been described by Moody and Patera in [25]. In [6] one can find a more general construction of $C&P$ sets with rotational symmetry of order $2n + 1$, for $n \in \mathbb{N}, n \geq 2$.

Consider the lattice $L \subset \mathbb{R}^4$ to be generated by unit vectors $\alpha_1, \ldots, \alpha_4$ whose mutual position is given by the following diagram.

$$A_4 \equiv \begin{array}{cccc}
\alpha_1 & \alpha_2 & \alpha_3 & \alpha_4
\end{array}$$
In the diagram the vectors connected by an edge make an angle $\pi/3$, otherwise are orthogonal. Such vectors are root vectors of the group which is in physics denoted by $A_4$.

It can be verified that the lattice generated by $\alpha_1, \ldots, \alpha_4$ is invariant under 5-fold rotational symmetry. Let us mention that dimension 4 is the smallest which allows a lattice with such a rotational symmetry.

The physical space $V_1$ and the inner space $V_2$ in our example have both dimension 2, thus they are spanned by two vectors, say $v, u$ and $v^*, u^*$ respectively. We can choose them as unit vectors, such that $u$ and $v$ form an angle $4\pi/5$ and $u^* a v^*$ form an angle $2\pi/5$.

The following scheme shows the definition of the projection $\pi_1$, which is uniquely given if specified on the four basis vectors $\alpha_1, \ldots, \alpha_4$.

The irrational number $\tau$, usually called the golden ratio, is the greater root of the quadratic equation $x^2 = x + 1$. Recall that regular pentagon of side-length 1 has the diagonal of length $\tau$, whence the correspondence of the golden ratio with the construction of a point set having 5-fold rotational symmetry.

The projection $\pi_2$ is defined analogically, substituting vectors $u, v$ in the diagram by $v^*, u^*$, and the scalar factor $\tau$ by $\tau' = \frac{1+\sqrt{5}}{2}$, which is the other root of the quadratic equation $x^2 = x + 1$.

With this choice of projections $\pi_1$ and $\pi_2$, a point of a lattice given by four integer coordinates $(a, b, c, d)$ is projected as

$$
\pi_1(a, b, c, d) = (a + \tau b)v + (c + \tau d)u,
\pi_2(a, b, c, d) = (a + \tau' b)v^* + (c + \tau' d')u^* ,
$$
and the C&P set has the form

$$
\Sigma(\Omega) = \left\{ (a + \tau b)v + (c + \tau d)u \mid a, b, c, d \in \mathbb{Z}, (a + \tau' b)v^* + (c + \tau' d')u^* \in \Omega \right\} .
$$

To complete the definition of the C&P set $\Sigma(\Omega)$ we have to provide the acceptance window $\Omega$. Its choice strongly influences geometrical properties of $\Sigma(\Omega)$. In [12] it is shown that with the above cut-and-project scheme the set $\Sigma(\Omega)$ has 10-fold rotational symmetry if and only if the 10-fold symmetry is displayed by the acceptance window $\Omega$. Figure 3 shows a cut-and-project set $\Sigma(\Omega)$ where $\Omega$ is a disc centered at the origin.

If one studies the inter-atomic interactions, it is impossible to consider contribution of all atoms in the matter; one must limit the consideration to ‘neighbours’ of a given atom. Thus it is necessary to define the notion of neighbourhood in a general point set, which has not a lattice structure. A natural definition of neighbours is given in the notion of a Voronoi cell.

Consider a Delone set $\Sigma \subset \mathbb{R}^d$ and choose a point $x$ in it. The Voronoi cell of $x$ is the set
The Voronoi cell of the point $x$ is thus formed by such part of the space, which is closer to $x$ than to any other point of the set $\Sigma$. Since $\Sigma$ is a Delone set, the Voronoi cells of all points are well defined convex polytopes in $\mathbb{R}^d$, filling this space without thick overlaps. Therefore they form a perfect tiling of the space.

The notion of Voronoi cells allows a natural definition of neighbourhood of points in a Delone set $\Sigma \subset \mathbb{R}^d$. Two points may be claimed neighbours, if their Voronoi polytopes share a face of dimension $d - 1$. The Voronoi tiling of the cut-and-project set $\Sigma(\Omega)$ from Figure 2 is shown on Figure 3.

In the Voronoi tiling of Figure 3 one finds only 6 basic types of tiles (Voronoi polygones). They are all found together with their copies rotated by angles $\frac{\pi}{10}j$, $j = 0, 1, \ldots, 9$.

Let us mention that the Voronoi tiling shown at Figure 4 is aperiodic, since the C&P set $\Sigma(\Omega)$ is aperiodic. For certain classes of acceptance windows with 10-fold rotational symmetry, the collections of appearing Voronoi tiles are described in the series of articles [23].

The geometry of the Voronoi tilings generated by cut-and-project sets is, except several special cases, unknown. The only known fact is that the number of types of tiles is for every cut-and-project set finite, which follows from the finite local complexity of cut-and-project sets. The situation in dimensions $d \geq 2$ is quite complicated. Therefore we focus in the remaining part of the paper on one-dimensional cut-and-project sets.

4. One-dimensional C&P Sets and C&P Words

Let us describe in detail the construction of a one-dimensional C&P set, as illustrated on Figure 1. Consider the lattice $L = \mathbb{Z}^2$ and two distinct straight lines $V_1 : y = \varepsilon x$ and...
V₂ : \( y = \eta x, \varepsilon \neq \eta \). If we choose vectors \( \vec{x}_1 = \frac{1}{\varepsilon - \eta} (1, \varepsilon) \) and \( \vec{x}_2 = \frac{1}{\eta - \varepsilon} (1, \eta) \) then for any point of the lattice \( \mathbb{Z}^2 \) we have

\[
(p, q) = (q - p\eta)\vec{x}_1 + (q - p\varepsilon)\vec{x}_2 .
\]

Let us recall that the construction by cut and projection requires that the projection \( \pi_1 \) restricted to the lattice \( L \) is one-to-one, and that the set \( \pi_2(L) \) is dense in \( V_2 \).

If \( \eta \) and \( \varepsilon \) are irrational numbers, then these conditions are satisfied. The projection of the lattice \( L = \mathbb{Z}^2 \) on the straight lines \( V_1 \) and \( V_2 \) are written using additive abelian groups

\[
\mathbb{Z}[\eta] := \{ a + b\eta \mid a, b \in \mathbb{Z} \},
\]
\[
\mathbb{Z}[\varepsilon] := \{ a + b\varepsilon \mid a, b \in \mathbb{Z} \}.
\]

These groups are obviously isomorphic; the isomorphism \( \ast : \mathbb{Z}[\eta] \rightarrow \mathbb{Z}[\varepsilon] \) is given by the prescription

\[
x = a + b\eta \mapsto x^\ast = a + b\varepsilon .
\]

The cut-and-project scheme can then be illustrated by the following diagram.
Every projected point \( \pi_1(p, q) \) lies in the set \( \mathbb{Z}[\eta]x_1 \). The notation will be simplified by omitting the constant vector \( \bar{x}_1 \). In a similar way, we omit the vector \( \bar{x}_2 \) in writing the projection \( \pi_2(p, q) \). With this convention, one can define a one-dimensional cut-and-project set as follows.

**Definition 1.** Let \( \varepsilon, \eta \) be distinct irrational numbers, and let \( \Omega \subset \mathbb{R} \) be a bounded interval. Then the set

\[
\Sigma_{\varepsilon, \eta}(\Omega) := \{a + b\eta \mid a, b \in \mathbb{Z}, a + b\varepsilon \in \Omega\} = \{x \in \mathbb{Z}[\eta] \mid x^* \in \Omega\}
\]

is called a one-dimensional cut-and-project set with parameters \( \varepsilon, \eta \) and \( \Omega \).

From the properties of general cut-and-project sets, in particular from their finite local complexity, we derive that the distances between adjacent points of \( \Sigma_{\varepsilon, \eta}(\Omega) \) are finitely many. The following theorem [19] limits the number of distances to three.

**Theorem 2.** For every \( \Sigma_{\varepsilon, \eta}(\Omega) \) there exist positive numbers \( \Delta_1, \Delta_2 \in \mathbb{Z}[\eta] \) such that the distances between adjacent points in \( \Sigma_{\varepsilon, \eta}(\Omega) \) take values in \( \{\Delta_1, \Delta_2, \Delta_1 + \Delta_2\} \). The numbers \( \Delta_1, \Delta_2 \) depend only on the parameters \( \varepsilon, \eta \) and on the length \( |\Omega| \) of the interval \( \Omega \).

As the theorem states, the distances \( \Delta_1, \Delta_2 \) and \( \Delta_1 + \Delta_2 \) depend only on the length of the acceptance window \( \Omega \) and not on its position in \( \mathbb{R} \) or on the fact whether \( \Omega \) is open or closed interval. These properties can, however, influence the repetitivity of the set \( \Sigma_{\varepsilon, \eta}(\Omega) \). More precisely, they can cause that the largest or the smallest distance appears in \( \Sigma_{\varepsilon, \eta}(\Omega) \) at one place only.

From the proof of Theorem 2 it follows that if \( \Omega \) semi-closed, then \( \Sigma_{\varepsilon, \eta}(\Omega) \) is repetitive. Therefore in the sequel we consider without loss of generality the interval \( \Omega = [c, c + \ell] \). Nevertheless, let us mention that even if \( \Sigma_{\varepsilon, \eta}([c, c + \ell]) \) is repetitive, the distances between adjacent points may take only two values, both of them appearing infinitely many times.

The knowledge of values \( \Delta_1, \Delta_2 \) allows one to easily determine the neighbours of arbitrary point of the set \( \Sigma_{\varepsilon, \eta}([c, c + \ell]) \) and by that, generate progressively the entire set. Denote \( (x_n)_{n \in \mathbb{Z}} \) an increasing sequence such that \( \{x_n \mid n \in \mathbb{Z}\} = \Sigma_{\varepsilon, \eta}([c, c + \ell]) \). Then for the images of points of the set \( \Sigma_{\varepsilon, \eta}([c, c + \ell]) \) under the mapping \( \star \) one has

\[
x_{n+1}^* = \begin{cases} 
x_n^* + \Delta_1^* & \text{if } x_n^* \in [c, c + \ell - \Delta_1^*] =: \Omega_A, \\
x_n^* + \Delta_1^* + \Delta_2^* & \text{if } x_n^* \in [c + \ell - \Delta_1^*, c - \Delta_2^*] =: \Omega_B, \\
x_n^* + \Delta_2^* & \text{if } x_n^* \in [c - \Delta_2^*, c + \ell] =: \Omega_C.
\end{cases}
\]

The mapping, which to \( x_n^* \) associates the element \( x_{n+1}^* \) is a piecewise linear bijection \( f : [c, c + \ell] \rightarrow [c, c + \ell] \). Its action is illustrated on Figure 5. Such mapping is in the theory of dynamical systems called 3-interval exchange transformation. In case that
\[ \Delta_1^* - \Delta_2^* = |\Omega| = \ell, \text{ the interval denoted by } \Omega_B \text{ is empty. This is the situation when the } \\
\text{distances between adjacent points in } \Sigma_{\varepsilon,\eta}([c, c + \ell]) \text{ take only two values. The mapping } \\
f \text{ is then an exchange of two intervals.} \]

![Figure 5. The diagram illustrating the prescription (1). The function $f$ is a three-interval exchange transformation.](image)

In order to record some finite segment of the set $\Sigma_{\varepsilon,\eta}([c, c + \ell])$, one can write down to a list the individual elements of this set. However, this is not the most efficient way, since every point $x \in \Sigma_{\varepsilon,\eta}([c, c + \ell])$ is of the form $x = a + b\eta \in \mathbb{Z}[\eta]$ and with growing size of the considered segment, the integer coordinates $a, b$, of the points needed for recording $x = a + b\eta$ grow considerably. Much simpler is to find a point $x_0 \in \Sigma_{\varepsilon,\eta}([c, c + \ell])$ in the segment and record the sequence of distances between consecutive points on the left and on the right of $x_0$.

With this in mind, the entire set $\Sigma_{\varepsilon,\eta}([c, c + \ell])$ can be coded by a bidirectional infinite word $(u_n)_{n \in \mathbb{Z}}$ in the alphabet \{A, B, C\} given as

\[
u_n = \begin{cases} 
A & \text{if } x_{n+1} - x_n = \Delta_1, \\
B & \text{if } x_{n+1} - x_n = \Delta_1 + \Delta_2, \\
C & \text{if } x_{n+1} - x_n = \Delta_2.
\end{cases}
\]

Such an infinite word is denoted by $u_{\varepsilon,\eta}(\Omega)$.

**Example 1 (Mechanical words).** Let us choose irrational $\varepsilon \in (-1, 0)$ and irrational $\eta > 0$. We shall consider one-dimensional C&P set with acceptance window $\Omega = (\beta - 1, \beta]$, for some $\beta \in \mathbb{R}$. For simplicity of notation we shall put $\alpha = -\varepsilon \in (0, 1)$. From the definition of C&P sets it follows that

\[ a + b\eta \in \Sigma_{\varepsilon,\eta}(\Omega) \iff a + b\varepsilon \in \Omega \iff \beta - 1 < a - b\alpha \leq \beta \iff a = |b\alpha + \beta| \]

and therefore the C&P set is of the form

\[ \Sigma_{-\alpha,\eta}(\beta - 1, \beta] = \{ |b\alpha + \beta| + b\eta \mid b \in \mathbb{Z} \}. \]

Since $\alpha, \eta > 0$, the sequence $x_n := |n\alpha + \beta| + n\eta$ is strictly increasing and thus the distances between adjacent points of the C&P set $\Sigma_{-\alpha,\eta}(\beta - 1, \beta]$ are of the form

\[ x_{n+1} - x_n = \eta + |(n + 1)\alpha + \beta| - |n\alpha + \beta| = \begin{cases} 
\eta + 1 = \Delta_1, & \text{if } \eta = \Delta_1, \\
\eta = \Delta_2. & \end{cases} \]

(2)
This $C&P$ set can therefore be coded by an infinite word $(u_n)_{n \in \mathbb{Z}}$ in a binary alphabet. Usually one chooses the alphabet $\{0, 1\}$, so that the $n$-th letter of the infinite word can be expressed as

$$u_n = \lfloor (n + 1)\alpha + \beta \rfloor - \lfloor n\alpha + \beta \rfloor .$$

Such infinite words $(u_n)_{n \in \mathbb{Z}}$ were introduced already in [26] and since then, extensively studied, under the name mechanical words. The parameter $\alpha \in (0, 1)$ is called the slope and the parameter $\beta$ the intercept of the mechanical word.

5. Equivalence of One-dimensional $C&P$ Sets

In the previous section we have defined for a triplet of parameters $\varepsilon$, $\eta$ and $\Omega$ the set $\Sigma_{\varepsilon,\eta}(\Omega)$ and we have associated to it the infinite word $u_{\varepsilon,\eta}(\Omega)$. Natural question is how these objects differ for different triplets of parameters. Recall that our construction is based on the projection of the lattice $\mathbb{Z}^2$. The group of linear transformations of this lattice onto itself is known to have three generators:

$$G = \{ \mathbb{A} \in M_2(\mathbb{Z}) \mid \det \mathbb{A} = \pm 1 \} = \langle \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \rangle .$$

Directly from the definition of $C&P$ sets it follows that the action of these three generators on the lattice provides the identities

$$\Sigma_{\varepsilon,\eta}(\Omega) = \Sigma_{1+\varepsilon, 1+\eta}(\Omega) ,$$

$$\Sigma_{\varepsilon,\eta}(\Omega) = \Sigma_{-\varepsilon, -\eta}(-\Omega) ,$$

$$\Sigma_{\varepsilon,\eta}(\Omega) = \eta \Sigma_{\frac{1}{\varepsilon}, \frac{1}{\eta}}(\frac{1}{\varepsilon^2}\Omega) .$$

Another identity for $C&P$ sets is obtained using invariance of the lattice $\mathbb{Z}^2$ under translations.

$$a + b\eta + \Sigma_{\varepsilon,\eta}(\Omega) = \Sigma_{\varepsilon,\eta}(\Omega + a + b\varepsilon) , \quad \text{for any } a, b \in \mathbb{Z} .$$

The mentioned transformations were used in [19] for the proof of the following theorem.

**Theorem 3.** For every irrational numbers $\varepsilon$, $\eta$, $\varepsilon \neq \eta$ and every bounded interval $\Omega$, there exist $\tilde{\varepsilon}$, $\tilde{\eta}$ and an interval $\tilde{\Omega}$ satisfying

$$(P) \quad \tilde{\varepsilon} \in (-1, 0), \quad \tilde{\eta} > 0, \quad \max(1 + \tilde{\varepsilon}, -\tilde{\varepsilon}) < |\tilde{\Omega}| \leq 1$$

such that

$$\Sigma_{\varepsilon,\eta}(\Omega) = s\Sigma_{\tilde{\varepsilon},\tilde{\eta}}(\tilde{\Omega}) , \quad \text{for some } s \in \mathbb{R} .$$
Multiplying the set $\Sigma \tilde{e}, \tilde{\eta}(\tilde{\Omega})$ by a scalar $s$ can be understood as a choice of a different scale. From the physical point of view the sets are therefore de facto the same. In geometry such sets are said to be similar. In the study of one-dimensional $C&P$ sets, one can therefore limit the considerations only to parameters satisfying the condition $(P)$. One may ask whether the family of parameters can be restricted even more. More precisely, one asks whether for different triples of parameters satisfying $(P)$ the corresponding $C&P$ sets are essentially different. The answer to such question is almost always affirmative, except certain, in some sense awkward, cases. A detailed analysis can be found in [19].

Theorem 3 concerned geometrical similarity of $C&P$ sets. If interested only in the corresponding infinite words $u_{\varepsilon, \eta}(\Omega)$, we can restrict the consideration even more. This is a consequence of the following two assertions.

**Claim 1.** If the parameters $\varepsilon, \eta_1, \Omega$ and $\varepsilon, \eta_2, \Omega$ satisfy $(P)$ then the infinite word $u_{\varepsilon, \eta_1}(\Omega)$ coincides with $u_{\varepsilon, \eta_2}(\Omega)$.

Consequently, we can choose the slope of the straight line $V_2$ in the cut-and-project scheme to be $\eta = -\frac{1}{\varepsilon}$, where $\varepsilon$ is the slope of the straight line $V_1$. The straight lines $V_1$ and $V_2$ can therefore be chosen without loss of generality mutually orthogonal.

**Claim 2.** If the parameters $\varepsilon, \eta, \Omega$ satisfy $(P)$ then the infinite word $u_{\varepsilon, \eta}(\Omega)$ coincides with $u_{-1-\varepsilon, \eta}(-\Omega)$ up to permutation of assignment of letters.

This statement implies that for the study of combinatorial properties of infinite words associated with $C&P$ sets, one can limit the choice of the parameter $\varepsilon$ to the range $(-\frac{1}{2}, 0)$.

### 6. Factor and Palindromic Complexity of $C&P$ Words

For the description of combinatorial properties of infinite words associated to one-dimensional $C&P$ sets one uses the terminology and methods of language theory. Consider a finite alphabet $\mathcal{A}$ and a bidirectional infinite word $u = (u_n)_{n \in \mathbb{Z}}$,

$$u = \cdots u_{-2}u_{-1}u_0u_1u_2\cdots .$$

The set of factors of $u$ of the length $n$ is denoted

$$\mathcal{L}_n = \{u_{i}u_{i+1}\cdots u_{i+n-1} \mid i \in \mathbb{Z}\}.$$

The set of all factors of the word $u$ is the **language** of $u$,

$$\mathcal{L} = \bigcup_{n \in \mathbb{N}} \mathcal{L}_n .$$

If any factor occurs in $u$ infinitely many times, then the infinite word $u$ is called **recurrent**. If moreover for every factor the gaps between its individual occurrences in $u$ are bounded, then $u$ is called **uniformly recurrent**.

The factor complexity of the infinite word $u$ is a mapping $C : \mathbb{N} \to \mathbb{N}$ such that
\[ C(n) = \#\{u_i u_{i+1} \cdots u_{i+n-1} \mid i \in \mathbb{Z} \} = \#L_n. \]

The complexity of an infinite word is a measure of ordering in it: for periodic words it is constant, for random words it is equal to \((\#A)^n\).

Since every factor \(u_i u_{i+1} \cdots u_{i+n-1}\) of the infinite word \(u = (u_n)_{n \in \mathbb{Z}}\) has at least one extension \(u_i u_{i+1} \cdots u_{i+n}\), it is clear that \(C(n)\) is a non-decreasing function. If \(C(n) = C(n+1)\) for some \(n\), then every factor of the length \(n\) has a unique extension and therefore the infinite word \(u\) is periodic. The complexity of aperiodic words is necessarily strictly increasing function, which implies \(C(n) \geq n + 1\) for all \(n\). It is known that mechanical words (defined by (3)) with irrational slope are aperiodic words with minimal complexity, i.e. \(C(n) = n + 1\). Such words are called bidirectional sturmian words. A survey of which functions can express the complexity of some infinite word can be found in [16].

The following theorem has been proven in [19] for the infinite words obtained by the cut-and-project construction.

**Theorem 4.** Let \(u_{\varepsilon, \eta}(\Omega)\) be a C&P infinite word with \(\Omega = [c, c+\ell]\).

- If \(\ell \notin \mathbb{Z}[\varepsilon]\), then for any \(n \in \mathbb{N}\) we have \(C(n) = 2n + 1\).
- If \(\ell \in \mathbb{Z}[\varepsilon]\), then for any \(n \in \mathbb{N}\) we have \(C(n) \leq n + \text{const}\).

Moreover, the infinite word \(u_{\varepsilon, \eta}(\Omega)\) is uniformly recurrent.

From the theorem it follows that the complexity of the infinite word \(u_{\varepsilon, \eta}(\Omega)\) depends only on the length \(\ell = |\Omega|\) of the acceptance window and not on its position. This is the consequence of the fact that language of \(u_{\varepsilon, \eta}(\Omega)\) depends only on \(|\Omega|\).

If the parameters \(\varepsilon, \eta\) and \(\Omega = [c, c+\ell]\) satisfy the condition (P), then the complexity of the infinite word \(u_{\varepsilon, \eta}(\Omega)\) is minimal (i.e. \(C(n) = n + 1\)) if and only if \(\ell = 1\). Thus the infinite words \(u_{\varepsilon, \eta}([c, c+1])\) are sturmian words. Nevertheless, the sturmian structure can be found also in words \(u_{\varepsilon, \eta}([c, c+1])\) with \(\ell \in \mathbb{Z}[\varepsilon]\). For, one can prove the following proposition [18].

**Proposition 5.** If \(\ell \in \mathbb{Z}[\varepsilon]\) then there exists a sturmian word \(v = \cdots v_{-2} v_{-1} v_{0} v_{1} v_{2} \cdots\) in \(\{0, 1\}^{2}\) and finite words \(W_0, W_1\) over the alphabet \(\{A, B, C\}\) such that

\[ u_{\varepsilon, \eta}(\Omega) = \cdots W_{v_{-2}} W_{v_{-1}} W_{v_{0}} W_{v_{1}} W_{v_{2}} \cdots. \]

The proposition in fact states that the infinite word \(u_{\varepsilon, \eta}(\Omega)\) can be obtained by concatenation of words \(W_0, W_1\) in the order of 0’s and 1’s in the sturmian word \(v\). Let us mention that Cassaigne [11] has shown a similar statement for arbitrary one-directional infinite words with complexity \(n + \text{const}\). He calls such words quasisturmian.

A reasonable model of quasicrystalline material cannot distinguish between the ordering of neighbours on the right and on the left of a chosen atom. In terms of the infinite word, which codes the one-dimensional model of quasicrystal, it means that the language \(\mathcal{L}\) must contain, together with every factor \(w = w_1 w_2 \cdots w_n\) also its mirror image \(\overline{w} = w_n w_{n-1} \cdots w_1\). The language of C&P words satisfies such requirement.

A factor \(w\), which satisfies \(w = \overline{w}\), is called a palindrome, just as it is in natural languages. The study of palindromes in infinite words has a great importance for describing the spectral properties of one-dimensional Schrödinger operator, which is as-
sociated to \((u_n)_{n \in \mathbb{Z}}\) in the following way: To every letter of the alphabet \(a \in A\) one associates the potential \(V(a)\) in such a way that the mapping \(V : A \rightarrow \mathbb{R}\) is injective. The one-dimensional Schrödinger operator \(H\) is then defined as

\[(H\phi)(n) = \phi(n+1) + \phi(n-1) + V(u_n)\phi(n), \quad \phi \in l^2(\mathbb{Z}).\]

The spectral properties of \(H\) influence the conductivity properties of the given structure. Roughly speaking, if the spectrum is absolutely continuous, then the structure behaves like a conductor, while in the case of pure point spectrum, it behaves like an insulator. In [20] one shows the connection between the spectrum of \(H\) and the existence of infinitely many palindromes in the word \((u_n)_{n \in \mathbb{Z}}\).

The function that counts the number of palindromes of a given length in the language \(L\) of an infinite word \(u\) is called the palindromic complexity of \(u\). Formally, the palindromic complexity of \(u\) is a mapping \(P : \mathbb{N} \rightarrow \mathbb{N}\) defined by

\[P(n) := \# \{ w \in L_n \mid w = \overline{w} \}.\]

Upper estimates on the number \(P(n)\) of palindromes of length \(n\) in an infinite word \(u\) can be obtained using the factor complexity \(C(n)\) of \(u\). In [3] the authors prove a result which puts in relation between the factor complexity \(C(n)\) and the palindromic complexity \(P(n)\). For a non-periodic infinite word \(u\) it holds that

\[P(n) \leq \frac{16}{n} C \left( n + \left\lfloor \frac{n}{4} \right\rfloor \right).\]  \((4)\)

Combination of the above estimate with the knowledge of the factor complexity we obtain for \(C\&P\) infinite words that \(P(n) \leq 48\).

Infinite words constructed by cut and projection are uniformly recurrent. For such words, the upper estimate of the palindromic complexity can be improved, using the observation that uniformly recurrent words have either \(P(n) = 0\) for sufficiently large \(n\), or the language \(L\) of the infinite word is invariant under the mirror image, see [5]. If \(L\) contains with every factor \(w\) its mirror image \(\overline{w}\), then

\[P(n) + P(n+1) \leq 3\Delta C(n) := 3 \left( C(n+1) - C(n) \right).\]  \((5)\)

This estimate of the palindromic complexity is better than that of \((4)\) in case that the factor complexity \(C(n)\) is subpolynomial. In particular, for \(C\&P\) infinite words we obtain \(P(n) \leq 6\). In [14] one can find the exact value of the palindromic complexity for infinite words coding three-interval exchange transformation. Since this is the case of \(C\&P\) words, we have the following theorem.

**Theorem 6.** Let \(u_{\varepsilon,\eta}(\Omega)\) be a \(C\&P\) infinite word with \(\Omega = [c, c + \ell]\) and let \(\varepsilon, \eta, \Omega\) satisfy the conditions \((P)\). Then

\[P(n) = \begin{cases} 1 & \text{for } n \text{ even}, \\ 2 & \text{for } n \text{ odd and } \ell = 1, \\ 3 & \text{for } n \text{ odd and } \ell < 1. \end{cases}\]
7. Substitution Invariance of C&P Words

To generate the set \( \Sigma_{\xi, \eta}(\Omega) \) using the definition resumes in deciding for every point of the form \( a + b\eta \), whether \( a + b\varepsilon \) belongs to the interval \( \Omega \) or not. This is done by verifying certain inequalities between irrational numbers. If we use a computer working with finite precision arithmetics, the rounding errors take place and in fact, the computer generates a periodic set, instead of aperiodic \( \Sigma_{\xi, \eta}(\Omega) \). The following example gives a hint to much more efficient and in the same time exact generation of a C&P set.

Consider the most popular one-dimensional cut-and-project set, namely the Fibonacci chain. It is a C&P set with parameters \( \eta = \tau, \varepsilon = \tau' \) and \( \Omega = [0, 1) \). (Recall that the golden ratio \( \tau = \frac{1+\sqrt{5}}{2} \) and \( \tau' = \frac{1-\sqrt{5}}{2} \) are the roots of the equation \( x^2 = x + 1 \).)

Since \( \tau^2 = \tau + 1 \), the set of all integer combinations of 1 and \( \tau \) is the same as the set of all integer combinations of \( \tau^2 \) and \( \tau \), formally

\[
\tau \mathbb{Z}[\tau] = \mathbb{Z}[\tau].
\]

Moreover, \( \mathbb{Z}[\tau] \) is closed under multiplication, i.e. \( \mathbb{Z}[\tau] \) is a ring. Since \( \tau + \tau' = 1 \), we have also \( \mathbb{Z}[\tau] = \mathbb{Z}[\tau'] \), and the mapping \( \ast \) which maps \( a + b\tau \mapsto a + b\tau' \) is in fact an automorphism on the ring \( \mathbb{Z}[\tau] \). Note that \( \mathbb{Z}[\tau] \) is the ring of integers in the field \( \mathbb{Q}[\tau] \) and \( \ast \) is the restriction of the Galois automorphism of this field.

Using the mentioned properties one can derive directly from the definition of C&P sets that

\[
\tau^2 \Sigma_{\tau', \tau}(\Omega) = \Sigma_{\tau', \tau'}((\tau')^2 \Omega),
\]

which is valid for every acceptance window \( \Omega \). In the case \( \Omega = [0, 1) \) we moreover have \( (\tau')^2 \Omega \subset \Omega \). Therefore

\[
\tau^2 \Sigma_{\tau', \tau}(\Omega) \subset \Sigma_{\tau', \tau}(\Omega),
\]

i.e. \( \Sigma_{\tau', \tau}(\Omega) \) is selfsimilar with the scaling factor \( \tau^2 \), as illustrated on Figure 6.

Example 1 namely equation (2) implies that \( \Sigma_{\tau', \tau}(\Omega) \) has two types of distances between adjacent points, namely \( \Delta_1 = \tau^2 \) and \( \Delta_2 = \tau \). In Figure 6 the distance \( \Delta_1 \) is coded by the letter \( A \) and the distance \( \Delta_2 \) by the letter \( B \).

For our considerations it is important that every distance \( A \) scaled by the factor \( \tau^2 \) is filled by two distances \( A \) followed by \( B \). Similarly, every scaled distance \( B \) is filled by \( A \) followed by \( B \). This property can be proven from the definition of \( \Sigma_{\tau', \tau}(\Omega) \).

As a consequence, the Fibonacci chain can be generated by taking an initial segment of the set, scaling it by \( \tau^2 \) and filling the gaps by new points in the above described way, symbolically written as the rule

\[
A \mapsto AAB \quad \text{and} \quad B \mapsto AB.
\]

Repeating this, one obtains step by step the entire C&P set. Since the origin 0 as an element of \( \Sigma_{\tau', \tau}(\Omega) \) has its left neighbour in the distance \( \Delta_2 \) and the right neighbour in the distance \( \Delta_1 \), we can generate the Fibonacci chain symbolically as

\[
B|A \mapsto AB|AAB \mapsto AABAB|AABAABAB \mapsto \ldots
\]
A natural question arises, whether such efficient and exact generation is possible also for other one-dimensional cut-and-project sets, respectively their infinite words. Let us introduce several notions which allow us to formalize this question.

A mapping \( \varphi \) on the set of finite words over the alphabet \( \mathcal{A} \) is a morphism, if the \( \varphi \)-image of a concatenation of two words is concatenation of the \( \varphi \)-images of the individual words, i.e., \( \varphi(vw) = \varphi(v)\varphi(w) \) for every pair of words \( v, w \) over the alphabet \( \mathcal{A} \). For the determination of a morphism, it suffices to specify the \( \varphi \)-images of the letters of the alphabet. The action of a morphism can be naturally extended to infinite words,

\[
\varphi(u) = \varphi(u_{-2}u_{-1}|u_0u_1u_2u_3\ldots) := \ldots \varphi(u_{-2})\varphi(u_{-1})|\varphi(u_1)\varphi(u_2)\varphi(u_3)\ldots
\]

An infinite word \( u \) invariant under the action of the morphism, i.e., which satisfies \( \varphi(u) = u \), is called a fixed point of \( \varphi \). In this terminology, one can say that the Fibonacci chain (or the infinite word coding it) is a fixed point of the morphism \( \varphi \) over a two-letter alphabet \( \{A, B\} \), which is determined by the images of letters, \( \varphi(A) = AAB \), \( \varphi(B) = AB \).

The identity map, which maps every letter of the alphabet on itself, is also a morphism and arbitrary infinite word is its fixed point. However, one cannot use the identity map for generation of infinite words. Therefore we must put additional requirements on the morphism \( \varphi \).

The morphism \( \varphi \) over the alphabet \( \mathcal{A} \) is called a substitution, if for every letter \( a \in \mathcal{A} \) the length of the associated word \( \varphi(a) \) is at least 1, and if there exist letters \( a_0, b_0 \in \mathcal{A} \) such that the words \( \varphi(a_0) \) and \( \varphi(b_0) \) have length at least 2, the word \( \varphi(a_0) \) starts with the letter \( a_0 \), and the word \( \varphi(b_0) \) ends with the letter \( b_0 \).

A morphism, which is in the same time a substitution, necessarily has a fixed point \( u \), which can be generated by repeated application of the morphism on the pair of letters \( b_0|a_0 \). Formally,

\[
\varphi(u) = u = \lim_{n\to\infty} \varphi^n(b_0)|\varphi^n(a_0).
\]

To every substitution \( \varphi \) over the alphabet \( \mathcal{A} = \{a_1, a_2, \ldots, a_k\} \) one associates a \( k \times k \) square matrix \( M \) (the so-called \textit{incidence matrix} of the substitution). The element

\[
\begin{align*}
&\begin{array}{c}
\text{A} \quad \text{A} \quad \text{B} \\
\text{A} \quad \text{B} \quad \text{A} \\
\text{B} \quad \text{A} \quad \text{B}
\end{array} \\
&\begin{array}{c}
\tau^2\Delta_2 \\
0 \\
\tau^2\Delta_1
\end{array}
\end{align*}
\]
$M_{ij}$ is given as the number of letters $a_j$ in the word $\varphi(a_i)$. The incidence matrix of the substitution generating the Fibonacci word is $M = \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix}$.

The incidence matrix of a substitution is by definition a non-negative matrix for which Perron-Frobenius theorem holds \cite{17}. A substitution $\varphi$ is said primitive, if some power of its incidence matrix is positive. In this case the spectral radius of the matrix is an eigenvalue with multiplicity 1, the corresponding eigenvector (the so-called Perron eigenvector of the matrix) being also positive.

Although the incidence matrix $M$ does not allow to reconstruct the substitution $\varphi$, many properties of the fixed points of $\varphi$ can be derived from it. Let us mention some of them.

- If the infinite word $u$ is invariant under a substitution, then there exists a constant $K$ such that for the complexity function of the word $u$ we have
  \[ C(n) \leq Kn^2 \quad \text{for all } n \in \mathbb{N}. \]

- If the infinite word $u$ is invariant under a primitive substitution, then there exist constants $K_1$ and $K_2$ such that for the factor complexity and palindromic complexity of the word $u$ we have
  \[ C(n) \leq K_1 n \quad \text{and} \quad P(n) \leq K_2 \quad \text{for all } n \in \mathbb{N}. \]

- An infinite word which is invariant under a primitive substitution is uniformly recurrent.

- If the infinite word $u$ is invariant under a primitive substitution $\varphi$ over an alphabet $\mathcal{A} = \{ a_1, a_2, \ldots, a_k \}$, then every letter $a_i$ has well defined density in $u$, i.e. the limit
  \[ \rho(a_i) := \lim_{n \to \infty} \frac{\text{number of letters } a_i \text{ in the word } u_{-n} \ldots u_{-1} | u_0 u_1 \ldots u_{n-1}}{2n + 1} \]
  exists. Let $(x_1, x_2, \ldots, x_k)$ be the Perron eigenvector of the matrix $M^T$ (transpose of the incidence matrix $M$ of the substitution $\varphi$). Then the density $\rho(a_i)$ is equal to
  \[ \rho(a_i) = \frac{x_i}{x_1 + x_2 + \ldots + x_k}. \]

The question of describing all $CkP$ infinite words invariant under a substitution is still unsolved. A complete solution is known only for $CkP$ words over a binary alphabet, which can be, without loss of generality, represented by mechanical words \cite{1} with irrational slope $\alpha \in (0, 1)$ and intercept $\beta \in [0, 1)$.

The substitution invariance of mechanical words has first been solved in \cite{13} for the so-called homogeneous mechanical words, i.e. such that $\beta = 0$.

**Theorem 7.** The homogeneous mechanical word with slope $\alpha \in (0, 1)$ is invariant under a substitution if and only if $\alpha$ is a quadratic irrational number whose conjugate $\alpha'$ does not belong to $(0, 1)$.
A quadratic irrational number \( \alpha \in (0, 1) \) whose conjugate \( \alpha' \notin (0, 1) \) is called **Sturm number**. Let us mention that in the paper [13] the Sturm number is defined using its continued fraction expansion. The simple algebraic characterization was given in [2].

The substitution invariance for general (inhomogeneous) mechanical words is solved in [4] and [29].

**Theorem 8.** Let \( \alpha \) be an irrational number, \( \alpha \in (0, 1) \), and let \( \beta \in [0, 1) \). The mechanical word with slope \( \alpha \) and intercept \( \beta \) is invariant under a substitution if and only if the following three conditions are satisfied:

(i) \( \alpha \) is a Sturm number,

(ii) \( \beta \in \mathbb{Q}[\alpha] \),

(iii) \( \alpha' \leq \beta' \leq 1 - \alpha' \) or \( 1 - \alpha' \leq \beta' \leq \alpha' \), where \( \beta' \) is the image of \( \beta \) under the Galois automorphism of the field \( \mathbb{Q}[\alpha] \).

Unlike the case of binary C&P words, the question of substitution invariance for ternary C&P words has been so far solved only partially. The following result is the consequence of [1,9].

**Theorem 9.** Let \( \Omega = [c, d) \) be a bounded interval. If the infinite word \( u_{\varepsilon, \eta}(\Omega) \) is invariant under a primitive substitution, then \( \varepsilon \) is a quadratic irrational number and the boundary points \( c, d \) of the interval \( \Omega \) belong to the quadratic field \( \mathbb{Q}(\varepsilon) \).

All C&P words satisfying the properties of the theorem have a weaker property than substitution invariance, the so-called substitutivity [15]. It allows one to generate even those infinite words which are not fixed points of a morphism.

8. Conclusions

In the theory of mathematical quasicrystals, best known are the properties of the one-dimensional models, be it the geometric or the combinatorial aspects of these structures. However, this information can be used also in the study of higher dimensional models, since the one-dimensional ones are embedded in them. In fact, every straight line containing at least two points of a higher-dimensional cut-and-project set, contains infinitely many of them, and they ordering is a one-dimensional cut-and-project sequence.

Nevertheless, the notions of combinatorics on words, as they were presented here, are being generalized also to higher dimensional structures; for example, one speaks about complexity and substitution invariance of two-dimensional infinite words, even two-dimensional sturmian words are well defined [18].

Except cut-and-project sets, there are other aperiodic structures which can serve for quasicrystal models; they are based on non-standard numeration systems [10]. The set of numbers with integer \( \beta \)-expansions share many properties required from one-dimensional quasicrystal models, in particular, they are Meyer sets, are self-similar, and the corresponding infinite words are substitution invariant.

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