Singular continuous electron spectrum for a class of circle sequences

1995 J. Phys. A: Math. Gen. 28 479

(http://iopscience.iop.org/0305-4470/28/2/022)

J. Phys. A: Math. Gen. 28 (1995) 479–495. Printed in the UK

Singular continuous electron spectrum for a class of circle sequences

Michael Hörnquist† and Magnus Johansson‡

Department of Physics and Measurement Technology, Linköping University, S-581 83 Linköping, Sweden

Received 31 August 1994, in final form 8 November 1994

Abstract. We derive substitution rules for a class of binary quasiperiodic sequences generated by circle maps whose rotation numbers are obtained from the precious means. The nature of the electron spectra for the corresponding diatomic chains is studied in the nearest-neighbour on-site tight-binding approximation using the transfer-matrix technique. By studying properties of the trace maps, we find that the spectrum is purely singular continuous in most of the studied cases.

1. Introduction

During the last decade, much theoretical and experimental study has been devoted to the subject of one-dimensional deterministic aperiodic systems. Concerning the theoretical investigation of the electronic properties of such systems, the nearest-neighbour on-site tight-binding model or, equivalently, the discrete Schrödinger equation, described in natural units by

$$V_n c_n + t(c_{n-1} + c_{n+1}) = E c_n \tag{1}$$

has received the most attention. It has been realized that these systems exhibit a large variety in their spectral properties, depending on the explicit choice of the on-site potential. If the on-site potential V_n takes values from a continuous set, as in models for incommensurate crystals, the nature of the spectrum depends generically on the magnitude of the amplitude of the on-site potential compared to the hopping integral t. The spectrum is usually absolutely continuous when the potential amplitude is small, a pure point when the amplitude is large and has a mixed character with mobility edges separating regions with absolutely continuous and point character for intermediate amplitudes [1]. A notable exception from this generic behaviour is the famous Aubry–André model [2], where the on-site potential V_n is obtained from

$$V_n = V\cos(2\pi n\zeta + \varphi). \tag{2}$$

Due to duality, the character of the spectrum for this model will change from purely absolutely continuous to pure point at the critical value $V = 2|t|$, where the spectrum

† E-mail address: micho@ifm.liu.se

‡ E-mail address: majoh@ifm.liu.se

is purely singular continuous [3,4]. Moreover, if the incommensurability ζ is chosen as a Liouville number [3], the spectrum of this model will keep its singular continuous nature even for supercritical values of the potential strength.

If singular continuous energy spectra are somewhat exceptional in the study of incommensurate crystals, they appear much more frequently in models for one-dimensional quasicrystals or aperiodic superlattices, where the on-site potential is restricted to take values from a finite set of numbers. Examples of models where the spectrum has been rigorously proved to be singular continuous regardless of the potential strength are those obtained by choosing the on-site potential according to Fibonacci [5], Thue–Morse [6,7] and period-doubling [7] sequences. These results were obtained using the trace-map technique (see section 3) which is applicable to all sequences that can be generated by substitution rules.

In order to obtain a general description of the spectral properties of substitutionally generated systems, an important result was obtained recently by Bovier and Ghez [8,9]. In terms of some properties of the substitution rule and its corresponding trace map, they give sufficient conditions for the spectrum to be purely singular and singular continuous, respectively. (These results will be described in detail in section 3.) In this context, one may note that, although most of the sequences treated as examples in [8] fulfil at least the conditions to have a spectrum of zero Lebesgue measure, there is an exception in the Rudin–Shapiro sequence. For this sequence, numerical investigations have indicated that the spectral properties depend on the potential strength [10,11], and that for most values of the on-site amplitude the spectrum has a pure point character [11]. One should thus bear in mind that the class of sequences giving singular continuous spectra probably does not include all sequences that can be generated by substitutions, and that further investigation of the sequences which belong to this class is important.

One sequence shown in [8] to belong to this class is the one usually denoted in the literature as the 'circle sequence' [8,10,12,13]. It is a binary quasiperiodic sequence obtained from a circle map by dividing the circle into two equal parts representing the two values in the sequence and using a rotation number related to the golden mean (see section 2). It could also be viewed as the sequence obtained by taking the sign of the potential in the Aubry–André model (2). The rigorous treatment of the spectral properties for this system was possible due to the work of Aubry *et al* [14] who showed that the circle sequence could also be generated by a substitution rule using a process that will be described in section 2. However, this technique is by no means restricted to rotation numbers related to the golden mean, and one may ask the question whether other rotation numbers will also result in sequences giving singular continuous spectra. As a first step towards the answer to this question, we will, in this paper, treat the case with rotation numbers obtained from arbitrary precious means as defined by (15) below. To make the paper as self-contained as possible, we will state the main results from [14] and [8] in sections 2 and 3, respectively. As an illustrative example, we study here, in particular, a sequence related to the silver mean. We derive its substitution rule in section 2, its corresponding trace map in section 3 and show that it fulfils the conditions to give a singular continuous energy spectrum. The case of a general precious mean is then treated in section 4 and concluding remarks are made in section 5.

2. The sequences

One standard way of generating binary quasiperiodic sequences is by using a circle map (see, e.g., [14]). For completeness, we give here a short recapitulation of the method.

Consider a circle with unit circumference. Let Δ be the fraction of one of the two elements in the sequence and let ζ be an irrational number. Divide the circumference of the circle into two parts, of length Δ and $1-\Delta$, respectively, and associate the value $+V$ to one part and $-V$ to the other. By walking around the circle in steps of length ζ, and for each step picking the value of either $+V$ or $-V$, one obtains a binary quasiperiodic sequence with the two incommensurable frequencies ζ and 1. Analytically the sequence is given as

$$(V_n)_{n=0}^{\infty} \tag{3}$$

where

$$V_n = V\{-1 + 2[\mathrm{Int}(n\zeta) - \mathrm{Int}(n\zeta - \Delta)]\}. \tag{4}$$

Here $\mathrm{Int}(x)$ denotes the integer part of x, defined as $\mathrm{Int}(x) = \max\{j \in \mathbb{Z} : j \leqslant x\}$. All sequences which can be constructed in this way we will collectively call *circle sequences.* Note that this is a generalization compared to what is usually denoted as 'the circle sequence' [8, 10, 12, 13], which corresponds to $\Delta = \frac{1}{2}$ and $\zeta = \tau^{-2}$, where τ is the golden mean $(\sqrt{5}+1)/2$.

To facilitate analytical investigations of physical properties of systems generated by these sequences, Aubry *et al* [14] have proposed a way to obtain a *substitution rule* which generates a sequence equivalent to the one obtained from the circle map. We will now briefly discuss some formalism concerning substitution rules. The notation will mainly follow the one used in [8].

Let $\mathcal{A}$ be a finite set, called an alphabet, the elements of which we call letters. Any ordered combination of elements in $\mathcal{A}$, where each element can occur an arbitrary number of times, is called a word. The set of all words is denoted by $\mathcal{A}^*$, which makes it possible to define what we mean by a substitution ξ.

Definition 1. Let ξ be an operator $\mathcal{A} \to \mathcal{A}^*$. We then call ξ a substitution rule for the alphabet $\mathcal{A}$.

Since we want the substitution rule to apply to elements in $\mathcal{A}^*$ as well as in $\mathcal{A}$, we extend it to be an operator $\mathcal{A}^* \to \mathcal{A}^*$ by the rule

$$\xi(\omega) = \xi(\alpha_0)\xi(\alpha_1)\cdots\xi(\alpha_n) \tag{5}$$

where $\omega = \alpha_0\alpha_1\cdots\alpha_n \in \mathcal{A}^*$ and $\alpha_0, \alpha_1, \ldots, \alpha_n \in \mathcal{A}$. We will also use the notation ξ^k to denote a k times repeated application of the substitution rule. If a substitution rule is to be useful in generating an infinite sequence of the form $\xi^{\infty}(\alpha)$, where $\alpha \in \mathcal{A}$, it has to possess at least one fixpoint.

Definition 2. Let ξ be a substitution rule and ω a one-sided infinite word $\omega \in \mathcal{A}^*$. If

$$\xi(\omega) = \omega \tag{6}$$

we call ω a fixpoint to the substitution rule ξ.

We will use both right and left fixpoints, where the former corresponds to sequences such as $(V_n)_0^\infty$ and the latter to $(V_n)_{-\infty}^{-1}$. There is an easily verifiable criterion [15] for the existence of at least one right fixpoint to a substitution (namely $\xi^\infty(\alpha^{(0)})$).

(i) There exists a letter $\alpha^{(0)}$, $\alpha^{(0)} \in \mathcal{A}$, such that the word $\xi(\alpha^{(0)})$ begins with $\alpha^{(0)}$.

(ii) The length of the words $\xi^k(\alpha^{(0)})$ goes to infinity as $k \to \infty$.

In the same way, we can guarantee the existence of a left fixpoint by replacing the first condition above with 'there exists a letter $\alpha_l^{(0)}$ such that the word $\xi(\alpha_l^{(0)})$ ends with $\alpha_l^{(0)}$'.

The idea in [14] of obtaining a substitution rule for the binary sequence defined by (3) and (4) relies on the introduction of a set of elementary transformations, denoted by $\hat{S}$, $\hat{T}_1$, $\hat{T}_2$ and $\hat{T}_3$, resulting in an exact renormalization transform acting on the parameters (Δ, ζ). Each elementary transformation is associated with an elementary substitution rule, which we denote by $\xi_S, \xi_{T_1}, \xi_{T_2}$ and ξ_{T_3}, respectively. Although the final sequence should be binary, we have to use an alphabet with three elements, referred to as $\mathcal{A} = \{A, B, C\}$. Before we introduce these transformations, we have to review some number theoretical results. They will be stated here without proofs, which can be found in [14, 16]. We choose to rewrite ζ as a continued fraction expansion, i.e. as

$$\zeta = \cfrac{1}{a_1 + \cfrac{1}{a_2 + \cfrac{1}{\cdots}}} \tag{7}$$

where all a_n are non-negative integers. It is possible to show [16] that the sequence of best rational approximants to ζ is $(r_n/s_n)_{n=0}^\infty$, where

$$\begin{cases} r_n = a_n r_{n-1} + r_{n-2} \\ r_0 = 0 \qquad r_1 = 1 \end{cases} \tag{8}$$

and

$$\begin{cases} s_n = a_n s_{n-1} + s_{n-2} \\ s_0 = 1 \qquad s_1 = a_1. \end{cases} \tag{9}$$

Let δ_n be a measure of how close every rational approximation (r_n/s_n) is to ζ, i.e. set

$$\delta_n = s_n\zeta - r_n. \tag{10}$$

Now it is possible to show [14] that any Δ can be expanded in δ_n, i.e. we can always find non-negative integer coefficients p_n such that

$$\Delta = \sum_{n=0}^{\infty} p_n \delta_n. \tag{11}$$

There is also a unique way of determining the coefficients p_n to obtain the best approximation of Δ with a finite number of terms. Namely

$$\begin{cases} \text{set } R_0 = \Delta \\ p_n = \min\left\{a_{n+1}, 1 + \mathrm{Int}\left(\dfrac{R_n}{\delta_n}\right)\right\} \\ R_{n+1} = R_n - p_n\delta_n. \end{cases} \tag{12}$$

Once the p_n are obtained, it is straightforward to find the transformation which gives the substitution rule. First, define the elementary transformations $\hat{S}$, $\hat{T}_1$, $\hat{T}_2$ and $\hat{T}_3$ as:

$$\hat{S}: \quad \begin{aligned} & a'_1 = a_2 + 1 \\ & a'_n = a_{n+1} \qquad n \geqslant 2 \\ & p'_0 = p_1 + 1 \\ & p'_n = p_{n+1} \qquad n \geqslant 1 \\ & \xi_S(A) = C \qquad \xi_S(B) = B \qquad \xi_S(C) = A \end{aligned}$$

$$\hat{T}_1: \quad \begin{aligned} & a'_1 = a_1 - 1 \\ & a'_n = a_n \qquad n \geqslant 2 \\ & p'_n = p_n \qquad n \geqslant 0 \\ & \xi_{T_1}(A) = AC \qquad \xi_{T_1}(B) = BC \qquad \xi_{T_1}(C) = C \end{aligned}$$

$$\hat{T}_2: \quad \begin{aligned} & a'_1 = a_1 - 1 \\ & a'_n = a_n \qquad n \geqslant 2 \\ & p'_0 = 1 \\ & p'_n = p_n \qquad n \geqslant 1 \\ & \xi_{T_2}(A) = AB \qquad \xi_{T_2}(B) = AC \qquad \xi_{T_2}(C) = C \end{aligned}$$

$$\hat{T}_2: \quad \begin{aligned} & a'_1 = a_1 - 1 \\ & a'_n = a_n \qquad n \geqslant 2 \\ & p'_0 = p_0 - 1 \\ & p'_n = p_n \qquad n \geqslant 1 \\ & \xi_{T_3}(A) = AB \qquad \xi_{T_3}(B) = B \qquad \xi_{T_3}(C) = C. \end{aligned}$$

The A's, B's and C's are the elements of the alphabet $\mathcal{A}$ upon which the substitution acts, the p_n are from the algorithm in (12) and the a_n from the continued fraction expansion in (7). Then, acting on the a_n and p_n, let

(i) $\hat{S}$ apply when $a_1 = 1$;
(ii) $\hat{T}_1$ apply when $a_1 > 1$ and $p_0 = 1$;
(iii) $\hat{T}_2$ apply when $a_1 > 1$, $p_0 = 2$ and $p_1 > 0$; and
(iv) $\hat{T}_3$ apply when $a_1 > 1$ and either $p_0 > 2$ or $p_1 = 0$.

Finally, let $a_n = a'_n$ and $p_n = p'_n$ for all n and repeat the procedure.

If the a_n and p_n are periodic (at least for $n \geqslant N$, where N is some fixed integer) we will also, after a while, obtain periodicity in the string of $\hat{S}$ and $\hat{T}_i$, and the total transformation is obtained as a product of the elementary transformations in the period. This total transformation will be an exact renormalization operation which the associated substitution rule ξ is defined as the composition of the corresponding elementary substitution rules. In general, there will be a string of elementary transformations, a 'transient', preceding the period and in such a case we must apply to the word $\xi^{\infty}(\alpha^{(0)})$ the substitution rule corresponding to the transient in order to obtain the original sequence. Finally, introduce the operator $\nu : \mathcal{A} \to \mathbb{R}$ as

$$\begin{cases} \nu(A) \equiv +V \\ \nu(B) \equiv -V \qquad \text{if } \Delta < \zeta \\ \nu(C) \equiv -V \end{cases} \tag{13}$$

or

$$\begin{cases} \nu(A) \equiv +V \\ \nu(B) \equiv +V \qquad \text{if } \Delta > \zeta \\ \nu(C) \equiv -V \end{cases} \tag{14}$$

and set $V_n = \nu(\alpha_n)$, where $\alpha_n \in \mathcal{A}$ is the nth letter in the sequence $\xi^{\infty}(\alpha^{(0)})$. With this we are back to the sequence in (3).

Generalizing the ordinary 'circle sequence', we now turn our attention to the case when ζ is equal to the inverse of an arbitrary precious mean, i.e. when all non-negative integers a_n in (7) are equal, $a_n = a$, $n = 1, 2, \ldots$. Keeping the value $\Delta = \frac{1}{2}$, the pair (Δ, ζ) can be expressed as

$$\begin{cases} \Delta = \frac{1}{2} \\ \zeta = \frac{1}{2}\sqrt{a^2+4} - a. \end{cases} \tag{15}$$

The case $a = 1$ is just the image by S of the case $\zeta = \tau^{-2}$ discussed above. The sequences $(r_n)_{n=0}^{\infty}$ and $(s_n)_{n=0}^{\infty}$ from (8) and (9) are now connected as $r_n = s_{n-1}$, which turns the r_n into 'generalized Fibonacci numbers of order a'. Explicitly this means

$$\begin{cases} r_n = ar_{n-1} + r_{n-2} \\ r_0 = 0 \qquad r_1 = 1 \end{cases} \tag{16}$$

which is possible to write in closed form as

$$r_n = \frac{\zeta^{-n} - (-\zeta)^n}{\zeta^{-1} + \zeta}. \tag{17}$$

We will also need an expression for the δ_n, which can be obtained from (10) and (17) as

$$\delta_n = r_{n+1}\zeta - r_n = (-1)^n \zeta^{n+1}. \tag{18}$$

To illustrate the main ideas, we will now study the particular case $a = 2$. In section 4 we will return to the more general case of an arbitrary a.

With $a = 2$ in (15), we obtain

$$\begin{cases} \Delta = \frac{1}{2} \\ \zeta = \sqrt{2} - 1. \end{cases} \tag{19}$$

From the algorithm in (12), we obtain $(p_n)_{n=0}^{\infty} = (2, 2, 1, 2, 1, 2, 1, 2, \ldots)$. This sequence is periodic and so is the sequence of a_n. This makes it possible to associate a finite substitution rule with the sequence generated by the circle map. Before we arrive at the periodicity in the string, we have a transient. Here this transient turns out to be the $\hat{T}_2$-transformation, applied once. A calculation gives the period for the transformation as

$$\hat{T} = \hat{S}\hat{T}_3\hat{T}_2\hat{S}\hat{T}_2\hat{T}_1 \tag{20}$$

where the notation $\hat{T}$ has been used to denote the whole transformation. The substitution rule associated with this transformation is now obtained as $\xi = \xi_S\xi_{T_3}\xi_{T_2}\xi_S\xi_{T_2}\xi_{T_1}$, acting on the letters A, B and C, respectively. Explicitly,

$$\begin{cases} \xi(A) = ACBACBB \\ \xi(B) = ACBBCBB \\ \xi(C) = CBB. \end{cases} \tag{21}$$

To arrive at the sequence associated with the values of the parameters (Δ, ζ) given in (19), we start with a seed $\alpha^{(0)}$ upon which we let the substitution ξ act an infinite number of times. Subsequently, we apply to the generated sequence the elementary substitution that preceded the period, i.e. we apply the transient ξ_{T_2}, which means that we turn every A in the final sequence into AB and every B into AC. In the case when we do *not* use the transient, we obtain a sequence, which we will call the silver circle sequence, corresponding to parameters (Δ', ζ') with values

$$\begin{cases} \Delta' = \dfrac{\zeta}{2(1+\zeta)} = \dfrac{1}{2}\left(1 - \dfrac{1}{\sqrt{2}}\right) \\ \zeta' = \dfrac{1}{1+\zeta} = \dfrac{1}{\sqrt{2}}. \end{cases} \tag{22}$$

This can be seen from the formulae for the transient, i.e. from the elementary transformation $\hat{T}_2$ above. The last step is to obtain from the letters A, B, C the original sequence of $\pm V$. This is achieved by applying the operator ν in the form of (14), if we use the transient to obtain the sequence described by (19), and otherwise in the form of (13) to obtain the sequence described by (22).

For further use we introduce the concept of primitive substitution [15].

Definition 3. A substitution ξ on an alphabet $\mathcal{A}$ is called primitive if there exists an integer k such that for any two letters $\alpha, \beta \in \mathcal{A}$, the word $\xi^k(\alpha)$ contains the letter β.

We see immediately that our substitution rule (21) is primitive and that $k = 2$ in the definition is sufficient. We also see from the criterion below definition 2 that it has one left and two right fixpoints which are obtained for $\alpha_l^{(0)} = B$, $\alpha^{(0)} = A$ and $\alpha^{(0)} = C$. Note, however, that these two values of $\alpha^{(0)}$ result in the same sequence, except for the first two elements corresponding to $n = 0$ and $n = 1$, respectively.

3. Electron spectrum

Consider the sequence $(V_n)_{n=0}^{\infty}$ defined in (3) and (4) and extend it to negative n as described in [9]. This can always be achieved in the following by choosing an appropriate generator

$\alpha_l^{(0)}$, of a left fixpoint and then concatenate the two fixpoints to an infinite sequence $\xi^\infty(\alpha_l^{(0)})\xi^\infty(\alpha^{(0)})$, observing that the word $\alpha_l^{(0)}\alpha^{(0)}$ is contained in $\xi^\infty(\alpha^{(0)})$ as requested in [9]. With this extension, equation (4) holds also for negative n if we choose $\alpha_l^{(0)}$ properly. This is indeed the case for all sequences that we consider.

Let this sequence represent a one-dimensional quasiperiodic structure of two different types of atoms placed equidistantly on an abscissa. Let V_n also denote the potential on site n and stick to the form of the Schrödinger equation given in (1). If we define the transfer matrix T_n as

$$T_n = \begin{pmatrix} \frac{E-V_n}{t} & -1 \\ 1 & 0 \end{pmatrix} \tag{23}$$

we can rewrite (1) as

$$\begin{pmatrix} c_{n+1} \\ c_n \end{pmatrix} = T_n \begin{pmatrix} c_n \\ c_{n-1} \end{pmatrix}. \tag{24}$$

This makes it natural to consider the transfer matrices as operators $T : \mathcal{A} \to SL(2, \mathbb{R})$ via

$$T(\alpha) = \begin{pmatrix} \frac{E-\nu(\alpha)}{t} & -1 \\ 1 & 0 \end{pmatrix} \tag{25}$$

where $\alpha \in \mathcal{A}$ and ν is defined by (13) or (14). We can also let T operate on elements in $\mathcal{A}^*$, i.e. words, according to

$$T(\omega) = T(\alpha_n)T(\alpha_{n-1})\cdots T(\alpha_0) \tag{26}$$

where $\omega = \alpha_0\alpha_1\cdots\alpha_n \in \mathcal{A}^*$ and $\alpha_0, \alpha_1, \ldots, \alpha_n \in \mathcal{A}$. Note that the order of matrix multiplication is opposite to the order of the letters in the word. This can be seen from (24). Now we can combine the map T with the substitution rule ξ via

$$\xi^n[T(\omega)] \equiv T^n(\omega) \equiv T[\xi^n(\omega)] \qquad \omega \in \mathcal{A}^* \tag{27}$$

where ξ^n as before is understood to be the substitution rule applied n times. This makes it possible for us to write $T^n(\alpha)$ expressed as

$$T^n(\alpha) = \prod_{\beta \in X} T^{n-1}(\beta) \qquad \alpha, \beta \in \mathcal{A} \tag{28}$$

where X is the set having the letters from $\xi(\alpha)$ as elements. The two theorems from [8] that we use below, however, do not deal with the transfer matrices themselves, but with their traces. Therefore, we have to introduce the concept of trace map, and, also from [8], the concepts of reduced trace map and semi-primitive substitution.

Definition 4. Let $\omega \in \mathcal{A}^*$ and use the notation $x_n(\omega) \equiv \mathrm{Tr}[T^n(\omega)]$. Extending the action of ξ in the same way as in (27), we write $x_n(\omega) \equiv \xi[x_{n-1}(\omega)]$. With a trace map we mean a mapping $\mathbb{R}^k \to \mathbb{R}^k$ such that $x_n(\omega)$ is a function of $x_{n-1}(\omega)$, $x_n \in \mathbb{R}^k$, k is the cardinality of some set $\mathcal{B} \subset \mathcal{A}^*$ and $\omega \in \mathcal{B}$.

The reason why we introduce a new set $\mathcal{B}$ is because it is, in general, not possible to find a trace map just for $\mathcal{A}$ for an arbitrary substitution rule. However, if we enlarge to a finite set $\mathcal{B}$ such that $\mathcal{A} \subset \mathcal{B} \subset \mathcal{A}^*$, it is shown in [12] that we can always find such a trace map if we choose $\mathcal{B}$ in an appropriate way. In order to obtain an explicit expression for the trace map, one can, for example, use the formula

$$\mathrm{Tr}(\Theta\Lambda\Theta\Xi) = \mathrm{Tr}(\Theta\Lambda)\,\mathrm{Tr}(\Theta\Xi) + \mathrm{Tr}(\Lambda\Xi) - \mathrm{Tr}(\Lambda)\,\mathrm{Tr}(\Xi) \tag{29}$$

which is obtained from the Cayley–Hamilton theorem and valid for all matrices of the group $SL(2,\mathbb{R})$.

Consider now the special case of the silver circle sequence, defined from the substitution rule in (21) with $\alpha^{(0)} = A$ and $\alpha_l^{(0)} = B$ (or, equivalently, from the values (Δ', ζ') in (22)). The two theorems from [8] apply only to sequences generated by a substitution rule which acts on single letters and, therefore, we cannot keep the values (Δ, ζ) from (19). Note also that for the use of the theorems, it does not matter if we apply ν from (13) or from (14), or even if we let A, B and C take three different values. From an inequality in [12], it is clear that our set $\mathcal{B}$ will not contain more than eight letters. However, in [13] it is shown that a substitution rule consisting of m letters has $3m - 3$ as a minimum number of elements in $\mathcal{B}$. Here it turns out that we can choose the set as $\mathcal{B} = \{A, B, C, ACB, BC, AC\}$. Introduce the following abbreviated notation for the traces of the transfer matrices associated with the elements in $\mathcal{B}$:

$$\begin{cases} x_n = \mathrm{Tr}[T^n(A)] \\ y_n = \mathrm{Tr}[T^n(B)] \\ z_n = \mathrm{Tr}[T^n(C)] \\ r_n = \mathrm{Tr}[T^n(ACB)] = \mathrm{Tr}[T^n(B)T^n(C)T^n(A)] \\ v_n = \mathrm{Tr}[T^n(BC)] \\ w_n = \mathrm{Tr}[T^n(AC)]. \end{cases} \tag{30}$$

Using (29), it is simple but tedious to obtain a mapping from generation n to generation $n+1$. Performing the calculations in all cases (a detailed derivation of the first case can be found in the appendix) gives the following trace map:

$$\begin{cases} x_{n+1} = (y_n r_n - w_n) r_n - y_n \\ y_{n+1} = (y_n v_n - z_n)(y_n r_n - w_n) - x_n \\ z_{n+1} = y_n v_n - z_n \\ r_{n+1} = [(y_n v_n - z_n)(y_n r_n - w_n) - x_n][r_n(y_n v_n - z_n)(y_n r_n - w_n) - r_n x_n \\ \qquad\qquad - y_n(y_n v_n - z_n) + v_n] - y_n r_n + w_n \\ v_{n+1} = (y_n v_n - z_n)[(y_n v_n - z_n)(y_n r_n - w_n) - x_n] - y_n r_n + w_n \\ w_{n+1} = [(y_n v_n - z_n)(y_n r_n - w_n) - x_n] r_n - (y_n v_n - z_n) y_n + v_n. \end{cases} \tag{31}$$

Note that there is nothing unique about this specific trace map, or even with the set $\mathcal{B}$. Several different maps can be obtained for every substitution rule, which is clear from the construction above. In order to proceed from here, we need the corresponding reduced trace map, defined as the mapping that is obtained if, in the full trace map, we keep only the monomial of highest degree and neglect all other terms. With degree we mean the number of letters associated with each variable, i.e. $\deg(x_n) = \deg(y_n) = \deg(z_n) = 1$, $\deg(v_n) = \deg(w_n) = 2$ and $\deg(r_n) = 3$. For example, $\deg(y_n v_n) = 3$. Keeping this in mind, it is clear from (29) that every trace map has a unique reduced trace map with all coefficients equal to unity. In the case of the silver circle sequence, the reduced trace-map becomes

$$\begin{cases} x_{n+1} = y_n r_n^2 \\ y_{n+1} = y_n^2 r_n v_n \\ z_{n+1} = y_n v_n \\ r_{n+1} = y_n^4 r_n^3 v_n^2 \\ v_{n+1} = y_n^3 r_n v_n^2 \\ w_{n+1} = y_n^2 r_n^2 v_n . \end{cases} \tag{32}$$

Omitting all subscripts in the reduced trace map and changing the names of the elements in the set $\mathcal{B}$, such as $\mathcal{B} = \{x, y, z, r, v, w\}$, we can consider (32) as a mapping $\phi : \mathcal{B} \to \mathcal{B}^*$. This mapping ϕ is not uniquely defined because the order between the elements is not specified. The ambiguity will not, however, give rise to any problems. To characterize an important property of the mapping ϕ, we introduce the concept of semi-primitive substitution [8].

Definition 5. A substitution ϕ on an alphabet $\mathcal{B}$ is called semi-primitive if

(i) there exists a subset $\mathcal{C} \subset \mathcal{B}$ such that ϕ maps $\mathcal{C}$ into $\mathcal{C}^*$ (where $\mathcal{C}^*$ is defined from $\mathcal{C}$ in the same way as $\mathcal{A}^*$ from $\mathcal{A}$ above) and the restriction of ϕ to $\mathcal{C}$ is a primitive substitution (cf definition 3); and

(ii) there exists a positive integer m such that for each letter $\beta \in \mathcal{B}$, $\phi^m(\beta)$ contains at least one letter from $\mathcal{C}$.

To see that ϕ really is semi-primitive, we choose the set $\mathcal{C}$ as $\mathcal{C} = \{y, r, v\}$. Now it is clear that $\mathcal{C} \subset \mathcal{B}$ and that ϕ maps $\mathcal{C}$ into $\mathcal{C}^*$ (cf (32)). From definition 3, it is obvious that the restriction of ϕ to $\mathcal{C}$ is a primitive substitution with $k = 1$. Finally, we note that whatever letter in $\mathcal{B}$ we start with, in the next step when the substitution has been applied once, we will always have at least *two* letters from $\mathcal{C}$. Hence, the substitution ϕ associated with our reduced trace map is semi-primitive.

From [8] we now obtain the following theorem.

Theorem 1. Let ξ be a non-constant primitive substitution with no constant iterate defined on a finite alphabet $\mathcal{A}$. Let ν be a non-constant map $\mathcal{A} \to \mathbb{R}$ and H the Schrödinger operator implicitly defined by (1). Suppose there exists a trace map with an associated substitution ϕ, defined on an alphabet $\mathcal{B}$ as described above, which is semi-primitive. Assume further that there exists $k < \infty$ and $\alpha^{(0)} \in \mathcal{A}$ such that $\xi^k(\alpha^{(0)})$ contains the word $\beta\beta$ for some $\beta \in \mathcal{B}$. Then the spectrum of H is singular.

Proof. See [8].

We have already noticed that our substitution ξ is primitive and that ϕ is semi-primitive. Further, we have that with $\alpha^{(0)} = A \in \mathcal{A}$, $\xi(A) = ACBACBB$. Since $B \in \mathcal{B}$, the theorem applies and the spectrum is singular, i.e. supported on a set of zero Lebesgue measure. In [8] we also find the following theorem.

Theorem 2. Suppose the hypotheses of theorem 1 are satisfied. If, in addition, there exists $n_0 < \infty$ such that $\xi^{n_0}(\alpha^{(0)}) = \xi^m(\gamma_0)\xi^m(\gamma_0)\omega$, where $\gamma_0 \in \mathcal{C}$ and contains $\alpha^{(0)}$, $\omega \in \mathcal{A}^*$ and m are arbitrary, then the spectrum of H is purely singular continuous and supported on a generalized Cantor set (i.e. a perfect nowhere dense set) of zero Lebesgue measure.

Proof. See [8].

As before we have that $\alpha^{(0)} = A \in \mathcal{A}$ and that $\xi(A) = ACBACBB$, but this time we focus our attention upon the fact that $ACB \in \mathcal{C}$ (more correctly, $r \in \mathcal{C}$, but $r_n = \mathrm{Tr}[T^n(ACB)]$) and that $\alpha^{(0)} = A$ is contained in ACB. Hence, it suffices with $n_0 = 1$ and $m = 0$ for the theorem to apply and the conclusion is reached that the spectrum is purely singular continuous and supported on a generalized Cantor set. (Note that there is a more general formulation of this theorem in [9], but that the version stated here is sufficient for our purposes.)

4. General precious means

Now we drop the restriction $a = 2$ and instead let a be an arbitrary positive integer, i.e. we have the general values of (Δ, ζ) from (15). It turns out that we have to distinguish between the cases when a is even and odd, respectively. There is, however, no fundamental difference in the calculations between the cases. The odd case is just more tedious.

We will follow the same lines as for the silver circle sequence above. First, we need to determine the p_n from the expansion in (11). This is achieved with algorithm (12) and the values of δ_n from (18). For a even, we now have

$$\begin{cases} p_0 = \frac{1}{2}a + 1 \\ p_{2n+1} = a \\ p_{2n+2} = \frac{1}{2}a \end{cases} \qquad n = 0, 1, 2, \ldots \tag{33}$$

and for a odd

$$\begin{cases} p_0 = \frac{1}{2}a + 1 \\ p_{3n+1} = \frac{1}{2}a + 1 \\ p_{3n+2} = a \\ p_{3n+3} = \frac{1}{2}a - 1. \end{cases} \qquad n = 0, 1, 2, \ldots. \tag{34}$$

In deriving (33) and (34), we have used the relation $\zeta^{-1} = a + \zeta$. The periodicity can be shown with induction over R_n/δ_n in (12).

The substitution rules can now be derived for arbitrary values of a in the same way as before. Working with the elementary transformations defined in section 2, we obtain for a even the period

$$\hat{T}_{\text{even}} = \hat{S}\hat{T}_3^{a-1}\hat{T}_2\hat{S}\hat{T}_3^{a/2-1}\hat{T}_2\hat{T}_1^{a/2} \tag{35}$$

and the transient $\hat{T}_3^{a/2-1}\hat{T}_2\hat{T}_1^{a/2-1}$. Note that for $a = 2$ we recover the period given in (20) and the transient $\hat{T}_2$. When $a \geqslant 3$ and odd the period becomes

$$\hat{T}_{\text{odd}} = \hat{S}\hat{T}_3^{(a-1)/2}\hat{T}_2\hat{T}_1^{(a-1)/2}\hat{S}\hat{T}_3^{a-1}\hat{T}_2\hat{S}\hat{T}_3^{(a-3)/2}\hat{T}_2\hat{T}_1^{(a+1)/2} \tag{36}$$

and the transient $\hat{T}_3^{(a-3)/2}\hat{T}_2\hat{T}_1^{(a-1)/2}$. These transients are not the shortest possible, but instead we have chosen them in such a way that the sequences $(a_n)_{n=1}^{\infty}$ and $(p_n)_{n=0}^{\infty}$ turn into

$$\begin{cases} (a_n')_{n=1}^{\infty} = (1, a, a, a, \ldots) \\ (p_n')_{n=0}^{\infty} = (1, p_1, p_2, p_3, \ldots) \end{cases} \tag{37}$$

after they have been applied. This will correspond to values of (Δ, ζ) other than those in (15), depending on whether a is even or odd. From (7), (11), (18), (33) and (34), we obtain these new values for a even as

$$\begin{cases} \Delta'_{\text{even}} = \dfrac{\zeta}{2(1+\zeta)} = \dfrac{a+2-\sqrt{a^2+4}}{4a} \\ \zeta'_{\text{even}} = \dfrac{1}{1+\zeta} = \dfrac{a-2+\sqrt{a^2+4}}{2a} \end{cases} \tag{38}$$

and for a odd as

$$\begin{cases} \Delta'_{\text{odd}} = \Delta = \frac{1}{2} \\ \zeta'_{\text{odd}} = \dfrac{1}{1+\zeta} = \dfrac{a-2+\sqrt{a^2+4}}{2a}. \end{cases} \tag{39}$$

From (35) we now obtain the general substitution rules for all even $a \geqslant 2$ as

$$\begin{cases} \xi_{\text{even}}(A) = A(CB^{a-1}A)^{a/2}(CB^a)^{a/2} \\ \xi_{\text{even}}(B) = A(CB^{a-1}A)^{a/2-1}(CB^a)^{a/2+1} \\ \xi_{\text{even}}(C) = CB^a \end{cases} \tag{40}$$

and the corresponding transient as

$$\begin{cases} A \mapsto AB^{a/2}C^{a/2-1} \\ B \mapsto AB^{a/2-1}C^{a/2} \\ C \mapsto C. \end{cases} \tag{41}$$

For all odd $a \geqslant 3$ we obtain from (36)

$$\begin{cases} \xi_{\text{odd}}(A) = CB^{(a+1)/2}A^{(a-1)/2}[A(CB^{(a-1)/2}A^{(a+1)/2})^{a-1}CB^{(a+1)/2}A^{(a-1)/2}]^{(a-1)/2} \\ \qquad\qquad \times [A(CB^{(a-1)/2}A^{(a+1)/2})^{a}]^{(a+1)/2} \\ \xi_{\text{odd}}(B) = CB^{(a+1)/2}A^{(a-1)/2}[A(CB^{(a-1)/2}A^{(a+1)/2})^{a-1}CB^{(a+1)/2}A^{(a-1)/2}]^{(a-3)/2} \\ \qquad\qquad \times [A(CB^{(a-1)/2}A^{(a+1)/2})^{a}]^{(a+3)/2} \\ \xi_{\text{odd}}(C) = A(CB^{(a-1)/2}A^{(a+1)/2})^{a} \end{cases} \tag{42}$$

with the corresponding transient

$$\begin{cases} A \mapsto AB^{(a-1)/2}C^{(a-1)/2} \\ B \mapsto AB^{(a-3)/2}C^{(a+1)/2} \\ C \mapsto C. \end{cases} \tag{43}$$

Note that if we apply the transient and have $a \geqslant 2$ (i.e. with the values of (Δ, ζ) in (15)), then the operator ν should be applied in the form of (14). Otherwise (i.e. without transient, corresponding to the values of (Δ', ζ') in (38) or (39)) the operator applies in the form of (13). With formula (29) and the following relation from [17]:

$$\mathrm{Tr}(\Theta^n\Lambda) = d_n[\mathrm{Tr}(\Theta)]\,\mathrm{Tr}(\Theta\Lambda) - d_{n-1}[\mathrm{Tr}(\Theta)]\,\mathrm{Tr}(\Lambda) \tag{44}$$

we can obtain a trace map for the substitutions above. Here, $\Theta, \Lambda \in SL(2, \mathbb{R})$ and $d_n(x)$ is defined as

$$\begin{cases} d_{n+1}(x) = x d_n(x) - d_{n-1}(x) \\ d_0(x) \equiv 0 \qquad d_1(x) \equiv 1. \end{cases} \tag{45}$$

This means that if we set $d_n(x) = s_{n-1}(x)$, we have s_n as a Chebyshev polynomial of the first kind [18]. However, since the trace maps for general a involve very lengthy expressions and since we are not interested in their exact form, we choose not to write them down explicitly. What is important for our purposes is how many and which elements the set $\mathcal{B}$ will contain. General considerations yield that to obtain a trace map we do not need to enlarge it compared with the case of the silver circle sequence above, i.e. $\mathcal{B} = \{A, B, C, ACB, BC, AC\}$. We will also keep the notation from (30) concerning the traces.

When a is even, we obtain the reduced trace map for the substitution rules (40) as

$$\begin{cases} x_{n+1} = y_n^{a^2-3a/2} r_n^{a/2+1} v_n^{a/2-1} \\ y_{n+1} = y_n^{a^2-3a/2+1} r_n^{a/2} v_n^{a/2} \\ z_{n+1} = y_n^{a-1} v_n \\ r_{n+1} = y_n^{2a^2-2a} r_n^{a+1} v_n^{a} \\ v_{n+1} = y_n^{a^2-a/2} r_n^{a/2} v_n^{a/2+1} \\ w_{n+1} = y_n^{a^2-a/2-1} r_n^{a/2+1} v_n^{a/2} \end{cases} \tag{46}$$

and for the rules in (42) when $a \geqslant 3$ is odd as

$$\begin{cases} x_{n+1} = x_n^{a^3/2-a^2/2+a-1} y_n^{a^3/2-3a^2/2+a-1} r_n^{a^2+1} \\ y_{n+1} = x_n^{a^3/2-a^2/2+a} y_n^{a^3/2-3a^2/2+a-2} r_n^{a^2+1} \\ z_{n+1} = x_n^{a^2/2-a/2+1} y_n^{a^2/2-3a/2} r_n^{a} \\ r_{n+1} = x_n^{a^3-a^2/2+3a/2} y_n^{a^3-5a^2/2+a/2-3} r_n^{2a^2+a+2} \\ v_{n+1} = x_n^{a^3/2+a/2+1} y_n^{a^3/2-a^2-a/2-2} r_n^{a^2+a+1} \\ w_{n+1} = x_n^{a^3/2+a/2} y_n^{a^3/2-a^2-a/2-1} r_n^{a^2+a+1}. \end{cases} \tag{47}$$

The final step is to apply theorems 1 and 2 to show that the spectrum is purely singular continuous. First we consider a even. We see from (40) that ξ_{even} possesses one right fixpoint with, for example, $\alpha^{(0)} = A$ and one left fixpoint with $\alpha_l^{(0)} = B$. This choice is the appropriate one for (4) to hold for all n. It is not hard to realize that ξ_{even} is a primitive substitution (with $k = 2$ in definition 3) and with the set $\mathcal{C}_{\text{even}} = \{y, r, v\}$ that ϕ_{even}, defined from (46), is semi-primitive (with $m = 1$ in definition 5). With the observation from (40) that $\xi_{\text{even}}(A)$ contains BB, it is clear that theorem 1 is applicable. That the same is true also for theorem 2 is a more delicate problem for $a \geqslant 4$, since the word $\xi_{\text{even}}^{n_0}(\alpha^{(0)})$ does *not* begin with the square of any element in $\mathcal{C}_{\text{even}}$ (except for the case $a = 2$, which was treated in the previous section). However, if we let $\alpha^{(0)} = A$ and $n_0 \geqslant 1$ then $\xi_{\text{even}}^{n_0}(\alpha^{(0)})$ always begins with $(ACB^{a-1})^2$ and we are led to include into the set $\mathcal{B}$ the element $t_n = \mathrm{Tr}[T^n(ACB^{a-1})]$. This yields a possibility for enlarging the reduced trace map in (46) to a form better suited for our purposes. We choose to enlarge it as

$$\begin{cases} y_{n+1} = y_n^{a^2/2+a/2-1} r_n t_n^{a/2-1} v_n^{a/2} \\ t_{n+1} = y_n^{a^3-3a^2/2+2a-2} r_n^{a^2/2+1} v_n^{a^2/2} \\ x_{n+1}, z_{n+1}, r_{n+1}, v_{n+1}, w_{n+1} \text{ as in (46).} \end{cases} \tag{48}$$

Choose the set $C'_{\rm even}$ as $C'_{\rm even} = \{y, r, t, v\}$. It is shown as before that the associated substitution $\phi'_{\rm even}$, this time from (48), is semi-primitive and theorem 1 still applies. With this extension, the word $\xi_{\rm even}(A)$ starts with the square of an element in $C'_{\rm even}$, i.e. we can have $n_0 = 1$ and $m = 0$ in theorem 2. We also have that $\gamma_0 = ACB^{a-1}$ contains $\alpha^{(0)} = A$ so the conclusion is reached that for all even $a \geqslant 2$, the spectrum of the sequence with parameters (Δ', ζ') from (38) is purely singular continuous.

Next we turn our attention to the nature of the spectrum for all odd $a \geqslant 3$. That $\xi_{\rm odd}$ is a primitive substitution is easily seen from (42). This time, however, $\xi_{\rm odd}$ does not possess any right fixpoint, but since $\xi^2_{\rm odd}$ has, for example, a right fixpoint with $\alpha^{(0)} = A$ and a left fixpoint with $\alpha_l^{(0)} = A$, we can focus upon this substitution instead. With this choice, we also see that (4) holds for all n. Now let $\phi_{\rm odd}$ be defined from (47) and $C_{\rm odd} = \{x, y, r\}$. Then it is seen from definition 5 that $\phi_{\rm odd}$ is semi-primitive for all odd $a \geqslant 3$. Using the fact that $\alpha^{(0)} = A$, which implies that $\xi^2_{\rm odd}(\alpha^{(0)})$ contains AA and $A \in \mathcal{B}$, it is clear that theorem 1 is fulfilled. In order to show that theorem 2 also applies, we perform the same 'trick' as before, namely to enlarge the set $\mathcal{B}$. This time the set is enlarged with $s_n = \mathrm{Tr}[T^n(ACB^{(a-1)/2}A^{(a-1)/2})]$, which we choose to incorporate in the reduced trace map (47) as

$$\begin{cases} x_{n+1} = x_n^{a^2/2-1/2} y_n^{a^2/2-a+1/2} r_n^a s_n^{a^2-a+1} \\ s_{n+1} = x_n^{a^4/2-a^3/2+3a^2/2-a+1/2} y_n^{a^4/2-3a^3/2+3a^2/2-3a+1/2} r_n^{a^3+2a} \\ y_{n+1}, z_{n+1}, r_{n+1}, v_{n+1}, w_{n+1} \text{ as in (47).} \end{cases} \tag{49}$$

Now the set $C'_{\rm odd}$ is chosen to be $C'_{\rm odd} = \{x, y, r, s\}$ and the substitution $\phi'_{\rm odd}$ is from (49). That $\phi'_{\rm odd}$ is semi-primitive and that theorem 1 is still applicable is obvious. The main point here is that $\xi^2_{\rm odd}(A)$ begins with $(ACB^{(a-1)/2}A^{(a-1)/2})^2$ and $\mathrm{Tr}[T^n(ACB^{(a-1)/2}A^{(a-1)/2})] = s_n \in C'_{\rm odd}$ and that $\gamma_0 = ACB^{(a-1)/2}A^{(a-1)/2}$ contains $\alpha^{(0)} = A$. This also means that theorem 2 is fulfilled and, thus, we have shown that for the values of (Δ', ζ') given in (38) and (39), our physical model (1) has a purely singular continuous spectrum for all positive integers $a \geqslant 2$.

We see that the values in (39) for odd values of a are $\Delta = \frac{1}{2}$ and $(a_n)_{n=1}^{\infty} = (1, a, a, \ldots)$, but that $\Delta \neq \frac{1}{2}$ in (38) for a even. A natural question to ask is if we will then obtain a substitution rule without any transient if we also consider the values $\Delta = \frac{1}{2}$ and $(a_n)_{n=1}^{\infty} = (1, a, a, \ldots)$ for a even. The answer turns out to be in the affirmative, but we cannot guarantee the existence of a purely singular continuous spectrum in all cases. The calculations to show this are as before and we will not go into detail describing them, but instead just sketch them briefly. First, the p_n becomes

$$\begin{cases} p_0 = 1 \\ p_n = \frac{1}{2}a \qquad n = 1, 2, 3, \ldots \end{cases} \tag{50}$$

This yields the period for the transformation as

$$\hat{T} = \hat{S}\hat{T}_3^{a/2-1}\hat{T}_2\hat{T}_1^{a/2} \tag{51}$$

and now we do not have any transient. The corresponding substitution rule is

$$\begin{cases} \xi(A) = CB^{a/2}A^{a/2} \\ \xi(B) = CB^{a/2-1}A^{a/2+1} \\ \xi(C) = A. \end{cases} \tag{52}$$

In this case, the operator ν takes the form in (13) for all even values of a. Also, this time the set $\mathcal{B}$ can be chosen as $\mathcal{B} = \{A, B, C, ACB, BC, AC\}$ and we keep the notation from (30). For $a \geqslant 4$, we have the following form for the reduced trace map:

$$\begin{cases} x_{n+1} = x_n^{a/2-1} y_n^{a/2-1} r_n \\ y_{n+1} = x_n^{a/2} y_n^{a/2-2} r_n \\ z_{n+1} = x_n \\ r_{n+1} = x_n^a y_n^{a-3} r_n^2 \\ v_{n+1} = x_n^{a/2+1} y_n^{a/2-2} r_n \\ w_{n+1} = x_n^{a/2} y_n^{a/2-1} r_n. \end{cases} \tag{53}$$

We consider here ξ^2 instead of ξ which yields fixpoints for the substitution with $\alpha^{(0)} = \alpha_l^{(0)} = A$. This choice makes (4) valid for all n. Since ξ^2 is primitive and $\xi^2(A)$ contains AA, we have that with the set $\mathcal{C}$ chosen as $\mathcal{C} = \{x, y, r\}$, the substitution ϕ is semi-primitive and, hence, it is clear that theorem 1 is fulfilled. Using the same technique as before, we enlarge the set $\mathcal{B}$ with $t_n = \mathrm{Tr}[T^n(CB^{a/2-1}A^{a/2+1})]$. The reduced trace map can now be expanded via

$$\begin{cases} y_{n+1} = t_n \\ t_{n+1} = x_n^{a^2/2-a/2} y_n^{a^2/2-3a/2+1} r_n^a \\ x_{n+1}, z_{n+1}, r_{n+1}, v_{n+1}, w_{n+1} \text{ as in (53).} \end{cases} \tag{54}$$

With $\mathcal{C}' = \{x, y, r, t\}$, the word $\xi^2(A)$ begins with the square of an element in $\mathcal{C}$ and then it is not hard to see that both theorems 1 and 2 apply, i.e. the spectrum is purely singular continuous for $a \geqslant 4$. When $a = 2$, the full trace map is given by

$$\begin{cases} x_{n+1} = r_n \\ y_{n+1} = x_n w_n - z_n \\ z_{n+1} = x_n \\ r_{n+1} = (x_n w_n - z_n)(x_n r_n - v_n) - y_n \\ v_{n+1} = (x_n^2 - 1) w_n - x_n z_n \\ w_{n+1} = x_n r_n - v_n. \end{cases} \tag{55}$$

With $\mathcal{C} = \{x, r, w\}$, it is obvious that theorem 1 is fulfilled. However, this time there seems to be no way to fulfil the requirements in theorem 2. This is because the word $\xi^{n_0}(\alpha^{(0)})$ does *not* begin with the square of *any* word for $a = 2$ (as far as we can see). This means that for $a = 2$ we cannot exclude the possibility of eigenvalues in the spectrum. This statement is also true for the extended version of theorem 2 given in [9].

5. Summary and conclusions

The purpose of this paper has been to study the nature of the electron spectrum for a quasiperiodic tight-binding model with on-site potential chosen according to a class of circle sequences. To be able to apply the theorems from [8], giving sufficient conditions for the spectrum to be singular and singular continuous, respectively, we have derived substitution rules for the sequences following the procedure described in [14]. Explicit expressions for the rules generating sequences with parameter values according to (39) are given in (42) and (52) for a odd and even, respectively. By studying the corresponding reduced trace maps, we find that the spectrum for these parameter values is purely singular continuous for all $a \neq 2$. (The case $a = 1$ was treated already in [8].) For $a = 2$, the spectrum is shown to be singular (i.e. there is no absolutely continuous part), but we cannot exclude the existence of eigenvalues (point spectrum). However, one should note that also for the Thue–Morse sequence, the theorems in [8] and [9] could not be used to exclude the existence of eigenvalues, but that this could be achieved using a more detailed analysis [7]. Thus, a more detailed investigation of the dynamics of the full trace map in (55) might also lead here to a similar result.

The singular continuous nature of the spectrum was also shown for the class of circle sequences with parameter values from (38) for even values of a using the substitution rules in (40). Concerning the originally discussed case, with ζ equal to an inverse precious mean and $\Delta = \frac{1}{2}$ as in (15), we note that we cannot, with the method from [14], derive a substitution rule acting on single letters for $a \neq 1$. We can, however, use the rules (40) and (42) to generate the sequences for a even and odd, respectively, if each letter is replaced by a finite word according to (41) or (43) in the final sequence. In the transfer-matrix formalism, this means that we must consider basic matrices which are not of the simple type (25), but instead consist of products of such matrices. Since it is not clear to us to what extent the theorems from [8] can be extended to cover such a case, our analysis does not allow us to draw any conclusions about the nature of the spectrum for these sequences. We believe that this is a problem that deserves further investigation in the future.

Acknowledgments

We would like to thank Rolf Riklund for valuable discussions about physics in general, and aperiodic systems in particular. We would also like to thank Mihnea Dulea for pointing out [8] to us, and one of the referees for sending us a preprint of [9]. Financial support from the Swedish Natural Science Research Council is also gratefully acknowledged.

Appendix. Detailed derivation of a trace formula

To obtain the trace map in (31), we have to apply the relation in (29) several times and also use the fact that the value of a trace is always invariant with respect to cyclic permutations of the matrices. Explicitly this can be achieved as

$$\begin{aligned}
x_{n+1} = \mathrm{Tr}[T^{n+1}(A)] &= \mathrm{Tr}[T^n(ACBACBB)] \\
&= \mathrm{Tr}[T^n(B)T^n(ACB)T^n(ACB)] \\
&= \mathrm{Tr}[T^n(ACB)T^n(ACB)T^n(B)] \\
&= \mathrm{Tr}[T^n(ACB)]\,\mathrm{Tr}[T^n(ACB)T^n(B)] - \mathrm{Tr}[T^n(B)] \\
&= \mathrm{Tr}[T^n(ACB)]\,\mathrm{Tr}[T^n(BACB)] - \mathrm{Tr}[T^n(B)] \\
&= \mathrm{Tr}[T^n(ACB)]\,\mathrm{Tr}[T^n(BBAC)] - \mathrm{Tr}[T^n(B)] \\
&= \mathrm{Tr}[T^n(ACB)]\{\mathrm{Tr}[T^n(B)]\,\mathrm{Tr}[T^n(BAC)] - \mathrm{Tr}[T^n(AC)]\} \\
&\quad - \mathrm{Tr}[T^n(B)] \\
&= r_n(y_n r_n - w_n) - y_n.
\end{aligned}$$

In the same way, all the other formulae in (31) can be found.

References

[1] Soukoulis C M and Economou E N 1982 *Phys. Rev. Lett.* **48** 1043
Hiramoto H and Kohmoto M 1989 *Phys. Rev. Lett.* **62** 2714; 1989 *Phys. Rev.* B **40** 8225
Weisz J F, Johansson M and Riklund R 1990 *Phys. Rev.* B **41** 6032
Johansson M and Riklund R 1990 *Phys. Rev.* B **42** 8244
[2] Aubry S and André G 1980 *Ann. Isr. Phys. Soc.* **3** 133
[3] Avron J and Simon B 1983 *Duke Math. J.* **50** 369
[4] Last Y 1994 *Commun. Math. Phys.* **164** 421
[5] Kohmoto M, Kadanoff L P and Tang C 1983 *Phys. Rev. Lett.* **50** 1870
Ostlund S, Pandit R, Rand D, Schellnhuber H J and Siggia E G 1983 *Phys. Rev. Lett.* **50** 1873
Sütő A 1987 *Commun. Math. Phys.* **111** 409; 1989 *J. Stat. Phys.* **56** 525
Bellissard J, Iochum B, Scoppola E and Testard D 1989 *Commun. Math. Phys.* **125** 527
[6] Axel F and Peyrière J 1989 *J. Stat. Phys.* **57** 1013
Bellissard J 1990 *Number Theory and Physics (Springer Proceedings in Physics 47)* ed J M Luck, P Moussa and M Waldschmidt (Berlin: Springer) p 140
[7] Bellissard J, Bovier A and Ghez J-M 1991 *Commun. Math. Phys.* **135** 379
[8] Bovier A and Ghez J-M 1993 *Commun. Math. Phys.* **158** 45
[9] Bovier A and Ghez J-M Erratum to [8], to be published in *Commun. Math. Phys.*
[10] Luck J M 1989 *Phys. Rev.* B **39** 5834
[11] Dulea M, Johansson M and Riklund R 1993 *Phys. Rev.* B **47** 8547
[12] Kolář M and Nori F 1990 *Phys. Rev.* B **42** 1062
[13] Avishai Y and Berend D 1993 *J. Phys. A: Math. Gen.* **26** 2437
[14] Aubry S, Godrèche C and Luck J M 1988 *J. Stat. Phys.* **51** 1033
[15] Queffélec M 1987 *Substitution Dynamical Dystems—Spectral Analysis (Springer Lecture Notes in Mathematics 1294)* (Berlin: Springer)
[16] Lang S 1966 *Introduction to Diophantine Approximations* (Reading, MA: Addison-Wesley)
[17] Kolář M and Ali M K 1990 *Phys. Rev.* A **42** 7112
[18] Szegö G 1975 *Orthogonal Polynomials (Amer. Math. Soc. Coll. Publ. 23)* (Providence, RI: American Mathematical Society)