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1994 J. Phys. A: Math. Gen. 27 3689

(http://iopscience.iop.org/0305-4470/27/11/019)

J. Phys. A: Math. Gen. 27 (1994) 3689–3706. Printed in the UK

A natural class of generalized Fibonacci chains

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Received 15 November 1993, in final form 11 March 1994

Abstract. In this paper we propose a class of substitution rules that generate quasiperiodic chains sharing their typical properties with the quasiperiodic Fibonacci chain. For a subclass we explicitly construct the atomic surface. Moreover, scaling properties of the energy spectrum are discussed in relation to the dynamics of trace maps.

1. Introduction

One-dimensional (1D) quasiperiodic Schrödinger equations have been studied by many authors in recent years [1–24]. In particular, much attention has been focused on quasiperiodic potentials that are derived from the Fibonacci sequence, providing a kind of prototype model for studying quasiperiodic systems.

Starting from the Fibonacci sequence, some authors have proposed generalizations, mainly by generalizing the substitution rule that is characteristic for the quasiperiodic Fibonacci sequence [12–22]. However, in doing so, one should be aware of the consequences. As the main motivation for studying the Fibonacci sequence is its quasiperiodicity, it seems most appropriate to study in the first place generalizations of Fibonacci sequences which are also quasiperiodic.

In this paper quasiperiodic chains are considered that are related to a special class of substitution rule, preserving most properties that are typical for the Fibonacci sequence. Having given the motivation for our choice of generalizations, we discuss the scaling properties of the energy spectra of such quasiperiodic chains in a tight-binding approximation, using a trace-map analysis.

Before discussing the various aspects of generalized Fibonacci sequences in detail, some preliminaries are recalled first.

Let $S = \{a, b\}$ be an alphabet of two letters. Then any finite sequence composed of the elements of S is called a word, and we denote by S^* the collection of all possible words. The empty word ε is defined by

$$\varepsilon w = w\varepsilon = w \tag{1}$$

for any $w \in S^*$. A morphism

$$\tau : S^* \mapsto S^* \tag{2}$$

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0305-4470/94/113689+18$19.50

is defined by the property

$$\tau(u_1u_2) = \tau(u_1)\tau(u_2) \tag{3}$$

for any two words $u_1, u_2 \in S^*$. Note that any morphism over S^* is completely determined by $\tau(a)$ and $\tau(b)$. Moreover we adopt the following notation:

$$\tau = (u, v) \Leftrightarrow \tau(a) = u \qquad \tau(b) = v\,. \tag{4}$$

We use the morphisms over S^* as substitution rules that provide a systematic means of inflating the word a.

Let w be a word, then we denote by $|w|$ the length of w, and by $|w|_a$ (resp. $|w|_b$) the number of letters a (resp. b) appearing in w. Let the morphism τ define a substitution rule, then the substitution matrix of τ is defined by

$$M_\tau := \begin{pmatrix} |\tau(a)|_a & |\tau(b)|_a \\ |\tau(a)|_b & |\tau(b)|_b \end{pmatrix}. \tag{5}$$

If the substitution τ is primitive [25], i.e. all entries of M_τ^N are strictly positive for some $N \geqslant 1$, $\tau^N(a)$ converges towards an infinite word x in the limit $N \to \infty$ if $\tau(a)$ begins with a. This infinite word satisfies

$$x = \tau(x)\,. \tag{6}$$

A quasiperiodic physical structure corresponding to the word x of (6) can be constructed by regarding the two letters a, b as atoms of type a and b. In order to study the electronic energy spectrum of such a structure, we consider a tight-binding model with discretized Schrödinger equation

$$\Psi_{m+1} + \Psi_{m-1} + V_m\Psi_m = E\Psi_m\,. \tag{7}$$

Here m labels the lattice site on which the atom (a or b) is situated, V_m is the site potential (V_a or V_b) and Ψ_m is the electronic wavefunction with energy E. The nature of the energy spectrum for various substitution rules has been discussed by several authors [1–7, 11–14, 17–21].

For quasiperiodic but not periodic limit structures, the energy spectrum cannot be analysed directly. If we consider the finite sequence achieved after N iterations, $\tau^N(a)$, as the unit cell of a periodic infinite structure, then the spectrum for successive iterations can be compared in order to achieve information about the limit structure. The approximate energy spectra are found using a well known transfer-matrix technique (cf [3]). The Schrödinger equation (7) can be written in terms of transfer matrices as

$$T_m\Theta_m = \Theta_{m+1} \qquad T_m = \begin{bmatrix} E - V_m & -1 \\ 1 & 0 \end{bmatrix}. \tag{8}$$

If the unit cell contains q atoms, then Θ_m and $\Theta_{m+q} = T_{m+q-1} \circ \cdots \circ T_m\Theta_m$ differ by a constant phase factor, independent of m. A consequence is that an energy E is allowed if and only if

$$|\mathrm{Tr}(T_{m+q-1} \circ \ldots \circ T_m)| \leqslant 2 \tag{9}$$

where $\mathrm{Tr}(A)$ denotes the trace of A. The transfer matrix of a chain w, of atoms a and b, consists of a corresponding product of transfer matrices, T_w. For a given substitution rule τ, define

$$x_k = \mathrm{Tr}(T_{\tau^k(a)}) \qquad y_k = \mathrm{Tr}(T_{\tau^k(b)}) \qquad z_k = \mathrm{Tr}(T_{\tau^k(ab)})\,. \tag{10}$$

Then [26] $x_{k+1}, y_{k+1}, z_{k+1} \in \mathbb{Z}[x_k, y_k, z_k]$. We obtain the k-independent trace map

$$(x', y', z') = F_\tau(x, y, z)\,. \tag{11}$$

A very important question is of course, what the approximate spectra (based on (9)) tell us about the incommensurate limit spectrum. For the step potential tight-binding model (7) with

$$V_m = V(x + m\omega) = \begin{cases} V_0 & \text{for} \quad 1 - \omega \leqslant t < 1 \\ V_1 & \text{for} \quad 0 \leqslant t < 1 - \omega \end{cases} \tag{12}$$

it has been proved that the limit spectrum is the set $\{E | x_k(E)$ is bounded as $k \to \infty\}$ for every V_0, $V_1 \in \mathbb{R}$ and irrational ω and any $x \in \mathbb{R}$ [27–30].

Let us now regard some typical properties of the well known Fibonacci chain. The substitution rule, leading to the Fibonacci chain is given by

$$\sigma = (ab, a). \tag{13}$$

This substitution rule is invertible with inverse $\sigma^{-1} = (b, b^{-1}a)$ and the determinant of the substitution matrix M_σ is -1.

The diffraction spectrum of the Fibonacci chain contains Bragg peaks that can be labelled by two indices (two-dimensional $\mathbb{Z}$-module), i.e. the chain is quasiperiodic of rank-2 [31]. Moreover, the chain has an average lattice, i.e. a limiting average spacing and a bounded modulation with respect to this average lattice.

We are lead to investigate chains that are fixed points of substitution rules τ that are invertible and have $\det(M_\tau) = \pm 1$. As Peyrière [32] has pointed out, this leads us to an understanding of the Fibonacci sequence in the context of the free group $\mathcal{F}_2 = \langle a, b \rangle$ (see also [33, 34]). The Fibonacci substitution rule can be regarded as an automorphism of this free group, and the proposed generalization leads to a consideration of any $\tau \in \mathrm{Aut}(\mathcal{F}_2)$ that is physically meaningful, i.e. any $\tau \in \mathrm{Aut}(\mathcal{F}_2)$ that does not contain inverse letters. We call this set, the set of invertible substitutions $\mathrm{Inv}(S^*)$. In section 2 this class will be discussed in detail.

A substitution rule studied extensively is the rule $\tau = (a^m b^n, a)$ [12–22]. Two different classes can be distinguished. The class with $n = 1$ has $\det(M_\tau) = -1$. The chain is quasiperiodic with $\mathbb{Z}$-module of rank-2. For the other class with $n > 1$ we have $\det(M_\tau) < -1$ and $\tau \notin \mathrm{Aut}(F_2)$ (hence $\tau \notin \mathrm{Inv}(S^*)$). In literature, the infinite chain built by $\tau = (a^m b^n, a)$ is sometimes called a generalized Fibonacci chain [15, 17]. In our opinion, this term is only appropriate if $n = 1$, since only then the typical properties of the Fibonacci chain are recovered.

In table 1 a comparison is made between the different types of substitution rules and the properties of the chains they generate. One of the typical properties of the Fibonacci sequence is that it can be constructed by the so-called method of cut and project [35]. This

Table 1. Comparison of properties of chains that are generated by various types of substitution rule τ with substitution matrix M_τ (with $\det M_\tau \neq 0$). The properties labelled with # are conjectures. Examples confirming these conjectures can be found in e.g. [31].

	Fibonacci	$\tau \in \mathrm{Inv}(S^*)$	$\tau \notin \mathrm{Inv}(S^*)$		
Pisot property	yes	yes	yes		no
$\det M_\tau$	-1	± 1	± 1	not ± 1	not ± 1
Rank $\mathbb{Z}$ module	2	2	2	∞	–
Average lattice and bounded modulation	yes	yes	yes	yes	no
Cut-and-project (extension of atomic surface $\Delta\theta = 1$)	yes	yes#	no#	no#	no
Trace map preserves volume and invariant λ (cf (19))	yes	yes	no	no	no

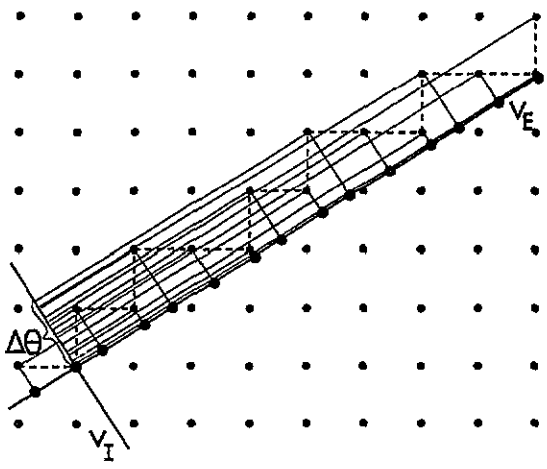

Figure 1. The method of cut-and-project for the Fibonacci chain and the construction of the atomic surface. The window is achieved by shifting the square unit cell along the eigenvector of the substitution matrix having the highest eigenvalue, coinciding with the physical space V_E. The projection of the unit cell along the other eigenvector, V_I, is the atomic surface of length $\Delta\theta$. All lattice points within the window represent a walk on this square lattice: each step in the horizontal direction is an a and each step in the vertical direction a b. The projection of all lattice points within the window on the external space V_E yields a quasiperiodic sequence of long and short intervals, corresponding to a, b, respectively. Their relative length is prescribed by construction.

method involves a projection of points on a square lattice to a line (the so-called physical space) with an irrational slope (the golden mean in the case of the Fibonacci chain). As a rule only points in a certain neighbourhood of this line, the window, are projected. The physical space lies in the direction of the eigenvector belonging to the largest eigenvalue of the substitution matrix. In figure 1, this method is illustrated. Regarding all the points on the square lattice that participate in this construction, one can also consider the projection of these points to the space that lies in the direction of the other eigenvector, the so-called internal space. The closure of this projection is called the atomic surface (for an illustration, see again figure 1).

By convention, usually the lattice constant of the square lattice is chosen such that the total length of the atomic surface (i.e. the sum of the lengths of all parts if it is disconnected) equals one [31]. For a discussion of other, but equivalent, definitions of the atomic surface we refer the reader to [31]. Now denote by θ_+ and θ_- the upper and lower extremities of the full atomic surface, and by $\Delta\theta = \theta_+ - \theta_-$ its extension. In the case of the Fibonacci chain the atomic surface consists of only one line element of length one. In fact a quasiperiodic chain can be obtained by the method of cut-and-project if and only if the atomic surface consists of one line segment†.

Bombieri and Taylor [36] have shown that any infinite chain obtained via a substitution rule possessing the Pisot property‡ is contained in a chain that can be obtained via the

† We prefer to reserve the term 'cut-and-project' to the cases in which there is an ordinary window within which each point is projected to the physical space (as in [36]). This excludes the cases in which the atomic surface is a fractal object.

‡ The substitution rule τ has the Pisot property if M_τ has one eigenvalue bigger than one, and the other eigenvalue of absolute value smaller than one. The Pisot property is sufficient for τ to generate a chain with an average lattice and a bounded modulation with respect to this average lattice.

method of cut-and-project as discussed above. In this case the atomic surface does not have to be a single line segment but may consist of (many) disconnected parts. However, the total length of (all parts) of the atomic surface is always equal to one [31].

It is an appealing question whether every quasiperiodic chain that is a fixed point of a physically meaningful $\tau \in \mathrm{Aut}(\mathcal{F}_2)$, i.e. $\tau \in \mathrm{Inv}(S^*)$, can be constructed via the method of cut-and-project. We conjecture that this question has a positive answer. In our support, in section 3 a large family of invertible substitution rules is presented for which we succeeded to prove this relation.

The trace map associated with the Fibonacci substitution rule is given by

$$F_\sigma : \begin{cases} x' = z \\ y' = x \\ z' = xz - y\,. \end{cases} \tag{14}$$

It is volume preserving and foliates its three-dimensional phase space with invariant surfaces $x^2 + y^2 + z^2 - xyz - 4 = \lambda$ [32–34, 37].

One other aspect of the energy spectrum of the Fibonacci chain is its self-similar (multifractal) structure [7, 9]. The scaling behaviour of this spectrum can be understood in relation to dynamical features of the trace map. In section 4 this relation is discussed in more detail.

2. Invertible substitution rules

In this section, some general properties of substitution rules are discussed that are in the automorphism class, and the quasiperiodic chains they generate.

It is well known [33, 34, 38] that the group of automorphisms $\mathrm{Aut}(\mathcal{F}_2)$ may be generated by the following morphisms:

$$\alpha = (b, a) \qquad \beta = (a, b^{-1}) \qquad \gamma = (ab, b^{-1})\,. \tag{15}$$

However, for our purpose of building words in S^*, we are only interested in those automorphisms τ that do not involve inverse letters. These automorphisms form a semigroup of invertible substitutions, $\mathrm{Inv}(S^*)$. It is generated by three morphisms [39]

$$\mathrm{Inv}(S^*) = \langle \alpha, \sigma, \varphi \rangle \tag{16}$$

where α is as defined in (15), σ is the Fibonacci substitution rule (13) and

$$\varphi = (ba, a)\,. \tag{17}$$

Because

$$\det(M_\alpha) = \det(M_\sigma) = \det(M_\varphi) = -1 \tag{18}$$

for any $\tau \in \mathrm{Inv}(S^*)$, we have $\det M_\tau = \pm 1$ and the Fourier transform of the diffraction pattern of the infinite chain generated by τ consists of a two-dimensional $\mathbb{Z}$-module, i.e. the chain is quasiperiodic of rank-2†. Other well known properties are related to the trace map. Let F_τ be the trace map associated with the substitution rule τ, and let

$$\lambda(x, y, z) = x^2 + y^2 + z^2 - xyz - 4 \tag{19}$$

then there is a polynomial Q_τ in x, y, z with integer coefficients such that [32]

$$\lambda \circ F_\tau = Q_\tau \cdot \lambda\,. \tag{20}$$

† In case τ is a substitution rule that possesses the Pisot property, but $\det M_\tau \neq \pm 1$, one speaks of a limit quasiperiodic chain (of rank-∞) [31].

Moreover,

$$\tau \in \mathrm{Aut}(\mathcal{F}_2) \Leftrightarrow Q_\tau = 1 \tag{21}$$

i.e. the trace map foliates the $\mathbb{R}^3$ with surfaces that are constants of the motion if and only if the substitution rule is invertible. F_τ is also volume preserving.

After having identified the subset of physically meaningful substitutions in $\mathrm{Aut}(\mathcal{F}_2)$ as the set of invertible substitutions $\mathrm{Inv}(S^*)$, the relevant set can be reduced even further considering locally isomorphic† chains as being equivalent.

Theorem. Let $\tau_1, \tau_2 \in \mathrm{Inv}(S^*)$ and let M_{τ_1} and M_{τ_2}, respectively, be their substitution matrices. Then the infinite word generated by τ_1 is locally isomorphic to the infinite word generated by τ_2 if and only if $M_{\tau_1} = M_{\tau_2}$.

The proof of the 'if' part of the above theorem can be found in [39]. The local isomorphism follows from the observation that if $M_{\tau_1} = M_{\tau_2}$ there exists a word $w \in S^*$ such that

$$\tau_1(a) = w\tau_2(a)w^{-1} \qquad \tau_1(b) = w\tau_2(b)w^{-1} \tag{22}$$

or such that

$$\tau_1(a) = w^{-1}\tau_2(a)w \qquad \tau_1(b) = w^{-1}\tau_2(b)w\,. \tag{23}$$

The proof of the 'only if' part will be given elsewhere [40].

Physical properties of interest that are invariant under local isomorphisms (such as the energy spectrum [18, 23]) of quasiperiodic chains generated by a substitution rule in $\mathrm{Inv}(S^*)$ are classified by their substitution matrix, rather than by the specific substitution rule. In that respect it is important to notice that for any 2×2 substitution matrix M with positive integer entries and determinant ± 1, there is a $\tau \in \langle \alpha, \sigma \rangle$ such that $M = M_\tau$ [39]. Hence, we conclude that if we are interested in properties that are invariant under local isomorphisms, we only need to consider substitution rules of the form

$$\sigma^{n_k} \circ \alpha \circ \sigma^{n_{k-1}} \circ \alpha \cdots \circ \sigma^{n_2} \circ \alpha \circ \sigma^{n_1} \tag{24}$$

where $n_1, n_k \geqslant 0$ and $n_2, \ldots, n_{k-1} \geqslant 1$.

In this section we have shown that many properties that are typical for the Fibonacci chain, are in fact typical for the class of chains that are generated by an invertible substitution $\tau \in \mathrm{Inv}(S^*)$. This leads us to conjecture that most of the physically relevant features that have been observed in the study of Fibonacci sequences, will persist throughout the entire class of quasiperiodic chains over S that are generated by invertible substitutions.

In the next section, to support our conjecture, we focus on a special class of invertible substitution rules to illustrate the persistence of the property to generate a quasiperiodic chain with the method of cut and project. In section 4 this same class will be discussed in relation to the scaling properties of the energy spectrum.

3. A special class of invertible substitutions

As indicated in the previous sections, the invertible substitution is a natural generalization of the Fibonacci substitution rule, conserving most of its typical features. In fact we conjecture that important features such as the method of cut-and-project are applicable if and only if the substitution rule is invertible (see also table 1).

† Let u and v be two infinite sequences over S. Then we say that u and v are locally isomorphic if any subsequence of u (or its mirror image) is also a subsequence of v and vice versa.

Therefore, we will consider a special class of invertible substitutions

$$\tau_k^n = (\sigma \circ \alpha)^n \circ \sigma^k . \tag{25}$$

This class contains the Fibonacci substitution rule τ_1^0 as well as the one-parameter family of substitution rules τ_1^n suggested by Kalugin *et al* [12]. It benefits from the special relations

$$(\sigma \circ \alpha)^n(a) = a \qquad (\sigma \circ \alpha)^n(b) = a^n b \tag{26}$$

and

$$|\sigma^k(a)| = f_k \qquad |\sigma^k(b)| = f_{k-1} \tag{27}$$

where f_k are the Fibonacci numbers with the initial conditions $f_{-1} = f_0 = 1$ and $f_k = 0$ for all $k \leqslant -2$, defined by the recurrent formula $f_{n+2} = f_{n+1} + f_n$.

Thus the substitution matrix of τ_k^n is

$$M_{\tau_k^n} = \begin{pmatrix} f_{k-1} + nf_{k-2} & f_{k-2} + nf_{k-3} \\ f_{k-2} & f_{k-3} \end{pmatrix} . \tag{28}$$

In the next subsection it will be shown that the extension of the atomic surface of a chain generated by the substitution rule τ_k^n always has length one, i.e. $\Delta\theta = 1$, implying that such a chain can be obtained by the method of cut-and-project [31].

3.1. The atomic surface

In this subsection we will discuss the proof of the fact that the extension of the atomic surface of a quasiperiodic chain generated by the invertible substitution τ_k^n is equal to one, for any $n \geqslant 0$ and $k \geqslant 1$, implying that such a chain can be obtained by the method of cut-and-project. For some details of the proof, we will refer to [41] in which an analogous problem has been discussed. Let us first define some useful notations.

We have a substitution rule τ on the alphabet $S = \{a, b\}$ with fixed point $x(\tau)$. We denote by n_a and n_b, respectively, the number of the letters a and b in the first n letters of $x(\tau)$. Moreover, we define

$$d_a(\tau) := \lim_{n\to\infty} \frac{n_a}{n} \qquad d_b(\tau) := \lim_{n\to\infty} \frac{n_b}{n} \tag{29}$$

which are, respectively, the frequencies of the letters a and b appearing in $x(\tau)$. Evidently, $d_a(\tau) + d_b(\tau) = 1$. Furthermore let $\mu(\tau) := d_a(\tau)/d_b(\tau)$, then

$$d_b(\tau)(1 + \mu(\tau)) = d_a(\tau) + d_b(\tau) = 1 . \tag{30}$$

Considering the substitution matrix M_τ, let $\Lambda(\tau)$ and $\lambda(\tau)$ be its eigenvalues with $\Lambda(\tau) > |\lambda(\tau)|$. It is well known [25] that $\Lambda(\tau) > 1$ and $(d_a(\tau), d_b(\tau))^T$ is an eigenvector of M_τ belonging to $\Lambda(\tau)$. (To simplify the notation in the rest of this section, if no confusion arises, we will omit the label τ if possible.)

With the notations as above, we define a sequence $\{u_n\}_{n\geqslant 1}$ as follows:

$$u_n := n_a - nd_a . \tag{31}$$

Then from (30) it is easy to check that

$$u_n = d_b(n_a - n_b\mu) . \tag{32}$$

We can also write

$$u_n = \frac{n_a - n_b\mu}{1 + \mu} . \tag{33}$$

The atomic surface of the chain generated by the substitution rule τ, which we denote by $A(\tau)$, is defined as

$$A(\tau) = \overline{\{u_n(\tau)\}_{n\geqslant 1}} \tag{34}$$

where the horizontal bar denotes the topological closure of a set.

Let $\theta_+(A) := \sup_{n\geqslant 1} u_n$ and $\theta_-(A) := \inf_{n\geqslant 1} u_n$, then the extension of A is defined as

$$\Delta\theta(A) := \theta_+(A) - \theta_-(A)\,. \tag{35}$$

Our purpose is to prove that $\Delta\theta(A(\tau_k^n)) = 1$. The proof consists of five successive steps.

(i) Because of the special relations (26), we can obtain the finite chain $\tau_k^n(a)$ from the chain $\sigma^k(a)$ in the following way: replace a and b, respectively, by a and $a^n b$ in the chain $\sigma^k(a)$.
(ii) We will determine $\theta_+(A)$ and $\theta_-(A)$ by a similar technique to that in [41], which requires $\lambda \geqslant 0$. For any $n \geqslant 0$ this requires $\det(M_{(\tau_k^n)}) = 1$ and hence k should be even. For the case of k being odd we can take $(\tau_k^n)^2$, which gives the same infinite chain as τ_k^n, but $\det(M_{(\tau_k^n)^2}) = 1$, thus $\lambda > 0$.
(iii) Let

$$\theta_+^{(n)}(\tau(a)) = \sup_{1\leqslant m\leqslant|\tau^n(a)|} u_m \tag{36}$$

$$\theta_-^{(n)}(\tau(a)) = \inf_{1\leqslant m\leqslant|\tau^n(a)|} u_m \tag{37}$$

then

$$\theta_+(A(\tau)) = \lim_{n\to\infty} \theta_+^{(n)}(\tau) \tag{38}$$

$$\theta_-(A(\tau)) = \lim_{n\to\infty} \theta_-^{(n)}(\tau) \tag{39}$$

and hence

$$\Delta\theta(A(\tau)) = \lim_{n\to\infty} [\theta_+^{(n)}(\tau) - \theta_-^{(n)}(\tau)]\,. \tag{40}$$

If we know $\theta_+^{(1)}$ and $\theta_-^{(1)}$, we can obtain inductively $\theta_+^{(n)}$ and $\theta_-^{(n)}$ by a method described in [41].
(iv) We consider first σ^{2k}. In this case

$$M_{\sigma^{2k}} = \begin{pmatrix} f_{2k-1} & f_{2k-2} \\ f_{2k-2} & f_{2k-3} \end{pmatrix}. \tag{41}$$

(Notice that we have $|\sigma^k(a)| = f_k$.)

In addition,

$$\Lambda(\sigma^{2k}) = \tau_g^{2k} \qquad \mu(\sigma^{2k}) = \tau_g \tag{42}$$

where τ_g is the golden mean $(\sqrt{5}+1)/2$.

It is not difficult to see that

$$\begin{cases} \theta_+^{(1)}(\sigma^{2k}) &= f_{2k-2} - (f_{2k-3} - 1)\mu(\sigma^{2k}) \\ \theta_-^{(1)}(\sigma^{2k}) &= f_{2k-1} - 1 - f_{2k-2}\mu(\sigma^{2k})\,. \end{cases} \tag{43}$$

(v) In view of (i), by using the facts $|\sigma^k(a)| = f_k$, $|\sigma^k(b)| = f_{k-1}$, $k \geqslant 1$, a simple calculation leads to

$$M_{\tau_{2k}^n} = \begin{pmatrix} f_{2k-1} + nf_{2k-2} & f_{2k-2} + nf_{2k-3} \\ f_{2k-2} & f_{2k-3} \end{pmatrix}. \tag{44}$$

Its characteristic equation is

$$\lambda^2 - (f_{2k-1} + f_{2k-3} + nf_{2k-2})\lambda + 1 = 0\,. \tag{45}$$

Hence the largest eigenvalue of $M_{\tau_{2k}^n}$ reads

$$\Lambda(\tau_{2k}^n) = \frac{f_{2k-1} + f_{2k-3} + nf_{2k-2} + \sqrt{(f_{2k-1} + f_{2k-3} + nf_{2k-2})^2 - 4}}{2}\,. \tag{46}$$

On the other hand, since $(d_a(\tau_{2k}^n), d_b(\tau_{2k}^n))^T$ is the eigenvector of $\Lambda(\tau_{2k}^n)$, we find with relation (30) that

$$f_{2k-2}d_a(\tau_{2k}^n) + f_{2k-3}d_b(\tau_{2k}^n) = \Lambda(\tau_{2k}^n)d_b(\tau_{2k}^n) \tag{47}$$

which yields that

$$\mu(\tau_{2k}^n) = \frac{\Lambda(\tau_{2k}^n) - f_{2k-3}}{f_{2k-2}}\,. \tag{48}$$

Since for any $n \geqslant 0$, $k \geqslant 1$ we have

$$f_{2k-1} + f_{2k-3} + nf_{2k-2} - 2 < \sqrt{(f_{2k-1} + f_{2k-3} + nf_{2k-2})^2 - 4} < f_{2k-1} + f_{2k-3} + nf_{2k-2} \tag{49}$$

it follows from (46) that

$$f_{2k-1} + f_{2k-3} + nf_{2k-2} - 1 < \Lambda(\tau_{2k}^n) < f_{2k-1} + f_{2k-3} + nf_{2k-2} \tag{50}$$

which yields

$$\frac{f_{2k-1}}{f_{2k-2}} + n - \frac{1}{f_{2k-2}} < \frac{\Lambda(\tau_{2k}^n) - f_{2k-3}}{f_{2k-2}} < \frac{f_{2k-1}}{f_{2k-2}} + n\,. \tag{51}$$

On the other hand, it is readily seen that

$$1 + \frac{1}{f_{2k-2}} < \frac{f_{2k-1}}{f_{2k-2}} < 2\,. \tag{52}$$

We thus obtain by (48) and (51) that

$$n + 1 < \mu(\tau_{2k}^n) < n + 2\,. \tag{53}$$

In view of (i) again, from the inequality (53) we see that if we replace a and b by a and $a^n b$, respectively, in $\sigma^{2k}(a)$, then $\theta_+(A(\tau_{2k}^n))$ and $\theta_-(A(\tau_{2k}^n))$ will be obtained in the same position as in the case of σ^{2k}, up to a translation n. More precisely, by (43) we have

$$\begin{cases} \theta_+^{(1)}(\tau_{2k}^n) &= f_{2k-2} + nf_{2k-3} - (f_{2k-3} - 1)\mu(\tau_{2k}^n) \\ \theta_-^{(1)}(\tau_{2k}^n) &= f_{2k-1} - 1 + nf_{2k-2} - f_{2k-2}\mu(\tau_{2k}^n)\,. \end{cases} \tag{54}$$

By using (54) it follows from an analogous argument to that used in [41] that

$$\Delta\theta(A(\tau_{2k}^n)) = \theta_+(A(\tau_{2k}^n)) - \theta_-(A(\tau_{2k}^n)) \tag{55}$$

$$= \frac{1}{1 + \mu(\tau_{2k}^n)}\left[\theta_+^{(1)}(\tau_{2k}^n) - \theta_-^{(1)}(\tau_{2k}^n)\right]\frac{1}{1 - \Lambda^{-1}(\tau_{2k}^n)} \tag{56}$$

$$= \frac{\Lambda(\tau_{2k}^n)[\theta_+^{(1)}(\tau_{2k}^n) - \theta_-^{(1)}(\tau_{2k}^n)]}{(1 + \mu(\tau_{2k}^n))(\Lambda(\tau_{2k}^n) - 1)}\,. \tag{57}$$

Moreover, from (54) we have

$$\theta_+^{(1)}(\tau_{2k}^n) - \theta_-^{(1)}(\tau_{2k}^n) = (f_{2k-2} - f_{2k-3} + 1)\mu(\tau_{2k}^n) - (f_{2k-1} - f_{2k-2} - 1 + n(f_{2k-2} - f_{2k-3})) \tag{58}$$

$$= (f_{2k-4} + 1)\mu(\tau_{2k}^n) - (f_{2k-3} - 1 + nf_{2k-4})\,. \tag{59}$$

We thus have

$$\Delta\theta(A(\tau_{2k}^n)) = \frac{\Lambda(\tau_{2k}^n)\left[(f_{2k-4}+1)\mu(\tau_{2k}^n) - (f_{2k-3}-1+nf_{2k-4})\right]}{(1+\mu(\tau_{2k}^n))(\Lambda(\tau_{2k}^n)-1)}. \tag{60}$$

Substituting (48) into (60), if we wish to prove that $\Delta\theta(A(\tau_{2k}^n)) = 1$, it suffices to prove that

$$\left(1+\frac{\Lambda(\tau_{2k}^n)-f_{2k-3}}{f_{2k-2}}\right)(\Lambda(\tau_{2k}^n)-1) = \Lambda(\tau_{2k}^n)\left[(f_{2k-4}+1)\frac{\Lambda(\tau_{2k}^n)-f_{2k-3}}{f_{2k-3}} - (f_{2k-3}-1+nf_{2k-4})\right]. \tag{61}$$

By using the recurrent relation $f_{k+2} = f_{k+1} + f_k$ and a known result about the Fibonacci numbers $f_{2k}f_{2k-2} + 1 = f_{2k-1}^2$, the equality (61) can be rewritten as

$$f_{2k-4}(\Lambda^2(\tau_{2k}^n) - (f_{2k-1} + f_{2k-3} + nf_{2k-2})\Lambda(\tau_{2k}^n) + 1) = 0. \tag{62}$$

If $k = 1$, then $f_{2k-4} = 0$ and (62) holds. If $k > 1$, then $f_{2k-4} \neq 0$ and (62) is reduced to

$$\Lambda^2(\tau_{2k}^n) - (f_{2k-1} + f_{2k-3} + nf_{2k-2})\Lambda(\tau_{2k}^n) + 1 = 0. \tag{63}$$

Notice that (63) is exactly the characteristic equation of the matrix $M_{\tau_{2k}^n}$ (45). Hence we find that (61) is always satisfied, completing the proof that the extension of the atomic surface $\Delta\theta(A(\tau_{2k}^n)) = 1$, implying that $\Delta\theta(A(\tau_k^n)) = 1$ for all k and n. □

4. Scaling properties of the energy spectrum

For every substitution rule τ we find a sequence of approximate periodic structures with corresponding energy spectra of the Schrödinger equation (7). In this section we will study the scaling behaviour of these approximate spectra, considering various invertible substitutions as well as a non-invertible one.

For a given substitution τ_k^n and approximation number l, for each energy E the vector $r_l(E) := F_{(\tau_k^n)^l} r_0(E)$ is determined by successive application of the trace maps F_α and F_σ occurring in $F_{(\tau_k^n)^l} = F_{\tau_k^n}^l$†. The first component of this vector determines whether an energy E occurs in the spectrum of the lth (periodic) approximation to the infinite quasiperiodic chain generated by the substitution τ_k^n, starting with a single a. That is, the first component $|x_l(E)| \leqslant 2$ (cf (9)). The initial conditions for this iteration process are

$$r_0(E) = (E - V_a, E - V_b, (E - V_a)(E - V_b) - 2) \tag{64}$$

i.e. a line parametrized by E on the invariant surface $\lambda = (V_a - V_b)^2$. In all explicit calculations we have set $V_a = -V_b = 0.6$.

In figure 2 the energy spectrum for the first few (periodic) approximations of quasiperiodic chains using the substitution rules τ_1^0, τ_1^1 and τ_2^1 are depicted. Note that τ_1^0 is the Fibonacci substitution rule.

In the Fibonacci case, it was observed [3, 5] that the substitution rule induces a band splitting that repeats itself at smaller scales in higher-order approximations. In figure 2 we observe a similar mechanism also in the case of other invertible substitutions.

With the above observation, it is natural to do a scaling analysis of the central band. In studies of Fibonacci spectra, non-uniform scaling was found, giving rise to a limit spectrum that is a Cantor set with multifractal properties [4, 9, 11].

† For all $\tau_1, \tau_2 \in \mathrm{Aut}(\mathcal{F}_2)$ we have [26, 32] $M_{\tau_2} \circ M_{\tau_1} = M_{\tau_2 \circ \tau_1}$ and $F_{\tau_2} \circ F_{\tau_1} = F_{\tau_1 \circ \tau_2}$. Hence any trace map F_τ (with $\tau \in \mathrm{Inv}(S^*)$) can be written as a composition of the trace maps F_α, F_σ, and F_φ, where F_σ is the Fibonacci trace map (14), $F_\varphi = F_\sigma$, and $F_\alpha : (x, y, z) \mapsto (y, x, z)$.

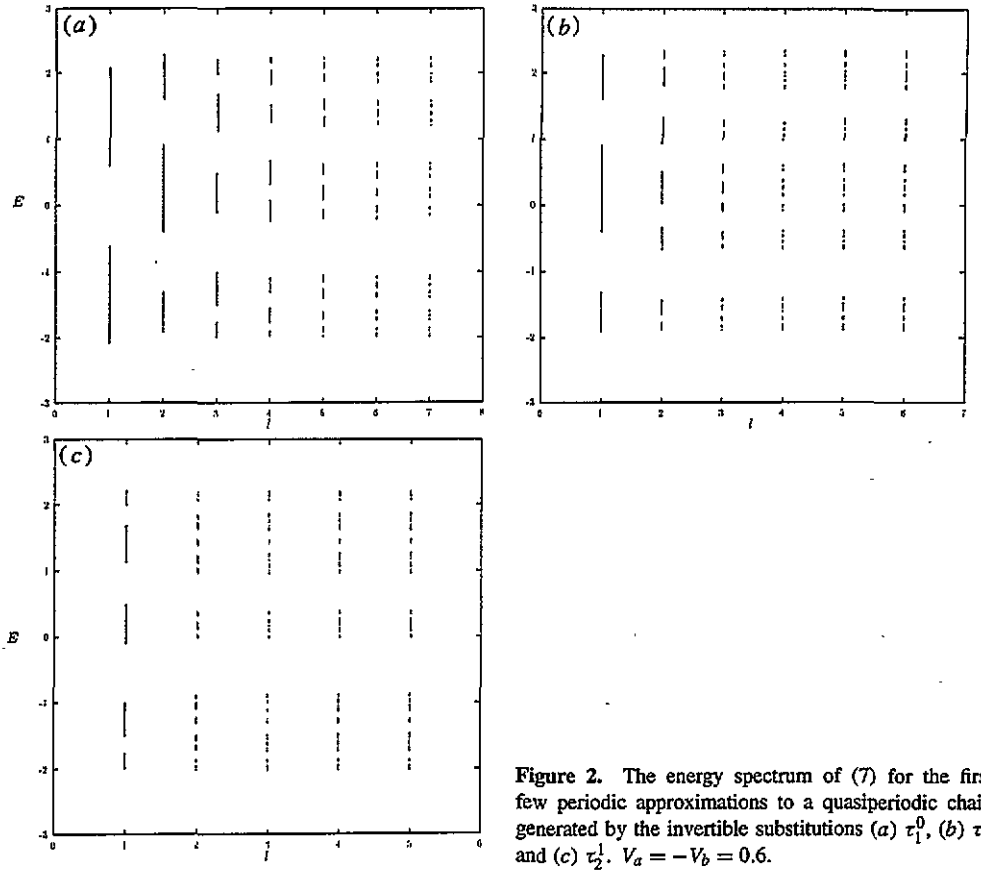

Figure 2. The energy spectrum of (7) for the first few periodic approximations to a quasiperiodic chain generated by the invertible substitutions (*a*) τ_1^0, (*b*) τ_1^1 and (*c*) τ_2^1. $V_a = -V_b = 0.6$.

We will focus on the scaling behaviour of central band, i.e. we will compare the width of the central band in successive approximate spectra. In table 2 we present the scaling parameter α, i.e. the ratio of the width of the central bands at level l and $l+\delta$, as obtained numerically for different substitution rules τ_k^n. A step size $\delta > 1$ is sometimes required to circumvent spectra that have no central band (e.g. τ_1^0, τ_1^2, τ_2^2) or to ensure convergent scaling (e.g. τ_2^1).

Table 2. Scaling parameter α of the centre band in approximate spectra generated by invertible substitution rules τ_k^n (cf (25)) for various values of k and n. α is the ratio of the width of the centre bands of approximations l and $l+\delta$. Max l indicates the highest approximation used in obtaining the scaling results.

k	n	δ	Max l	α
1	0	3	13	5.618 ± 0.007
1	1	1	13	2.702 ± 0.002
1	2	3	6	80.4 ± 0.5
1	3	1	6	4.8702 ± 0.0004
2	1	2	6	27.55 ± 0.02
2	2	3	6	375 ± 5

The scaling of the central band of the Fibonacci spectra was found to be related to the largest eigenvalue of the Jacobian matrix of F_σ^6 in $(a, 0, 0)$, which lies on a 6-cycle of F_σ [5]. Note in this respect that volume preservation together with the invariant λ (cf (19)) implies the eigenvalue spectrum to be of the form $\{1, \mu, \mu^{-1}\}$ ($\lambda > 0$ moreover implies that $\mu \in \mathbb{R}$).

In [5], Kohmoto and Oono argue that the central band appears as the result of the intersection of the stable manifold of the 6-cycle with the initial line $r_0(E)$. To explain the other results of table 2, consider the set

$$\mathcal{A} := \{x_a, y_a, z_a, x_{-a}, y_{-a}, z_{-a}\} \tag{65}$$

where $x_a = (a, 0, 0)$, $y_a = (0, a, 0)$, etc. Considering the invariant surface of the trace map $\lambda = (V_a - V_b)^2 = a^2 - 4 > 0$, these points are situated on the central part of the surface right between its four cones (for a picture of this surface see, for example, [5]).

The set $\mathcal{A}$ consists of periodic orbits of F_τ for any $\tau \in \mathrm{Inv}(S^*)$ because $F_\tau(\mathcal{A}) = \mathcal{A}$, as can easily be verified from the fact that F_σ and F_α map $\mathcal{A}$ onto itself. These periodic orbits may be written as permutation cycles, e.g.

$$F_\sigma(\mathcal{A}) = (x_a y_a z_{-a} x_{-a} y_{-a} z_a)\,. \tag{66}$$

Now, let us investigate the eigenvalues of the periodic orbits of $\mathcal{A}$ and compare them to scaling factors α of table 2.

For our special class of invertible substitutions τ_k^n (25) we find

$$F_{\tau_k^n}(\mathcal{A}) = (x_a y_a z_{-a} x_{-a} y_{-a} z_a)^k \circ (z_a y_a z_{-a} y_{-a})^n \tag{67}$$

giving rise to 24 different periodic orbit structures within $\mathcal{A}$. In table 3 we present the explicit orbits and their largest eigenvalues for the substitutions considered in table 2. Comparing table 2 and table 3 we find that in all cases the observed scaling coincides with the largest eigenvalue of a periodic orbit in $\mathcal{A}$.

Table 3. Periodic orbits of trace maps of invertible substitutions τ_k^n (cf (25)) their periods p, their largest eigenvalue $\mu(a)$ for general a, the value of δ as used in table 2, and $|\mu^{\delta/p}(a)|$ for $a^2 = 5.44$ for comparison with α in table 2 (with $V_a = -V_b = 0.6$). Only periodic orbits within the set $\mathcal{A}$ (cf (65)) are considered.

k	n	$F_{\tau_k^n}(\mathcal{A})$	p	$\mu(a)$	δ	$\lvert\mu^{\delta/p}(\sqrt{5.44})\rvert$
1	0	$(x_a y_a z_{-a} x_{-a} y_{-a} z_a)$	6	$8a^4 + 1 + \sqrt{(8a^4+1)^2 - 1}$	3	5.618
1	1	$(x_a y_a x_{-a} y_{-a})$	4	$2a^4 - 4a^2 + 1 + \sqrt{(2a^4 - 4a^2 + 1)^2 - 1}$	1	2.960 73
		$(z_a z_{-a})$	2	$\frac{1}{2}[a^2 + 2 + \sqrt{(a^2+2)^2 - 4}]$	1	2.702 4
1	2	$(x_a y_a z_a x_{-a} y_{-a} z_{-a})$	6	$\frac{1}{2}[16a^8 - 56a^6 + 49a^4 + 2 + \sqrt{(16a^8 - 56a^6 + 49a^4 + 2)^2 - 4}]$	3	80.31
1	3	$(x_a y_a)\ (x_{-a} y_{-a})$	2	$\frac{1}{2}[3a^4 - 8a^2 + 2 + \sqrt{(3a^4 - 8a^2 + 2)^2 - 4}]$	1	6.873 11
		$(z_a)\ (z_{-a})$	1	$-a - \sqrt{a^2 + 1}$	1	4.870 10
2	1	$(x_a z_{-a})\ (x_{-a} z_a)$	2	$\frac{1}{2}[2 - a^4 - \sqrt{(2 - a^4)^2 - 4}$	2	27.557
		$(y_a y_{-a})$	2	$1 - 2a^2 - \sqrt{(1 - 2a^2)^2 - 1}$	2	19.709
2	2	$(x_a z_{-a} y_a)\ (x_{-a} z_a y_{-a})$	3	$\frac{1}{2}[9a^4 - 4a^6 + 2 - \sqrt{(9a^4 - 4a^6 + 2)^2 - 4}]$	3	375.611

In table 3, note that δ is not always equal to the period of the cycle that is related to the scaling factor α, although one would expect them to be equal from the stable manifold argument. The reason for this is to be found in the symmetry properties of the periodic orbits. In the cases τ_1^0, τ_1^1, and τ_1^2, where δ equals half the period of the determining cycle, the period-two orbits of $F_{\tau_k^n}^\delta$ appear to be symmetric with respect to a symmetry of $F_{\tau_k^n}^\delta$,

causing local dynamics near the two points to be similar and hence giving rise to a uniform scaling behaviour.

In most cases the value of δ needed to circumvent spectra without central bands automatically gives convergent scaling behaviour. Only in the case of τ_2^1 this does not happen: one is tempted to take $\delta = 1$ because in all approximations there is an odd number of bands and hence a central band. However, the determining period-two orbit is not symmetric. As a result, if we take $\delta = 1$ we find α oscillating around the root of the largest eigenvalue. Taking $\delta = 2$ avoids the oscillation and we find α to be in correspondence to the eigenvalue. In the appendix the symmetry properties of the trace maps are discussed in more detail, in particular in relation to this problem.

Considering the initial conditions $r_0(E)$ and the points contained in $\mathcal{A}$, we find that z_{-a} is closest to $r_0(E)$ (in fact even near $r_0(0)$). Hence one would expect the orbit containing z_{-a} to determine the scaling of the central band. The results in table 2 and table 3 support this line of reasoning.

In the earlier work of Wijnands [19], quasiperiodic chains generated by juxtaposition rules

$$S_{k+1} = S_k^{n+1} S_{k-1} \qquad S_0 = b \qquad S_1 = ab^n \tag{68}$$

with $n = 0, 1, 2, 3$ were studied. With different initial conditions ($S_0 = b$, $S_1 = a$), these juxtaposition rules are equivalent to the invertible substitution rules τ_1^n. The energy spectrum in successive approximations generated by the juxtapositution rules (68) is governed by the same trace maps as in the case of the substitution rules τ_1^n, but (if $n > 0$) with initial conditions $r_0(E)$ different from (64). In the case $n = 1, 2, 3$ the scaling behaviour was also found to correspond exactly to the largest eigenvalue of periodic orbits in $\mathcal{A}$. However, in the cases $n = 1$ and $n = 3$ the scaling of the central band is dominated by the eigenvalue of a 2-cycle and, respectively, a 4-cycle, i.e. not the fixed point, respectively, the 2-cycle as found for the substitution rules (cf table 2 and table 3).

We would like the reader to note that it is not clear to us why precisely some orbit in $\mathcal{A}$ (and not some other periodic orbit) determines the scaling behaviour of the central band. The argument in [5] is mainly heuristic to our opinion. Nevertheless, it is remarkable that in all cases the scaling behaviour can be explained with periodic orbits in the set $\mathcal{A}$. A profound discussion of this phenomenon is beyond the scope of the present paper. Note that in a slightly different model [8] the scaling behaviour of the central band can be explained rigorously because the initial condition $r_0(0)$ coincides with the point z_{-a}.

In order to make a comparison between scaling properties of the spectrum of quasiperiodic chains generated by invertible and non-invertible substitutions†, we calculated the energy spectrum of chains generated by the non-invertible substitution rule

$$\tilde{\sigma} = (a^2 b, ba) \tag{69}$$

where $\tilde{\sigma}$ is a so-called Fibonacci-squared substitution [31] since

$$M_{\tilde{\sigma}} = M_\sigma \cdot M_\sigma \tag{70}$$

with σ denoting the Fibonacci substitution rule. Because of (70), $\tilde{\sigma}$ obviously possesses the Pisot property and has $\det M_{\tilde{\sigma}} = 1$. Therefore it generates a quasiperiodic chain of rank-2.

The atomic surface of the quasiperiodic chain generated by $\tilde{\sigma}$ has a fractal atomic surface with $\Delta\theta > 1$ [31]. Thus this chain cannot be generated with the method of cut-and-project.

† For a comparison with scaling properties of chains, generated by a substitution rule, that are neither periodic nor quasiperiodic see, for example, [10].

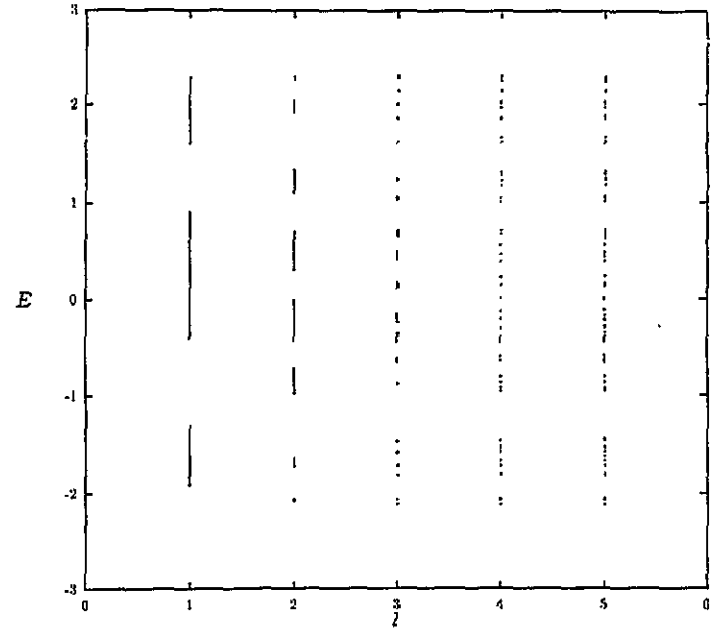

Figure 3. The energy spectrum for the first few periodic approximations to a quasiperiodic chain generated by the non-invertible substitution $\tilde{\sigma}(a)$ (cf (69)).

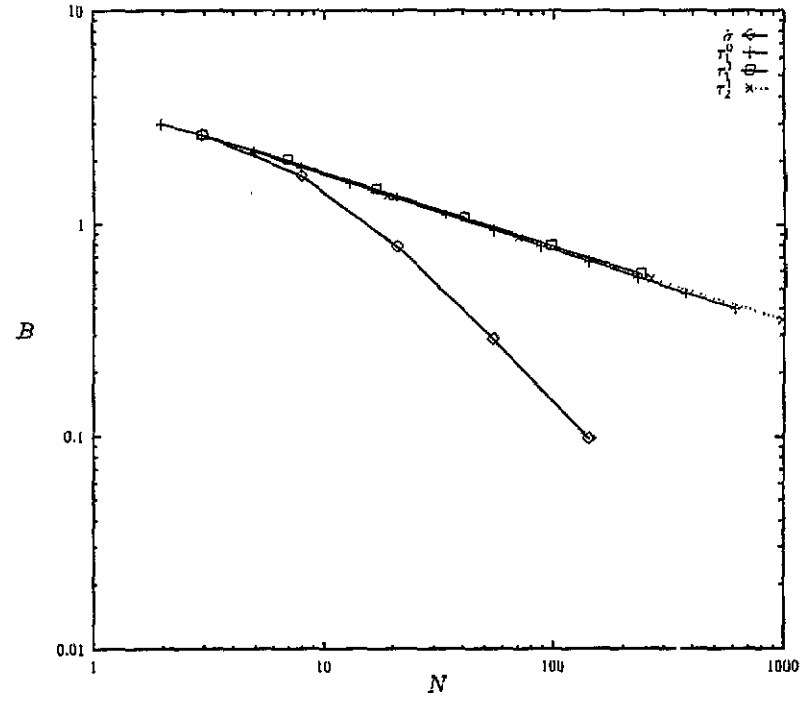

Figure 4. *Total bandwidth (B) against number of atoms N in the unit cell for the invertible substitutions* τ_1^0, τ_1^1, τ_2^1 and the non-invertible substitution $\tilde{\sigma}$.

In figure 3 we have plotted the energy spectrum for the first few approximations $\tilde{\sigma}^l(a)$. One immediately observes a striking difference: in the case of the non-invertible substitution the width of the energy bands tends to zero much more quickly than in the case of the invertible substitutions in figure 2 (particularly in comparison to the case of τ_1^0). Moreover, the typical large gaps in the Fibonacci spectrum are absent in the spectrum of $\tilde{\sigma}$.

In figure 4 the total bandwidth B, i.e. the Lebesgue measure of the energy spectrum, is set out on a double logarithmic scale against the number of atoms N of the unit cell in the periodic approximation. In the case of the invertible substitutions τ_1^0, τ_1^1 and τ_2^1 we find that $B \sim N^{-\beta}$ with $\beta = 0.347 \pm 0.005$. The non-invertible substitution $\tilde{\sigma}$ clearly shows a different behaviour.

An explanation for this difference can be found on the level of the trace maps. The speed with which B approaches zero is roughly speaking determined by the escape rate of points on the inner domain of the phase space of the trace map, and can be interpreted as a diffusion coefficient. As mentioned before, the dynamics of the trace maps of non-invertible substitutions differs in many respects from the dynamics of invertible substitutions. Whereas in the case of invertible substitutions the diffusion process, governed by the hyperbolic points on the invariant surface, is found to be uniform, the (in general) dissipative dynamics of trace maps of non-invertible substitutions induces a different diffusion process, giving rise to different scaling behaviour.

5. Summary and concluding remarks

In this paper the construction of quasiperiodic chains using substitution rules has been discussed. It was found that chains generated by invertible substitution rules share their typical properties with the well studied Fibonacci chain. In particular, we conjecture that quasiperiodic chains generated by a substitution rule can be obtained also with the method of cut-and-project if and only if the substitution rule is invertible. This conjecture is supported by an explicit calculation of the atomic surface for a two-parameter family of invertible substitutions.

Following the energy spectrum of a quasiperiodic tight-binding Hamiltonian we also find that the spectra of quasiperiodic chains generated by invertible substitutions behave Fibonacci-like. In particular, the scaling of the central band can be explained by the largest eigenvalue of the periodic point $(0, 0, -a)$ and the total bandwidth B shows universal scaling behaviour. Quasiperiodic chains generated by non-invertible substitution rules show a rather different behaviour. This is for instance illustrated by the scaling properties of the spectrum. The differences between spectra of quasiperiodic chains generated by invertible and non-invertible substitutions can be inferred directly from the spectra-determining trace maps. In the invertible case the maps preserve the volume and a one-parameter family of surfaces, giving rise to two-dimensional measure-preserving dynamics. However, in the non-invertible case the trace maps are truly three-dimensional and (in general) dissipative. One consequence of this difference is nicely illustrated in figure 4. These findings are confirmed by an independent study of Janssen [42].

Many other properties of the Fibonacci chain were studied over the years, which we have not discussed in this paper. For example, the energy spectrum of the tight-binding Fibonacci Hamiltonian has been shown to form a purely singular continuous Cantor set of Lebesque measure zero [28–30]. Another property which has been studied extensively is the nature of the electronic wavefunctions, in particular whether the wavefuctions are extended, localized or whether they have a different nature [7, 8, 11]. For these and all other properties of physical interest we conjecture their typical behaviour to extend throughout the class of

quasiperiodic chains generated by invertible substitutions. Quasiperiodic chains generated by non-invertible substitutions have a different nature.

Acknowledgments

We gratefully acknowledge valuable discussions with M Baake, T Janssen and JAG Roberts. Part of this research was carried out in the context of the research program of the Stichting voor Fundamenteel Onderzoek der Materie (FOM) which is financially supported by the Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO).

Appendix. Symmetry properties of trace maps of invertible substitutions

The trace map F_τ of an invertible substitution $\tau \in \mathrm{Inv}(S^*)$ is a dynamical system in $\mathbb{R}^3$. Such maps are volume preserving and moreover have a constant of the motion λ (cf equation (19)) giving rise to a foliation of the phase space. In case $\lambda > 0$, as in the tight-binding problem, the constant of motion is a non-compact surface with tetrahedral symmetry consisting of four cones connected to each other via a centre part. In this appendix some symmetry properties of the dynamics of the trace maps of invertible substitutions are pointed out, in particular for the special class introduced in section 3, and we discuss some consequences for the scaling behaviour of the centre band of the energy spectrum.

Let us first introduce the concept of $\tilde{k}$-symmetry in dynamical systems†. Consider a dynamical system which is an invertible map $L : \Omega \mapsto \Omega$, then we say that an invertible map $U : \Omega \mapsto \Omega$ is a $\tilde{k}$-symmetry of L if $\tilde{k}$ is the smallest positive integer such that [43]

$$U \circ L^{\tilde{k}} \circ U^{-1} = L^{\tilde{k}}. \tag{A1}$$

1-symmetries are usually called symmetries. In fact, $\tilde{k}$-symmetries of L are symmetries of $L^{\tilde{k}}$, but not vice-versa.

On the set of all symmetries of $L^{\tilde{k}}$ (the symmetry group of $L^{\tilde{k}}$), denoted $\mathcal{G}_{\tilde{k}}$, we define a map $\phi_L : \mathcal{G}_{\tilde{k}} \mapsto \mathcal{G}_{\tilde{k}}$ that acts on $M \in \mathcal{G}_{\tilde{k}}$ as

$$\phi_L(M) = L \circ M \circ L^{-1}. \tag{A2}$$

As such, $\tilde{k}$-symmetries of L correspond to $\tilde{k}$-cycles of ϕ_L.

It has been realized recently [43,44] that trace maps of substitutions $\tau \in \mathrm{Aut}(\mathcal{F}_2)$ possess $\tilde{k}$-symmetries. Let us consider these $\tilde{k}$-symmetries of trace maps of invertible substitutions $\tau \in \mathrm{Inv}(S^*)$. In particular, let us focus on $\tilde{k}$-symmetries of trace maps of invertible substitutions that are elements of the group $\mathcal{P}_\lambda$ of polynomial maps in $\mathbb{R}^3$ with integer coefficients that leave the surface λ (19) invariant. In [34] it has been shown that this group, independent of the value of λ, is given by

$$\mathcal{P}_\lambda = \langle F_\sigma, F_\alpha, F_\beta, I_{xy}, I_{yz}, P_{xy}, P_{yz} \rangle \tag{A3}$$

where F_σ, F_α and F_β are the trace maps of the corresponding substitutions in $\mathrm{Aut}(\mathcal{F}_2)$, with F_σ and F_α as given in section 4 and $F_\beta : (x, y, z) \mapsto (x, y, xy - z)$. In (A3), I_{ij} denotes the reflection in the line $i = j = 0$ and P_{ij} is the reflection in the plane $i = j$, with $i, j \in \{x, y, z\}$ and $i \neq j$. In fact $\langle I_{xy}, P_{xy}, P_{yz} \rangle$ is the tetrahedral group.

† To avoid confusion we use $\tilde{k}$ instead of k in the symmetry property because k already occurs as a label of the special class of invertible substitutions.

Let $\Sigma = \langle I_{xy}, I_{yz} \rangle$. Then, Σ is a $\tilde{k}$-symmetry group of F_τ, for any $\tau \in \mathrm{Inv}(S^*)$, where $\tilde{k} \in \{1, 2, 3\}$ (cf [43, 44]). In particular, ϕ_L induces a permutation on Σ, among its three non-trivial elements. Writing the action of ϕ_{F_τ} on Σ in a cycle notation we obtain

$$\phi_{F_\sigma}(\Sigma) = (I_{xy} I_{yz} I_{xz}) \qquad \phi_{F_{\sigma\alpha}}(\Sigma) = (I_{xy} I_{xz}) \tag{A4}$$

yielding

$$\phi_{F_{\tau_k^n}}(\Sigma) = (I_{xy} I_{yz} I_{xz})^k \circ (I_{xy} I_{xz})^n \,. \tag{A5}$$

Because the group Σ is closed under $\phi_{F_{\tau_k^n}}$ it is called a $\tilde{k}$-symmetry group of $F_{\tau_k^n}$. Here, $\tilde{k} = 3$ if $k \neq 0 \pmod 3$ and n is even, $\tilde{k} = 2$ if n is odd, and $\tilde{k} = 1$ if $k = 0 \pmod 3$ and n is even.

In table A1 we give for the same values of n and k as used in section 4, $\phi_{F_{\tau_k^n}}(\Sigma)$ and $F^\delta_{\tau_k^n}(\mathcal{A})$, with δ as in table 2.

Table A1. The action of $\phi_{F_{\tau_k^n}}$ on the group Σ and the orbits of $F^\delta_{\tau_k^n}(\mathcal{A})$.

k	n	$\phi_{F_{\tau_k^n}}(\Sigma)$	δ	$F^\delta_{\tau_k^n}(\mathcal{A})$
1	0	$(I_{xy}I_{yz}I_{xz})$	3	$(x_a x_{-a})\ (y_a y_{-a})\ (z_a z_{-a})$
1	1	$(I_{yz}I_{xz})\ (I_{xy})$	1	$(z_a z_{-a})\ (x_a y_a)\ (x_{-a} y_{-a})$
1	2	$(I_{xy}I_{yz}I_{xz})$	3	$(x_a x_{-a})\ (y_a y_{-a})\ (z_a z_{-a})$
1	3	$(I_{yz}I_{xz})\ (I_{xy})$	1	$(x_a y_a)\ (x_{-a} y_{-a})\ (z_a)\ (z_{-a})$
2	1	$(I_{xy}I_{yz})\ (I_{xz})$	1	$(x_a z_{-a})\ (x_{-a} z_a)\ (y_a y_{-a})$
			2	$(x_a)\ (y_a)\ (z_a)\ (x_{-a})\ (y_{-a})\ (z_{-a})$
2	2	$(I_{xy}I_{xz})(I_{yz})$	3	$(x_a)\ (y_a)\ (z_a)\ (x_{-a})\ (y_{-a})\ (z_{-a})$

From table A1 we find in the case of τ_1^0 and τ_1^2 that the scaling determining two-orbits of $F^\delta_{\tau_k^n}$ are symmetric. Moreover, their two points x and y are related through a symmetry M, i.e. $Mx = y$. Hence, the dynamics near x is equivalent to the dynamics near y: in case we follow such a symmetric periodic orbit, we find uniform scaling behaviour. In the case of τ_2^1 we find the determining two-orbit $x_a z_{-a}$ (or $x_{-a} z_a$) to be asymmetric. This asymmetry causes the oscillatory behaviour in the scaling constant that is found if one considers $\delta = 1$ in stead of $\delta = 2$.

Note that in this appendix we confined the discussion to $\tilde{k}$-symmetries, although trace maps are well known to also possess reversing $\tilde{k}$-symmetries (cf [43, 44]). Although many trace maps of invertible substitutions are reversible, there seem to be ones that possess no reversing symmetries at all [44]. However, the physical relevance of these reversing symmetries, e.g. for the energy spectrum, are as yet unclear.

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