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1998 J. Phys. A: Math. Gen. 31 L331

(http://iopscience.iop.org/0305-4470/31/18/001)

J. Phys. A: Math. Gen. **31** (1998) L331–L336. Printed in the UK PII: S0305-4470(98)91391-9

LETTER TO THE EDITOR

On the canonical projection method for one-dimensional quasicrystals and invertible substitution rules

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Received 5 February 1998

Abstract. We show that if a quasiperiodic two-symbol sequence obtained by the canonical projection method has an infinite number of predecessors with respect to a substitution rule σ, then σ is an invertible substitution rule. *Vice versa*, we show that every quasiperiodic two-symbol sequence that has an infinite number of predecessors with respect to a non-trivial invertible substitution rule can be obtained by the canonical projection method.

1. Introduction and summary

There are several methods currently known by which one-dimensional quasiperiodic sequences of two symbols can be generated, cf for example Senechal [10, 11]. However, the relationship between these different methods has not received much attention. This letter aims to clarify the situation by explicitly pointing out the equivalence between quasiperiodic two-symbol sequences obtained by the canonical projection method and quasiperiodic two-symbol sequences that have an infinite number of predecessors with respect to an invertible substitution rule. The main result is stated in theorem 1.4.

The most celebrated method for constructing quasiperiodic two-symbol sequences is certainly the *canonical projection* method. In this method, one considers the intersection of the standard lattice $\mathbb{Z}^2$ with the strip $V + \mathcal{E}$, where V is a square 1×1 unit cell and $\mathcal{E}$ is a linear subspace of $\mathbb{R}^2$ (without loss of generality, we will assume here always that the slope of $\mathcal{E}$ is positive). A two-symbol sequence can be obtained from the orthogonal projection of the subset $\mathbb{Z}^2 \cap (V + \mathcal{E})$ of $\mathbb{Z}^2$ to $\mathcal{E}$. In the case when the boundary of $V + \mathcal{E}$ has no intersections with $\mathbb{Z}^2$ (regular case), then this tiling contains only two types of tiles. Assigning symbols a and b to these tiles produces a bi-infinite sequence of a's and b's. The remaining singular cases may be interpreted as two-symbol sequences obtained as limit points of regular sequences, cf [6].

Another popular approach towards quasicrystal sequences uses substitution rules. A substitution rule defines a procedure of replacing the symbols in a sequence.

We say that a sequence S' is a predecessor of a sequence S with respect to the substitution rule σ if $\sigma S' = S$. Certain types of quasicrystal sequences are characterized by the fact that they have an infinite number of predecessors with respect to a substitution rule. We will call such sequences *substitution sequences*, cf definition 1.3. In this approach we follow De Bruijn [3, 4] and Senechal [12].

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A well known example of a substitution rule is the *Fibonacci substitution* rule τ. It is defined on a two-symbol alphabet $A = \{a, b\}$ as

$$\tau : \begin{cases} a \to ab \\ b \to a. \end{cases} \quad (1)$$

In short notation, we will write $\tau(a, b) = (ab, a)$.

Bi-infinite two-symbol sequences that have an infinite number of predecessors with respect to τ are known as *Fibonacci sequences*. The Fibonacci sequences form a local isomorphism class, i.e. any finite subsequence of a Fibonacci sequence occurs in every other Fibonacci sequence. In general, whenever S is a Fibonacci sequence, $\tau S = S'$ is also a Fibonacci sequence (but S and S' need not be the same)†.

We now give definitions of what we call a two-symbol sequence and a *substitution sequence*.

Definition 1.1. We say that $S : \mathbb{Z} \to \{a, b\}$ is a bi-infinite *two-symbol* sequence, if there exist $n, m \in \mathbb{Z}$ such that $S[n] = a$ and $S[m] = b$.

Definition 1.2. A bi-infinite two-symbol sequence S is called a substitution sequence whenever there exists a non-trivial substitution rule σ so that S has an infinite number of predecessors with respect to σ, i.e. if for all $n \in \mathbb{Z}^+$ there exists a sequence $S^{(n)}$ such that $\sigma^n S^{(n)} = S$. A substitution rule σ over $\{a, b\}$ is non-trivial whenever σ is not equal to the identity substitution $1(a, b) = (a, b)$ or to the twofold substitution $\chi(a, b) = (b, a)$‡.

De Bruijn [3, 4] discussed certain explicit examples of substitution sequences that can be obtained by the canonical projection method. Among the examples he discussed are Fibonacci sequences: when the slope of the line $\mathcal{E}$ is exactly the golden mean $(1 + \sqrt{5})/2$, the two-symbol sequence describing the canonical projection tiling is a Fibonacci sequence.

However, Luck *et al* [5] have given examples of substitution sequences that are not canonical projection sequences.

These observations naturally lead to the following questions:

(A) Which substitution sequences can be obtained by the canonical projection method?

(B) Which canonical projection sequences are substitution sequences?

Wen *et al* [15] conjectured that a σ-self-similar two-symbol sequence can be obtained by the canonical projection method if and only if the corresponding substitution rule σ is *invertible*. The notion of invertibility used in this context is defined in relation to the free group $F_2(a, b)$. $F_2(a, b)$ consists of all sequences of a's, b's *and* their 'inverses' a^{-1} and b^{-1}. Here, $aa^{-1} = bb^{-1} = e$, the *empty* sequence. In this context, an invertible substitution rule can be interpreted as an automorphism of the free group F_2.

Definition 1.3. A substitution rule σ on two-symbol sequences is called *invertible* if σ has an inverse σ^{-1}, i.e. if $\sigma \in \mathrm{Aut}(F_2)$.

The Fibonacci substitution rule $\tau(a, b) = (ab, a)$ is invertible. Namely, $\tau^{-1}(a, b) = (b, b^{-1}a)$, and it is readily verified that indeed $\tau \circ \tau^{-1}(a, b) = (a, b)$§.

We now need one more definition before we can state our main result.

† We say that two sequences are the same whenever they are shift-equivalent: two bi-infinite sequences S and S' are shift-equivalent when there exists an $m \in \mathbb{Z}$ such that $S[n] = S'[n + m]$ for all $n \in \mathbb{Z}$.

‡ Note that every bi-infinite two-symbol sequence over $\{a, b\}$ has an infinite number of predecessors with respect to the substitutions 1 and χ.

§ Although the inverse of a substitution rule may involve inverse symbols, it should be noted that in our context substitution rules are not allowed to involve inverse symbols.

Definition 1.4. $\mu > 1$ is a *reduced quadratic irrational* when μ is a root of a quadratic equation with integer coefficients and its conjugate μ' (the other root of this equation) satisfies $-1 < \mu' < 0$.

Finally, we call a canonical projection sequence quasiperiodic when the slope of $\mathcal{E}$ is irrational (and not equal to ∞ or 0).

The main result of this letter is the following theorem establishing the intimate relationship between quasiperiodic two-symbol sequences obtained by the canonical projection method and two-symbol sequences generated by invertible substitution rules. It answers the questions (A) and (B) posed above.

Theorem 1.5. Let S be a bi-infinite two-symbol sequence. Then,

(i) if S is a quasiperiodic canonical projection sequence *and* a substitution sequence for a substitution rule σ, then σ is an invertible substitution rule;

(ii) if S is a substitution sequence for an invertible substitution rule, then S is non-periodic and can be obtained by the canonical projection method;

(iii) if S is a quasiperiodic canonical projection sequence, then S is a substitution sequence if and only if the slope μ of $\mathcal{E}$—or μ^{-1} (if $0 < \mu < 1$)—is a reduced quadratic irrational.

Our proof of this theorem will rely on earlier results of Series [13], Lunnon and Pleasants [6], Wen and Wen [14], and Séébold [10], and will be discussed in section 2†.

We now proceed with a discussion of the implications of theorem 1.5.

Theorem 1.5 settles a question raised by Luck *et al* [5] in a study of the *atomic surfaces* of two-symbol chains generated by substitution rules. Different types of *atomic surfaces* were observed, ranging from one closed interval to fractal-shaped atomic surfaces. However, the question on which property of the substitution rule decides the type of atomic surface was left unanswered. If the two-symbol chain is defined as the orthogonal projection to a linear subspace $\mathcal{E}$ in $\mathbb{R}^2$ of points in $\mathbb{Z}^2$ representing the chain as a monotonic walk in $\mathbb{Z}^2$, then the *atomic surface* is the orthogonal projection of the subset of $\mathbb{Z}^2$ to the orthogonal complement $\mathcal{E}^\perp$ of $\mathcal{E}$. (For a more careful definition, see [5].) We now note that the atomic surface of a substitution chain consists of precisely one closed interval if and only if the substitution chain can be obtained by the canonical projection method. Hence, we find:

Corollary 1.6. Let S be a bi-infinite two-symbol substitution sequence for a substitution rule σ. Then the atomic surface of this sequence consists of precisely one closed interval if and only if σ is an invertible substitution rule.

Indeed, the examples given in [5] nicely illustrate the conclusion of theorem 1.5 (and corollary 1.6).

Bombieri and Taylor [2] found that if a substitution rule on two symbols possess the so-called *Pisot property* (satisfied by non-trivial invertible substitution rules, the substitution sequence can be obtained as the subset of a sequence obtained by some projection method involving the orthogonal projection of a subset of the intersection of $\mathbb{Z}^2$ with a strip in $\mathbb{R}^2$. From corollary 1.6 it follows that the projection method of Bombieri and Taylor is precisely the canonical projection method if and only if the substitution rule is invertible.

† It should be noted that some of these papers deal with the setting of infinite, rather than bi-infinite two-symbol symbol sequences. However, the ingredients we need here do not crucially depend on whether the sequences are infinite or bi-infinite.

The link provided by theorem 1.5 will be useful in the study of physical properties of one-dimensional canonical projection quasicrystals. In particular, in the context of trace maps related to discrete Schrödinger equations on two-symbol substitution chains, it has become clear that the invertible substitution rules form a subclass of all substitution rules that possess very particular properties [7, 8, 14]. It was mainly in this context that the result of theorem 1.5 was anticipated in [15].

It remains an important open problem to understand the general relationship between substitution rules and the canonical projection method in constructing bi-infinite symbol sequences of more than two symbols and two- and three-dimensional quasicrystal tilings.

2. Proof of theorem 1.5

Every bi-infinite two-symbol sequence S that is constructed by the canonical projection method can also be obtained by recording where the boundary of $V + \mathcal{E}$ intersects the lines $x \in \mathbb{Z}$ and $y \in \mathbb{Z}$ and assigning symbols a and b to the respective intersection points. A sequence obtained by the latter construction was called a *cutting sequence* by Series [13]. Lunnon and Pleasants [6] proved the following equivalence.

Theorem 2.1. ([6].) Let S be a bi-infinite two-symbol sequence. Then S is a cutting sequence if and only if S is a characteristic sequence.

In order to appreciate this result, we need the definition of a characteristic sequence.

Definition 2.2. (Characteristic sequence.) A bi-infinite two-symbol (a, b) sequence S is called *characteristic*, if it can be reduced in a unique way into a sequence of predecessors with respect to the substitution rules $\alpha(a, b) = (a, ab)$ and $\beta(a, b) = (ba, b)$.

With each characteristic sequence there is associated an infinite sequence of the following operations:

$\bar{\alpha} = a$-reduction: remove every a preceding each b;

$\bar{\beta} = b$-reduction: remove every b preceding each a.

We call $\bar{\alpha}$ and $\bar{\beta}$ the *composition rules* associated with the substitution rules α and β. The sequence of compositions $\bar{\alpha}$ and $\bar{\beta}$ is completely determined because at one time a characteristic sequence has either no consecutive b's or no consecutive a's. We refer to [6] for details of the proofs.

Importantly, the substitution rules α and β used to define reduction processes for characteristic sequences are invertible. Namely,

$$\alpha^{-1}(a, b) = (a, a^{-1}b) \qquad \beta^{-1}(a, b) = (b^{-1}a, b).$$

Wen and Wen [14] proved that every invertible substitution σ can be written as the composition of a finite number of the simple invertible substitutions

$$\phi(a, b) = (a, ab) \qquad \psi(a, b) = (a, ba) \qquad \chi(a, b) = (b, a). \tag{2}$$

We see that $\alpha = \phi$ and $\beta = \chi \circ \phi \circ \chi$. In the reduction process for characteristic sequences we thus only use ϕ and χ.

We will now proceed to show that substitution sequences for invertible substitution rules are characteristic.

Lemma 2.3. Let S be a bi-infinite quasiperiodic two-symbol sequence that is obtained by the canonical projection method. Then if S is a substitution sequence, the slope μ of $\mathcal{E}$—or μ^{-1} if $0 < \mu < 1$—is a reduced quadratic irrational, and S has an infinite number of predecessors with respect to an invertible substitution rule.

Proof. We first recall that when a quasiperiodic canonical projection sequence has an infinite number of predecessors with respect to a substitution rule, then $\mathcal{E}$ must be an eigenspace of the substitution matrix M associated with the substitution rule, which is a 2×2 matrix with non-negative integer entries and determinant ± 1 [5].

Series [13] has pointed out that the reduction process associated with a cutting sequence of a line $\mathcal{E}$ in terms of compositions $\bar{\alpha}$ and χ corresponds to a linear geometric algorithm for calculating the continued fraction of the slope of $\mathcal{E}$, involving the linear transformation induced by the substitution matrices of ϕ and χ:

$$\Phi = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} \qquad \text{and} \qquad \mathcal{X} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

Importantly, Wen and Wen [14] showed that every matrix M with determinant ± 1 and non-negative integer entries can be decomposed as a product of Φ's and $\mathcal{X}$'s.

Hence, invariance of $\mathcal{E}$ with respect to M implies that the slope μ of $\mathcal{E}$ (or its inverse) must have a purely periodic continued fraction expansion (which is equivalent to saying that μ (or μ^{-1}) is a reduced quadratic irrational [7]) and that the cutting sequence is a substitution sequence for an invertible substitution rule (composition of ϕ's and χ's). □

Lemma 2.4. S is a quasiperiodic cutting sequence that has an infinite number of predecessors with respect to the invertible substitution $\sigma = \gamma_n \circ \cdots \circ \gamma_0$, with $\gamma_i \in \{\phi, \chi\}$ if and only if S has an infinite number of predecessors with respect to the invertible substitution rules $\sigma' = \gamma'_n \circ \cdots \circ \gamma'_0$, where $\gamma'_i \in \{\phi, \psi\}$ when $\gamma_i = \phi$, and $\gamma'_i = \chi$ when $\gamma_i = \chi$.

Proof. We sketch the main idea. Every quasiperiodic two-symbol cutting sequence S is a so-called *two-distance sequence* and consists of consecutive blocks of the form ba^n and ba^{n-1} (or ab^n and ab^{n-1}) for some $n \in \mathbb{Z}^+$ [6]. Now, it is not difficult to see that whenever there exists a sequence S' such that $S = \phi S'$, $\psi S'$ is also identical (i.e. shift-equivalent) to S. It namely does not matter whether one reduces from the left or from the right. □

From lemma 2.4 it follows that whenever a sequence is a substitution sequence for an invertible substiution, then it is also a substitution sequence for a substitution consisting of a composition of α's and β's (recall that $\alpha = \phi$ and $\beta = \chi \circ \phi \circ \chi$).

Corollary 2.5. Let S be a substitution sequence for an invertible substitution rule. Then S is a characteristic sequence.

Proof of theorem 1.5. Parts (ii) and (iii) follow from theorem 2.1, lemma 2.3, and corollary 2.5†. It thus remains to prove part (i). Lemma 2.3 asserts that every quasiperiodic two-symbol canonical projection sequence is a substitution sequence for an invertible substitution rule. It remains to verify that such a sequence does not have an infinite number of predecessors with respect to some non-invertible substitution rule. This follows from a

† Note that a canonical projection sequence that is a substitution sequence is almost always quasiperiodic. The exceptions correspond to non-interesting singular cases when the invertible substitution is equal to ϕ^n, ψ^n, $\chi \circ \phi^n \circ \chi$, or $\chi \circ \psi^n \circ \chi$ (for some n).

recent result of Séébold [10], who showed that when σ is invertible (Sturmian) and σ and τ generate the same subwords, τ must be invertible (Sturmian) too. This concludes the proof of theorem 2.1. □

As a final remark, we would like to note that many detailed results on cutting sequences (*Sturmian sequences*) and substitution rules (*morphisms*) have been obtained in recent years in the context of theoretical computer science, cf Séébold [10] and the survey by Berstel [1].

The discussions with Zhi-Ying Wen in 1993 (see [15]) formed the basis for my interest in the relation between substitution sequences and canonical projection sequences. This research was partially supported by a *Talent Stipendium* of the Netherlands Organisation for Scientific Research (NWO).

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