

Spectral Properties of One-Dimensional Schrödinger Operators with Potentials Generated by Substitutions

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Abstract: We investigate one-dimensional discrete Schrödinger operators whose potentials are invariant under a substitution rule. The spectral properties of these operators can be obtained from the analysis of a dynamical system, called the trace map. We give a careful derivation of these maps in the general case and exhibit some specific properties. Under an additional, easily verifiable hypothesis concerning the structure of the trace map we present an analysis of their dynamical properties that allows us to prove that the spectrum of the underlying Schrödinger operator is singular and supported on a set of zero Lebesgue measure. A condition allowing to exclude point spectrum is also given. The application of our theorems is explained on a series of examples.

1. Introduction

In this article we present general results on the spectral properties of a class of one-dimensional discrete Schrödinger operators of the form

$$H_v = -\Delta + V \quad \text{on } l^2(\mathbb{Z}), \quad (1.1)$$

where Δ is the discrete Laplacian and V is a diagonal operator whose diagonal elements V_n are obtained from a *substitution sequence* [1]. By a substitution sequence we mean the following. Let \mathcal{A} be a finite set, called an *alphabet*. Let \mathcal{A}^k be the set of *words* of length k in the alphabet, $\mathcal{A}^* \equiv \bigcup_{k \in \mathbb{N}} \mathcal{A}^k$ the set of all words of finite length, and $\mathcal{A}^{\mathbb{N}}$ the set of one-sided infinite sequences of letters. A map $\xi: \mathcal{A} \rightarrow \mathcal{A}^*$ is called a *substitution*. A substitution ξ naturally induces maps from $\mathcal{A}^* \rightarrow \mathcal{A}^*$ and $\mathcal{A}^{\mathbb{N}} \rightarrow \mathcal{A}^{\mathbb{N}}$, which we will denote by the same name and which are obtained simply by applying ξ to each letter in the respective words or sequences (e.g. $\xi(abc) = \xi(a)\xi(b)\xi(c)$). A substitution may possess fix-points in $\mathcal{A}^{\mathbb{N}}$, and such fix-points, u , will be called substitution sequences. There are two natural conditions that guarantee the existence of at least one fix-point, namely $\xi^\infty 0$, and that we will assume to be satisfied for all substitutions we discuss [1]:

- (C1) There exists a letter, called 0, in \mathcal{A} , such that the word $\xi(0)$ begins with 0.
 (C2) The length of the words $\xi^n(0)$ tends to infinity, as $n \uparrow \infty$.

A class of substitutions we will in general deal with are the so-called *primitive* substitutions [1]. They are characterized by the fact that there exists an integer, k , such that for any two letters α_i, α_j in \mathcal{A} the word $\xi^k \alpha_i$ contains the letter α_j .

Given a fix-point $u = (\alpha_0 \alpha_1 \alpha_2 \dots)$ of a substitution ξ , the associated sequence of potentials is now obtained as follows. Consider a map $v: \mathcal{A} \rightarrow \mathbb{R}$ (which we will always assume to be non-constant), we set, for $n \geq 0$, $V_n = v(\alpha_n)$. This sequence is then completed to the negative side by setting, say, $V_{-n-1} = V_n$.

Schrödinger operators with potentials of this type have attracted considerable attention over the last years in connection with the discovery of quasi-crystals [2, 3]. For, indeed, the prototypical one-dimensional quasi-crystal is associated to the Fibonacci-sequences, which are substitution sequences associated to the substitutions ξ on the alphabet $\mathcal{A} = \{a, b\}$, where

$$\xi(a) = ab^n, \quad \xi(b) = a. \quad (1.2)$$

(The most studied example (also called the Kohmoto model) corresponds to the case $n = 1$ and the Fibonacci sequence associated to the golden number.) There is a host of numerical and analytical work which has been done for these models [4], with amongst the most notable mathematical results those by Casdagli [5], Sütö [6] and Bellissard et al. [7], in which it was shown that the spectrum of these operators is always singular continuous and supported on a Cantor set of zero Lebesgue measure. All these results relied heavily on the very fact that the Fibonacci sequences are substitution sequences (in more technical terms, they employed the so-called *trace map*, whose existence is a direct consequence of the substitution, as we will discuss in detail below), and this observation stimulated the investigation of other examples of substitution sequences. The first and most heavily studied [8] example was the *Thue–Morse sequence* [9], defined by the substitution

$$\xi(a) = ab, \quad \xi(b) = ba \quad (1.3)$$

which offers an additional interesting feature in that it is not quasi-periodic. Again it was proven that the spectrum of the corresponding Hamiltonian is purely singular continuous [10, 11] and, moreover, a complete description of the gap-structure of the spectrum, including the dependence of the gap-width on the potential strength could be given [10]. A further example, where the same type of results could be proven [11], is provided by the *period-doubling sequence*, with substitution

$$\xi(a) = ab, \quad \xi(b) = aa. \quad (1.4)$$

These results required, in each example, a rather detailed analysis of some dynamical system associated to the so-called trace map. Unfortunately, for more complicated substitutions (e.g. on more than two letters), these become prohibitively complicated. Nonetheless, one would expect that certain qualitative properties of the spectra of such Hamiltonians should not depend on the details, but only on some general features of the substitution.

There are, indeed, two promising approaches attempting to obtain more general results. One is the perturbative method of Luck [12] that establishes, on a heuristic level, a connection between the Fourier spectrum of the sequences themselves and the gap structure of the spectrum of the Hamiltonians and that allows even to compute the behaviour of the gap-widths. A shortcoming of this approach is, besides the difficulties to give mathematically rigorous justifications of some of the steps involved, that it fails to make clear predictions in situations where the Fourier spectrum of the underlying sequence is not of the pure-point type. Unfortunately, singular continuous and even absolutely continuous Fourier spectra are not at all uncommon for substitution sequences. Nonetheless we emphasize that this perturbation method is so far the most powerful tool to get fast quantitative predictions.

Another attempt to obtain general information on these systems is based on the K -theory of C^* -algebras. It was realized [13, 14] that general gap-labelling theorems [15, 16] can be applied particularly well in these cases as substitution sequences allow for an easy computation of the corresponding K_0 -groups. This allows then to predict all possible spectral gaps from a simple computation of a Perron–Frobenius eigenvector of a (not too large) matrix. The shortfall of this approach is, so far, that it cannot predict whether the allowed gaps will actually be open for given values of the potentials, and in the known examples, closed gaps do occasionally occur. In particular, the K -theory makes no predictions on the type of spectrum one may expect.

In this article we attempt to obtain general results on the nature of the spectrum from a careful analysis of the trace maps. Indeed, it is natural to conjecture that the existence of an exact renormalization group structure, as is presented by the trace map, is responsible for the particular spectral properties observed in the examples. In particular, one may be led to believe that due to the existence of the trace map the singular spectral type should be the rule rather than the exception. We will prove here that this is true in some sense: namely, that under some conditions that can be verified fairly easily (there is a simple algorithmic procedure to verify them) and that appear to hold in most examples (the Rudin–Shapiro sequence [17] being a notable exception), the spectrum of our operators is always singular and supported on a set of zero Lebesgue measure. This result is based on the analysis of some general properties of the trace maps and of the ensuing characteristics of large time behaviour of the associated dynamical systems. These will allow to identify the spectrum with the set of energies for which the Lyapunov exponent vanishes. A general theorem proven already in [11] which is based on a profound lemma of Kotani [18] will then yield the result.

A more subtle question relates to the existence of point spectrum: there is a simple supplementary condition under which the existence of eigenvalues can be excluded, but this condition is not satisfied in all examples where the singular continuous nature of the spectrum was proven.

The remainder of this article is organized as follows. In Chap. II we review the derivation of the trace maps and exhibit some of their properties. We will define a new substitution rule on an extended alphabet that encodes the principal part of the trace map and formulate the assumptions entering in our theorem in terms of this substitution. In Chap. III we formulate our main theorem and present its proof. We also discuss the problem of eigenvalues. In Chap. IV we elucidate our results with some examples.

II. The Trace Map

In this section we give a careful review of the derivation of the so-called *trace map* and establish some crucial properties of these maps. The trace map was originally introduced by Allouche and Peyrière [19], but we also refer to the paper [20] by Kolár and Nori in which a more general and systematic construction is given.

As usual for one-dimensional discrete Schrödinger operators like (1.1), the analysis of their spectra is based on the discussion of the associated Schrödinger equation, written in vector form as

$$\Psi_E(n+1) = \begin{pmatrix} E - V_n & -1 \\ 0 & 0 \end{pmatrix} \Psi_E(n), \quad (2.1)$$

where $\Psi_E(n) \equiv \begin{pmatrix} \psi_E(n) \\ \psi_E(n-1) \end{pmatrix}$ with ψ_E the solution of the usual Schrödinger equation $H_v \psi_E = E \psi_E$. Iterating Eq. (2.1) we get, of course, the solution of the initial value problem in the form of a product of matrices as

$$\Psi_E(n+1) = \prod_{k=n}^0 \begin{pmatrix} E - V_k & -1 \\ 1 & 0 \end{pmatrix} \Psi_E(1). \quad (2.2)$$

In the case of substitution sequences we are naturally led to define the maps $T_E: \mathcal{A} \rightarrow SL(2, \mathbb{R})$ via

$$T_E(\alpha) = \begin{pmatrix} E - v(\alpha) & -1 \\ 1 & 0 \end{pmatrix}. \quad (2.3)$$

Again, by some abuse of notation we denote by the same symbol the maps $T_E: \mathcal{A}^* \rightarrow SL(2, \mathbb{R})$ where for $\omega = (\alpha_0 \dots \alpha_{n-1}) \in \mathcal{A}^n$,

$$T_E(\omega) \equiv T_E(\alpha_{n-1}) \dots T_E(\alpha_0). \quad (2.4)$$

The map T_E allows us to introduce the induced action of ξ on $\text{Im}(T_E)$ via

$$\xi T_E(\omega) \equiv T_E^{(1)}(\omega) \equiv T_E(\xi \omega), \quad (2.5)$$

and we will also use the notation

$$\xi^n T_E(\omega) \equiv T_E^{(n)}(\omega) = T_E(\xi^n \omega). \quad (2.6)$$

It is obvious from (2.4) that the action of ξ defines a dynamical system on $SL(2, \mathbb{R})^{|\mathcal{A}|}$, since $T_E^{(n)}(\alpha)$, $\alpha \in \mathcal{A}$, can be expressed as a product of matrices $T_E^{(n-1)}(\alpha)$, $\alpha \in \mathcal{A}$. The analysis of this dynamical system could in principle yield all desired information on the spectrum of (1.1). In practice, however, it turns out to be difficult to work with this system directly and it is advantageous to pass to a new dynamical system based on the traces of the matrices $T_E^{(n)}(\omega)$.

Let us define, for $\omega \in \mathcal{A}^*$, $x_E(\omega) \equiv \text{tr} T_E(\omega)$. Of course we may write also $x_E^{(n)}(\omega) \equiv \text{tr} T_E^{(n)}(\omega)$ and obviously we may extend the action of ξ to write $\xi x_E^{(n-1)}(\omega) = x_E^{(n)}(\omega)$, however this time there is no immediate expression of $\xi x_E^{(n-1)}(\alpha)$ as a function of the $x_E^{(n-1)}(\alpha)$, i.e. a realization of this action as a dynamical system on $\mathbb{R}^{|\mathcal{A}|}$ and in general such a realization will not exist. However, it is always possible to find a finite subset, $\mathcal{B} \subset \mathcal{A}^*$ such that for all $\omega \in \mathcal{B}$, $x_E^{(n)}(\omega)$ can be expressed as a function of the $x_E^{(n-1)}(\omega)$, with $\omega \in \mathcal{B}$, that is a realization of the

action of ξ as a dynamical system on $\mathbb{R}^{|\mathcal{B}|}$. Such a dynamical system is called a trace map. Note that in the sequel we will use the names β or β_i for the elements of \mathcal{B} to distinguish them from generic words ω . Following [20], such a trace map can be constructed for any substitution in the following way.

Notice first that for unimodular 2×2 -matrices A, B , the Cayley–Hamilton theorem yields

$$\operatorname{tr}(AB) = \operatorname{tr} A \operatorname{tr} B - \operatorname{tr}(BA^{-1}). \quad (2.7)$$

It is easy to deduce from this relation (see [20]) that for three such matrices A, B, C , one has

$$\operatorname{tr}(ABAC) = \operatorname{tr}(AB)\operatorname{tr}(AC) + \operatorname{tr}(BC) - \operatorname{tr} B \operatorname{tr} C. \quad (2.8)$$

Let us label the letters in \mathcal{A} by $\alpha_1, \dots, \alpha_K$, with $K \equiv |\mathcal{A}|$. Starting with α_1 we write

$$x_E^{(n+1)}(\alpha_1) = \operatorname{tr} \prod_{\alpha \in \xi \alpha_1} T_E^{(n)}(\alpha). \quad (2.9)$$

Now there are two possibilities: if $\xi \alpha_1$ contains no letter of \mathcal{A} twice, then we set $\beta_{K+1} \equiv \xi \alpha_1$. The word β_{K+1} will then be considered as a “letter” in the new alphabet \mathcal{B} (which also contains all the letters α_i from \mathcal{A}) that we will construct. More precisely, due to the invariance of the trace under cyclic permutations it is natural to identify words $\xi \alpha_1$ that differ only by a cyclic permutation of their letters, so that the elements of \mathcal{B} will really be equivalence classes of words in \mathcal{A}^* .

If $\xi \alpha_1$ contains a letter, say α , in \mathcal{A} twice, then an element in its equivalence class may be written in the form $\alpha \omega_1 \alpha \omega_2$, and thus by (2.8),

$$\begin{aligned} x_E^{(n+1)}(\alpha_1) &= \operatorname{tr} T_E^{(n)}(\alpha \omega_1) \operatorname{tr} T_E^{(n)}(\alpha \omega_2) + \operatorname{tr} T_E^{(n)}(\omega_1 \omega_2) \\ &\quad - \operatorname{tr} T_E^{(n)}(\omega_1) \operatorname{tr} T_E^{(n)}(\omega_2). \end{aligned} \quad (2.10)$$

We now proceed with each of the traces appearing in (2.10) just as before, that is if a corresponding word (say $\alpha \omega_1$) contains no letter twice it is included into \mathcal{B} , whereas for words that still contain a letter twice, (2.8) is again applied. The important point is that with each application of (2.8) the words that may appear become strictly shorter so that this process necessarily terminates after a finite number of steps, leaving us with $x_E^{(n+1)}(\alpha_1)$ expressed as a polynomial in the variables $x_E^{(N)}(\beta_i)$, with β_i elements of some finite set \mathcal{B} . The same procedure is now applied on the remaining letters α_i in \mathcal{A} , and finally on the new letters $\beta_i \in \mathcal{B}$ that have been introduced in the process. But since the elements of \mathcal{B} are equivalence classes of words in \mathcal{A}^* that contain no letter twice, the length of these words is a priori bounded by K , and the cardinality of \mathcal{B} by [20]

$$|\mathcal{B}| \leq \sum_{l=1}^K \frac{K!}{l(K-l)!} \quad (2.11)$$

so that the algorithm described above will terminate after a finite number of steps. In the end we have, for each $\beta_i \in \mathcal{B}$, an expression

$$x_E^{(n+1)}(\beta_i) = f_i(x_E^{(n)}(\beta_1), \dots, x_E^{(n)}(\beta_{|\mathcal{B}|})), \quad (2.12)$$

where each f_i is a polynomial map from $\mathbb{R}^{|\mathcal{B}|}$ to $\mathbb{R}^{|\mathcal{B}|}$, and where we have fixed, for notational convenience, the numbering of the letters $\beta_i \in \mathcal{B}$ once and for all.

An important further characterization of these maps can be given through the following notion of a “degree,” d , defined as follows: Put, for $x \in \mathbb{R}^{|\mathcal{B}|}$,

$$d(x_i) \equiv |\beta_i|, \quad (2.13)$$

and let for any two polynomials, p and q in the variables $\{x_i\}_{i=1}^{|\mathcal{B}|}$

$$d(pq) \equiv d(p) + d(q) \quad (2.14)$$

and

$$d(p + q) \equiv \max(d(p), d(q)). \quad (2.15)$$

Obviously, these three relations allow to compute the “degree,” $d(p)$, of any such polynomial.

We collect the properties of the trace map in the following

Proposition 2.1. *Let ξ be a substitution on an alphabet \mathcal{A} of cardinality K . Then there exists an alphabet \mathcal{B} whose elements are words modulo cyclic permutations in $\bigcup_{l=1}^K \mathcal{A}^l$, such that $\mathcal{A} \subset \mathcal{B}$ and $|\mathcal{B}| \leq \sum_{l=1}^K \frac{K!}{l(K-l)!}$, and a polynomial map $f: \mathbb{R}^{|\mathcal{B}|} \rightarrow \mathbb{R}^{|\mathcal{B}|}$, such that if $f^{(n)}(x)$ is the n^{th} iterate of f on the initial vector x , then,*

$$x_E^{(n)} = f^{(n)}(x_E^{(0)}). \quad (2.16)$$

Equation (2.12) holds for each $\beta_i \in \mathcal{B}$. Moreover f satisfies

$$d(f_i) = |\xi \beta_i|_{\mathcal{A}}, \quad (2.17)$$

where $|\omega|_{\mathcal{A}}$ denotes the number of letters of ω considered as a word in \mathcal{A}^* . Finally, there exists a unique monomial of highest “degree” (whose coefficient is one) in f_i which we shall denote by \tilde{f}_i .

Proof. Most of the proposition is evident from the construction given above and has already been noticed earlier [20]. The statement (2.17) on the degree is also evident from the fact that only (2.8) is used in the construction of the trace map and that there is exactly one term on the right-hand side of (2.8) that has the same degree as the term on the left. \diamond

Remark. The reader may notice that the construction of the trace map (and even the alphabet \mathcal{B}) is not unique, and that in general several trace maps can be obtained for the same substitution. They will all, however, enjoy the properties stated in Proposition 2.1. For practical purposes, one may try to minimize the size of \mathcal{B} and consider the trace map on invariant submanifolds. For our general considerations here this will be of no importance.

The map \tilde{f} , introduced in Proposition 2.1, will be called the *reduced trace map* and is of central importance for our analysis. We find it useful – and natural – to associate with \tilde{f} a substitution, $\phi: \mathcal{B} \rightarrow \mathcal{B}^*$, in the following way: Let us first define the map $X: \mathcal{B}^* \rightarrow \mathbb{R}$ such that for any $\omega = (\beta_{i_1} \dots \beta_{i_k}) \in \mathcal{B}^*$,

$$X(\omega) \equiv x_{i_1} \dots x_{i_k}. \quad (2.18)$$

Then ϕ is a substitution such that for any $\beta_i \in \mathcal{B}$,

$$X(\phi \beta_i) \equiv \tilde{f}_i(x_1, \dots, x_{|\mathcal{B}|}). \quad (2.19)$$

Properties of the substitution ϕ will be crucial for our analysis. The substitutions ϕ associated to trace maps will typically not be primitive, but have a structure that we will call *semi-primitive*:

Definition 2.1. *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}^* and the restriction of ϕ to \mathcal{C} is a primitive substitution on the alphabet \mathcal{C} .*
- (ii) *There exists a positive integer k such that for each letter $\beta \in \mathcal{B}$, $\phi^k \beta$ contains at least one letter from \mathcal{C} .*

Note that although (2.19) does not uniquely define the substitution ϕ , (since $X(\omega)$ does not depend on the order in which the letters appear in ω but only on their multiplicity) either all or none of the substitutions satisfying (2.19) for a given \tilde{f} are semi-primitive. In most examples of trace maps associated to primitive substitutions ξ we have analyzed (see Sect. IV), the associated substitutions ϕ turned out to be semi-primitive, the Rudin–Shapiro sequence being the only counterexample.

To conclude this section, we note that semi-primitive substitutions arising from primitive substitutions ξ in the above described way have the following additional property:

Lemma 2.1. *Let ξ be a primitive substitution satisfying conditions C1 and C2. Let ϕ be a substitution on \mathcal{B} associated to its reduced trace map. Let \mathcal{C} be a subset of \mathcal{B} such that the restriction of ϕ to \mathcal{C} is primitive. Then there exists a letter $\gamma_0 \in \mathcal{C}$, such that γ_0 as a word in \mathcal{A}^* contains the letter 0.*

Proof. To prove the lemma, just notice that for any letter $\beta_i \in \mathcal{B}$, the word $\phi \beta_i \in \mathcal{B}^*$ considered as a word in \mathcal{A}^* is made of the same letters as the word $\xi \beta_i \in \mathcal{A}^*$. The same holds true for the k^{th} iterates of ϕ and ξ , respectively. Now if ξ is primitive, then there exists k such that for any letter α , and a fortiori for any word $\omega \in \mathcal{A}^*$, $\xi^k \omega$ contains the letter 0. Therefore, for any letter $\gamma \in \mathcal{C}$, $\phi^k \gamma$ must contain a letter from \mathcal{B} containing 0. But by assumption, $\phi^k \gamma$ is a word in \mathcal{C}^* , and thus \mathcal{C} must contain at least one letter which, considered as a word in \mathcal{A}^* , contains the letter 0, which was to be proven. \diamond

III. Trace Map and Spectrum

In this section we review the determination of the spectrum of H through the dynamical spectrum of the trace map and some of its consequences. In particular, we will prove the main result of this article, that is

Theorem 1. *Let ξ be a non-constant primitive substitution with no constant iterate defined on a finite alphabet \mathcal{A} . Let v be a non-constant map from \mathcal{A} to \mathbb{R} and H_v the Schrödinger operator defined in (1.1). Suppose there exists a trace map whose associated substitution ϕ , defined on an alphabet \mathcal{B} , as described in Sect. II, is semi-primitive. Assume further that there exists $k < \infty$ such that $\xi^k 0$ contains the word $\beta\beta$ for some $\beta \in \mathcal{B}$. Then the spectrum of H_v is singular and supported on a set of zero Lebesgue measure.*

The strategy of the proof follows the one used in [11] to prove that the spectrum of H_v is singular continuous in the particular case of the period doubling sequence.

Let us begin by defining the so-called unstable set \mathcal{U} .

Definition 3.1. Let γ_0 denote a letter in \mathcal{C} that contains the letter $0 \in \mathcal{A}$. Let \mathcal{U}_n denote the set

$$\mathcal{U}_n \equiv \{x \in \mathbb{R}^{|\mathcal{B}|} \mid \forall_{m \geq n} |f_{i(\gamma_0)}^{(m)}(x)| > 2\}, \quad (3.1)$$

where $i(\gamma_0)$ is defined such that $\gamma_0 = \beta_{i(\gamma_0)}$. Then

$$\mathcal{U} \equiv \bigcup_{n=0}^{\infty} \text{int } U_n. \quad (3.2)$$

Remark. Notice that in general \mathcal{C} may contain several letters containing the letter 0, and thus the set \mathcal{U} depends a priori on which of these letters was chosen. However, as will become clear later, \mathcal{U} is really independent of this choice. Note also that we may choose the labelling of the letters in \mathcal{B} in such a way that our chosen γ_0 is β_1 (i.e. $i(\gamma_0) = 1$), which will simplify further notation.

Since in the sequel we will want to speak, for fixed v , of the set of energies such that $x_E^{(0)}$ belongs to \mathcal{U} or in fact other sets we will define later, it will be convenient to define, for any set $Y \subset \mathbb{R}^{|\mathcal{B}|}$, $\mathcal{E}(Y) \subset \mathbb{R}$, by

$$\mathcal{E}(Y) \equiv \{E \mid x_E^{(0)} \in Y\}. \quad (3.3)$$

Notice that $\mathcal{E}(Y^c) = \mathcal{E}(Y)^c$, where the superscript c indicates the complement of a set. The definition of \mathcal{U} (notice that it differs from the one given e.g. in Sütő [6]) implies immediately

Lemma 3.1. For given v , $\mathcal{E}(\mathcal{U}) \subset \sigma(H_v)^c$.

The proof of this lemma in this form has been given by Bellissard [10]. A similar result was also proven by Sütő [6]. Essentially it is contained in Theorem VIII.24a of Reed–Simon, Vol. 1 [21].

In principle we would like to prove also the converse of Lemma 3.1 which would allow to compute the spectrum of H_v from the trace map. In [11] we have seen that if \mathcal{U} is such that the Lyapunov exponent vanishes for $E \in \mathcal{E}(\mathcal{U}^c)$, then not only the converse of Lemma 3.1 holds, but also, applying some general results of Kotani [18], the spectrum has zero Lebesgue measure. However, while the definition of \mathcal{U} is convenient to prove Lemma 3.1, it is inconvenient to describe \mathcal{U} in more detail since in order to decide whether $x_E^{(0)}$ is in \mathcal{U} we need to control $x_E^{(n)}$ for all n . In [6, 10 and 11] a simpler characterization was found in the cases of the Fibonacci, Thue–Morse and period-doubling sequences which required information on $x_E^{(n)}$ only for *some* n . This implied in particular that the sets \mathcal{U}_n were open. We will give such a characterization in the general case. In fact, we will define a set $\tilde{\mathcal{U}}$ that a priori is contained in \mathcal{U} but that is big enough such that for energies $E \in \mathcal{E}(\tilde{\mathcal{U}})^c$, the Lyapunov exponent vanishes.

To define this set, let us introduce the maps $\rho^{(n)}: \mathcal{B} \rightarrow \mathbb{R}$ by

$$\rho^{(n)}(\beta_i) \equiv |f_i^{(n)}(x)|^{\frac{1}{2^n |\beta_i|}}, \quad (3.4)$$

and let

$$\rho_{\max}^{(n)} \equiv \max_{\beta_i \in \mathcal{B}} \rho^{(n)}(\beta_i). \quad (3.5)$$

Note that for notational convenience we have dropped the explicit mentioning of the dependence of $\rho^{(n)}$ on the initial condition x .

From now on we will always consider a trace map whose associated substitution ϕ is semi-primitive. Recall that this means that ϕ is primitive on an alphabet $\mathcal{C} \subset \mathcal{B}$.

Definition 3.2. Let $\tilde{\mathcal{U}}_{\varepsilon, c, n}$ be the subset of $\mathbb{R}^{|\mathcal{B}|}$ such that $x \in \tilde{\mathcal{U}}_{\varepsilon, c, n}$ implies

(i)

$$\min_{\gamma \in \mathcal{C}} \rho^{(n)}(\gamma) > [\rho_{\max}^{(n)}]^{1-\varepsilon}, \quad (3.6)$$

(ii)

$$\left[\min_{\gamma \in \mathcal{C}} \rho^{(n)}(\gamma) \right]^{\min_{\alpha \in \mathcal{A}} |\xi^n \alpha|} > c. \quad (3.7)$$

We have the following

Lemma 3.2. *There exists $n_0 < \infty$ such that for all $\varepsilon > 0$ small enough and $\varepsilon' > \varepsilon$, there exists $1 < c < \infty$ such that for all $n \geq n_0$ and for all $n' > n$, $\tilde{\mathcal{U}}_{\varepsilon, c, n} \subset \tilde{\mathcal{U}}_{\varepsilon', c, n'}$.*

Proof. Note first that a priori $\tilde{\mathcal{U}}_{\varepsilon, c, n} \subset \tilde{\mathcal{U}}_{\varepsilon', c', n}$ if $\varepsilon' \geq \varepsilon$ and $c' \leq c$. We will now show that $\tilde{\mathcal{U}}_{\varepsilon, c, n} \subset \tilde{\mathcal{U}}_{\varepsilon', c', n+1}$, for all $\varepsilon' \geq \varepsilon + 2c^{-\delta\bar{\theta}}$ and $c' \leq c^{\bar{\theta}(1-\varepsilon)}$, where $\delta > 0$ is some constant that depends only on the substitutions ξ and ϕ , and $\bar{\theta} > 1$ depends only on the substitution ξ (in fact, as $n \uparrow \infty$, $\bar{\theta} \uparrow \theta$, where θ is the largest eigenvalue of the “substitution matrix,” i.e. the matrix whose entries M_{ij} are the number of times the letter α_i appears in the word $\xi \alpha_j[1]$). Iterating this result one sees that $\tilde{\mathcal{U}}_{\varepsilon, c, n} \subset \tilde{\mathcal{U}}_{\varepsilon_k, c_k, n+k}$, where c_k grows like $c^{[\bar{\theta}(1-\varepsilon)]^k}$ and ε_k needs only to satisfy $\varepsilon_k \geq \varepsilon + \sum_{l=1}^k c_k^{-\delta}$. But since $\varepsilon + \sum_{l=1}^k c_k^{-\delta} \leq \varepsilon + \sum_{l=1}^{\infty} c_k^{-\delta} \equiv \tilde{\varepsilon}$ it suffices to choose $\varepsilon_k \geq \tilde{\varepsilon}$. Moreover, if c is chosen sufficiently large, $\tilde{\varepsilon}$ will be as close to ε as desired. This obviously will imply the lemma.

The crucial idea of the proof is the observation that for c sufficiently large $x \in \tilde{\mathcal{U}}_{\varepsilon, c, n}$ implies that $f \sim \tilde{f}$. Indeed, for any i ,

$$\begin{aligned} |\tilde{f}_i(f^{(n)}(x))| &\leq \sup_{\{n_i\}: \sum_{i=1}^{|\mathcal{B}|} n_i |\xi^n \beta_i| = |\xi^{n+1} \beta|} \prod_{i=1}^{|\mathcal{B}|} |f_i^{(n)}(x)|^{n_i} \\ &= \sup_{\{n_i\}: \sum_{i=1}^{|\mathcal{B}|} n_i |\xi^n \beta_i| = |\xi^{n+1} \beta|} \prod_{i=1}^{|\mathcal{B}|} [\rho^{(n)}(\beta_i)]^{n_i |\xi^n \beta_i|} \\ &\leq \sup_{\{m_i\}: \sum_{i=1}^{|\mathcal{B}|} m_i = |\xi^{n+1} \beta|} \prod_{i=1}^{|\mathcal{B}|} [\rho^{(n)}(\beta_i)]^{m_i} \\ &\leq [\rho_{\max}^{(n)}]^{|\xi^{n+1} \beta|}. \end{aligned} \quad (3.8)$$

Using the fact that by assumption for any $\gamma \in \mathcal{C}$, $\phi(\gamma)$ contains only letters in \mathcal{C} , in a similar way we obtain for any $\gamma \in \mathcal{C}$,

$$\begin{aligned} |\tilde{f}_{i(\gamma)}(f^{(n)}(x))| &\geq \inf_{\{n_i\}: \sum_{i=1}^{|\mathcal{C}|} n_i |\xi^n \gamma_i| = |\xi^{n+1} \gamma|} \prod_{j=1}^{|\mathcal{B}|} |f_{i(\gamma_j)}^{(n)}(x)|^{n_{i(\gamma_j)}} \\ &\geq \left[\min_{\gamma \in \mathcal{C}} \rho^{(n)}(\gamma) \right]^{|\xi^{n+1} \gamma|} \\ &\geq [\rho_{\max}^{(n)}]^{|\xi^{n+1} \gamma|(1-\varepsilon)}. \end{aligned} \quad (3.9)$$

On the other hand

$$\begin{aligned}
|\tilde{f}_i(f^{(n)}(x)) - f_i(f^{(n)}(x))| &\leq \text{const.} \sup_{\{n_i\}: \sum_{i=1}^{|\mathcal{B}|} n_i |\xi^n \beta_i| < |\xi^{n+1} \beta|} \prod_{i=1}^{|\mathcal{B}|} |f_i^{(n)}(x)|^{n_i} \\
&\leq \text{const.} [\rho_{\max}^{(n)}]^{|\xi^{n+1} \beta| - \inf_{\beta_i \in \mathcal{B}} |\xi^n \beta_i|} \\
&\leq [\rho_{\max}^{(n)}]^{|\xi^{n+1} \beta|(1-\kappa)}, \tag{3.10}
\end{aligned}$$

where κ is some strictly positive constant. Here we have used that

$$|\xi^{n+1} \beta| = \sum_{\alpha \in \beta} |\xi^{n+1} \alpha| \leq K \max_{\alpha \in \mathcal{A}} |\xi^{n+1} \alpha| \tag{3.11}$$

and

$$\inf_{\beta_i \in \mathcal{B}} |\xi^n \beta_i| = \inf_{\alpha \in \mathcal{A}} |\xi^n \alpha|. \tag{3.12}$$

Moreover, for primitive substitutions (see e.g. [1]), there exists a finite constant b such that

$$-r_n + \theta \leq \frac{|\xi^{n+1} \alpha|}{\inf_{\alpha \in \mathcal{A}} |\xi^n \alpha|} \leq b\theta + r_n, \quad \text{uniformly in } \alpha \in \mathcal{A}, \tag{3.13}$$

where r_n converges to zero exponentially fast as $n \uparrow \infty$. In particular, (3.13) is uniformly bounded from above by some constant $1/\kappa$, and for n sufficiently large, it is bounded from below by a constant $\tilde{\theta} > 1$. The uniform upper bound then implies the last inequality in (3.10). For c sufficiently large, the constant in (3.10) can be bounded by an arbitrarily small power of $[\rho_{\max}^{(n)}]^{|\xi^{n+1} \beta|}$, and thus it can be absorbed in κ .

Putting together (3.8) and (3.10), we get for all $\beta_i \in \mathcal{B}$ the upper bound

$$\begin{aligned}
|f_i(f^{(n)}(x))| &\leq |\tilde{f}_i(f^{(n)}(x))| + |f_i(f^{(n)}(x)) - \tilde{f}_i(f^{(n)}(x))| \\
&\leq [\rho_{\max}^{(n)}]^{|\xi^{n+1} \beta|} + [\rho_{\max}^{(n)}]^{|\xi^{n+1} \beta|(1-\kappa)} \\
&= [\rho_{\max}^{(n)}]^{|\xi^{n+1} \beta|} (1 + [\rho_{\max}^{(n)}]^{-\kappa |\xi^{n+1} \beta|}). \tag{3.14}
\end{aligned}$$

Thus

$$\begin{aligned}
\rho^{(n+1)}(\beta) &\leq \rho_{\max}^{(n)} [1 + [\rho_{\max}^{(n)}]^{-\kappa |\xi^{n+1} \beta|}]^{\frac{1}{|\xi^{n+1} \beta|}} \\
&\leq \rho_{\max}^{(n)} \exp \left\{ \frac{[\rho_{\max}^{(n)}]^{-\kappa |\xi^{n+1} \beta|}}{|\xi^{n+1} \beta|} \right\} \\
&\leq [\rho_{\max}^{(n)}]^{1 + (\ln [\rho_{\max}^{(n)}]^{|\xi^{n+1} \beta|} [\rho_{\max}^{(n)}]^{-\kappa |\xi^{n+1} \beta|})^{-1}} \\
&\leq [\rho_{\max}^{(n)}]^{1 + c^{-\tilde{\theta} \kappa}}, \tag{3.15}
\end{aligned}$$

where we have used the lower bound on $\rho_{\max}^{(n)}$ implied by (3.8), and the uniform lower bound on (3.13) given by θ . We have also readjusted the constant κ in the last line to absorb the $\ln [\rho_{\max}^{(n)}]$ in the exponent. Since the bound in (3.15) is uniform in i , the last line in (3.15) is an upper bound for $\rho_{\max}^{(n+1)}$. In much the same way we obtain

a lower bound on $\rho^{(n+1)}(\gamma)$ for $\gamma \in \mathcal{C}$, namely

$$\begin{aligned} \rho^{(n+1)}(\gamma) &\geq [\rho_{\max}^{(n)}]^{1-\varepsilon} [1 - [\rho_{\max}^{(n)}]^{(\kappa-\varepsilon)|\xi^{n+1}\gamma|}]^{\frac{1}{|\xi^{n+1}\gamma|}} \\ &\geq [\rho_{\max}^{(n)}]^{1-\varepsilon - (\ln[\rho_{\max}^{(n)}]^{|\xi^{n+1}\gamma|} [\rho_{\max}^{(n)}]^{(\kappa-\varepsilon)|\xi^{n+1}\gamma|})^{-1}(1+\tau)} \\ &\geq [\rho_{\max}^{(n)}]^{1-\varepsilon - c^{-\tilde{\theta}(\kappa-\varepsilon)}(1+\tau)}. \end{aligned} \quad (3.16)$$

Here we assumed that ε is smaller than κ (since κ is some absolute constant that depends only on the trace map, we may always choose ε , for instance, smaller than $\kappa/2$), and τ may be chosen as $c^{-(\kappa-\varepsilon)\tilde{\theta}}/2$ (note that the second inequality in (3.16) uses that for $a > 0$, $e^{-a} \leq 1 - a + \frac{a^2}{2} \leq 1 - a(1 - \tau)$, if $\tau \geq \frac{a}{2}$). Putting (3.15) and (3.16) together, we get that

$$\min_{\gamma \in \mathcal{C}} \rho^{(n+1)}(\gamma) \geq [\rho_{\max}^{(n+1)}]^{1-\varepsilon - c^{-\tilde{\theta}\kappa} - c^{\tilde{\theta}(\kappa-\varepsilon)}(1+\tau)} \quad (3.17)$$

and

$$\left[\min_{\gamma \in \mathcal{C}} \rho^{(n+1)}(\gamma) \right]^{\min_{\alpha \in \mathcal{A}} |\xi^{n+1}\alpha|} \geq c^{\tilde{\theta}} (1 - \varepsilon - c^{-\tilde{\theta}(\kappa-\varepsilon)}(1+\tau)), \quad (3.18)$$

as claimed above and the proof of Lemma 3.2 is completed. \diamond

Corollary 3.1. *Let ε and $c > 2$ and n_0 be chosen such that the conclusion of Lemma 3.2 holds. Then, for all $n \geq 0$,*

$$\tilde{\mathcal{U}}_{\varepsilon, c, n} \subset \text{int } \mathcal{U}_n. \quad (3.19)$$

Moreover, defining (for a given choice of ε , c and n_0)

$$\tilde{\mathcal{U}} \equiv \bigcup_{n=n_0}^{\infty} \tilde{\mathcal{U}}_{\varepsilon, c, n}, \quad (3.20)$$

we have that

$$\tilde{\mathcal{U}} \subset \mathcal{U}. \quad (3.21)$$

Proof. By Lemma 3.2 we have that if $x \in \tilde{\mathcal{U}}_{\varepsilon, c, n}$, then for all $m \geq n$,

$$\begin{aligned} |f_{i(\gamma_0)}^{(m)}(x)| &\geq \min_{\gamma \in \mathcal{C}} ([\rho^{(m)}(\gamma)]^{|\xi^m \gamma|}) = \min_{\gamma \in \mathcal{C}} ([\rho^{(m)}(\gamma)]^{\min_{\alpha \in \mathcal{A}} |\xi^m \alpha| \frac{|\xi^m \gamma|}{\min_{\alpha \in \mathcal{A}} |\xi^m \alpha|}}) \\ &\geq \frac{|\xi^m \gamma|}{c_{m-n}^{\min_{\alpha \in \mathcal{A}} |\xi^m \alpha|}} \geq c > 2 \end{aligned} \quad (3.22)$$

which by definition of \mathcal{U}_n proves that $\tilde{\mathcal{U}}_{\varepsilon, c, n} \subset \mathcal{U}_n$. But since the sets $\tilde{\mathcal{U}}_{\varepsilon, c, n}$ are manifestly open, they are also contained in the interiors of the sets \mathcal{U}_n . The final conclusion (3.21) is then obvious from the definition (3.20), which proves the corollary. \diamond

Proposition 3.1. *Suppose ϕ is semi-primitive. Then $x \in \tilde{\mathcal{U}}^c$ implies that for all $\beta_i \in \mathcal{B}$,*

$$\limsup_{n \uparrow \infty} \frac{1}{|\xi^n \beta_i|} \ln |f_i^{(n)}(x)| \leq 0. \quad (3.23)$$

Proof. Proving the proposition is equivalent to proving that $\limsup_{n \uparrow \infty} \rho_{\max}^{(n)} \leq 1$. Notice first that if $\rho_{\max}^{(n)} \leq D^{\theta^{-n}}$ for some n -independent constant D that may be chosen as large as desired, then a trivial estimate similar to the one used in obtaining the upper bound in the proof of Lemma 3.2 shows that there exists, for any m , a constant D_1 , depending only on D , m and f , such that

$$\rho_{\max}^{(n+m)} \leq D_1^{\theta^{-n}}. \quad (3.24)$$

On the other hand, if $\rho_{\max}^{(n)} > D^{\theta^{-n}}$, with D chosen sufficiently large, we will prove that there exist k, k' and $\delta > 0$, (independent of n), such that

$$\rho_{\max}^{(n+k+k')} \leq [\rho_{\max}^{(n)}]^{1-\delta}. \quad (3.25)$$

Before proving (3.25), let us show how (3.24) and (3.25) imply the proposition. Let us fix D and $m = k + k'$. Obviously, to prove (3.23), it is enough to show that for any $1 \leq n_0 \leq m$, we have that

$$\limsup_{i \uparrow \infty} \rho_{\max}^{(n_0+im)} \leq 1. \quad (3.26)$$

Now by (3.24) and (3.25) we get that for any n_0 ,

$$\rho_{\max}^{(n_0+m)} \leq \max \{ D_1^{\theta^{-n_0}}, [\rho_{\max}^{(n_0)}]^{1-\delta} \}, \quad (3.27)$$

and iterating this

$$\begin{aligned} \rho_{\max}^{(n_0+2m)} &\leq \max \{ D_1^{\theta^{-n_0-2m}}, D_1^{\theta^{-n_0}(1-\delta)}, [\rho_{\max}^{(n_0)}]^{(1-\delta)^2} \}, \dots, \\ \rho_{\max}^{(n_0+im)} &\leq \max \{ D_1^{\theta^{-n_0-(i-1)m}}, D_1^{\theta^{-n_0-(i-2)m}(1-\delta)}, \dots, D_1^{\theta^{-n_0}(1-\delta)^{i-1}}, \dots, [\rho_{\max}^{(n_0)}]^{(1-\delta)^i} \}. \end{aligned} \quad (3.28)$$

As a matter of fact, depending on whether θ^m is smaller or greater than $(1-\delta)$ the last line in (3.28) is bounded by either $\max \{ D_1^{\theta^{-n_0-im}}, [\rho_{\max}^{(n_0)}]^{(1-\delta)^i} \}$ or $\max \{ D_1^{\theta^{-n_0}(1-\delta)^{i-1}}, [\rho_{\max}^{(n_0)}]^{(1-\delta)^i} \}$. Obviously, whatever D_1 or $\rho_{\max}^{(n_0)}$, this bound converges to one as $i \uparrow \infty$, proving (3.26) and hence (3.23).

To prove (3.25) we proceed in two steps: First, we use the fact that ϕ is primitive on \mathcal{C} to show that there exist k and $\delta' > 0$ such that for all n ,

$$\max_{\gamma \in \mathcal{C}} \rho^{(n+k)}(\gamma) \leq [\rho_{\max}^{(n)}]^{1-\delta'}. \quad (3.29)$$

Then we use this inequality together with the second condition from the definition of semi-primitivity to show that there exist k' and $\delta > 0$ such that (3.25) holds.

Let us now prove (3.29). For each $\beta_i \in \mathcal{B}$,

$$f_i^{(n+k)}(x) = f_i^{(k)}(f^{(n)}(x)), \quad (3.30)$$

where $f_i^{(k)}$ is a polynomial s.t.

$$d(f_i^{(k)}) = |\xi^k \beta_i| \quad (3.31)$$

and

$$d(f_i^{(k)} - \tilde{f}_i^{(k)}) \leq |\xi^k \beta_i| - 1, \quad (3.32)$$

so that as in the proof of Lemma 3.2,

$$\begin{aligned} |f_i^{(k)}(f^{(n)}(x)) - \tilde{f}_i^{(k)}(f^{(n)}(x))| &\leq \text{const}_k [\rho_{\max}^{(n)}]^{|\xi^{n+k}\beta_i| - \min_{\alpha \in \mathcal{A}} |\xi^n \alpha|} \\ &\leq [\rho_{\max}^{(n)}]^{|\xi^{n+k}\beta_i|(1 - \tilde{\kappa})}, \end{aligned} \quad (3.33)$$

where $1 > \tilde{\kappa} > 0$ depends only on k , provided $[\rho_{\max}^{(n)}]^{|\xi^{n+k}\beta_i|}$ is sufficiently large, which is guaranteed by the condition $\rho_{\max}^{(n)} > D^{\theta^{-n}}$. In particular, $\tilde{\kappa}$ can be chosen such that (3.33) holds for all $0 \leq k \leq m$.

Now, to prove (3.29), notice that, since $x \in \mathcal{U}^c$, there exists $\tilde{\gamma} \in \mathcal{C}$, such that either

$$|f_{i(\tilde{\gamma})}^{(n)}(x)| \leq c_1 \quad (3.34)$$

with $c_1 \leq c^b$ (recall (3.13)) or

$$|f_{i(\tilde{\gamma})}^{(n)}(x)|^{|\xi^{n\tilde{\gamma}}|} \leq [\rho_{\max}^{(n)}]^{1-\varepsilon}. \quad (3.35)$$

Now choose k such that $\phi^k \gamma$ contains all letters in \mathcal{C} (and in particular $\tilde{\gamma}$) so that

$$\begin{aligned} |\tilde{f}_{i(\tilde{\gamma})}^{(k)}(f^{(n)}(x))| &\leq \sup_{\{n_i\}: \sum_{i=1}^{|\mathcal{C}|} n_i |\xi^n \gamma_i| = |\xi^{n+k}\gamma|} \prod_{j=1}^{|\mathcal{C}|} |f_{i(\tilde{\gamma}_j)}^{(n)}(x)|^{n_j} \times |f_{i(\tilde{\gamma})}^{(n)}(x)| \\ &\leq [\rho_{\max}^{(n)}]^{|\xi^{n+k}\gamma| - |\xi^{n\tilde{\gamma}}|} [\rho_{\max}^{(n)}]^{(1-\varepsilon)|\xi^{n\tilde{\gamma}}|} \\ &= [\rho_{\max}^{(n)}]^{|\xi^{n+k}\gamma| - \varepsilon|\xi^{n\tilde{\gamma}}|}. \end{aligned} \quad (3.36)$$

Since $|\xi^{n\tilde{\gamma}}| \geq \kappa|\xi^{n+k}\gamma|$, uniformly in γ , $\tilde{\gamma} \in \mathcal{C}$, this yields

$$|\tilde{f}_{i(\tilde{\gamma})}^{(k)}(f^{(n)}(x))| \leq [\rho_{\max}^{(n)}]^{|\xi^{n+k}\gamma|(1-\kappa\varepsilon)} \quad (3.37)$$

which together with (3.33) gives (3.26).

Finally, we choose k' such that for all $\beta_i \in \mathcal{B}$, $\phi^{k'} \beta_i$ contains a letter, say $\tilde{\gamma}$, from \mathcal{C} . Then, for all $\beta_j \in \mathcal{B}$,

$$\begin{aligned} |\tilde{f}_j^{(k'+k)}(f^{(n)}(x))| &\leq \sup_{\{n_i\}: \sum_{i=1}^{|\mathcal{B}|} n_i |\xi^{n+k'}\beta_i| = |\xi^{n+k+k'}\beta_j|} \prod_{i=1}^{|\mathcal{B}|} |\tilde{f}_i^{(k)}(f^{(n)}(x))|^{n_i} \\ &\quad \times |\tilde{f}_{i(\tilde{\gamma})}^{(k')} (f^{(n)}(x))| \\ &\leq [\rho_{\max}^{(n)}]^{|\xi^{n+k+k'}\beta_j| - |\xi^{n+k}\tilde{\gamma}|} [\rho_{\max}^{(n)}]^{(1-\delta)|\xi^{n+k}\tilde{\gamma}|} \\ &\leq [\rho_{\max}^{(n)}]^{|\xi^{n+k+k'}\beta_j| - \delta|\xi^{n+k}\tilde{\gamma}|} \end{aligned} \quad (3.38)$$

from which (3.25) follows as before. This concludes the proof of the proposition. \diamond

Remark. Proposition 3.1 provides us with a nice dichotomy: for substitutions with semi-primitive reduced trace maps, for any initial condition x , *either* all components of $f^{(n)}(x)$ diverge in absolute value exponentially fast with the same rate, *or* no component grows exponentially fast. To prove this it was crucial that for primitive substitutions the lengths of the words $|\xi^n \alpha|$ grow with n exponentially fast with the same rate, i.e. $|\xi^n \alpha| \sim \theta^n$, where θ is the largest eigenvalue of the substitution matrix (see e.g. [1, 14]).

Our next task will be to show that $\bar{\nu}$ under some extra conditions – the Lyapunov exponent will be zero if $E \in \mathcal{E}(\mathcal{M})^c$. This is the contents of

Proposition 3.2. *Suppose \tilde{f} satisfies the assumptions of Proposition 3.1. Assume further that there exists $k < \infty$ such that $\xi^k 0$ contains the word $\beta\beta$, for some $\beta \in \mathcal{B}$. Then $E \in \mathcal{E}(\tilde{\mathcal{U}})^c$ implies that*

$$\gamma(E, v) = \lim_{n \uparrow \infty} \frac{1}{|n|} \ln \|T_E(u^{(n)})\| = 0. \quad (3.39)$$

(Here $u^{(n)}$ denotes the word consisting of the first n letters of the substitution sequence $u \equiv \xi^\infty 0$.)

Proof. We show first that

$$\lim_{n \uparrow \infty} \frac{1}{|\xi^n 0|} \ln \|T_E(\xi^n 0)\| = 0. \quad (3.40)$$

Now let us denote

$$R_{\max}^{(n)} = \max_{\alpha \in \mathcal{A}} \|T_E^{(n)}(\alpha)\| \frac{1}{|\xi^n \alpha|}. \quad (3.41)$$

Using the Schwarz inequality, one finds that

$$\|T_E^{(n+1)}(\alpha)\| \leq [R_{\max}^{(n)}]^{|\xi^{n+1} \alpha|}. \quad (3.42)$$

Now choose k such that $\xi^k 0$ contains $\beta\beta$, for some $\beta \in \mathcal{B}$, and use that

$$(T_E^{(n)}(\beta))^2 = x_E^{(n)}(\beta) T_E^{(n)}(\beta) - \mathbf{1}, \quad (3.43)$$

where by Proposition 3.1 $\limsup_{n \uparrow \infty} |x_E^{(n)}(\beta)|^{1/|\xi^n \beta|} \leq 1$. Thus

$$\begin{aligned} \|T_E^{(n+k)}(\alpha)\| &\leq |x_E^{(n)}(\beta)| \sup_{\{n_i\}: \sum n_i |\xi^{n_i} \alpha_i| = |\xi^{n+k} \alpha| - |\xi^n \beta|} \prod_{i=1}^{|\mathcal{A}|} \|T_E^{(n)}(\alpha_i)\|^{n_i} \\ &\quad + \sup_{\{n_i\}: \sum n_i |\xi^{n_i} \alpha_i| = |\xi^{n+k} \alpha| - 2|\xi^n \beta|} \prod_{i=1}^{|\mathcal{A}|} \|T_E^{(n)}(\alpha_i)\|^{n_i} \\ &\leq [R_{\max}^{(n)}]^{|\xi^{n+k} \alpha|(1 - \tau_k)} \end{aligned} \quad (3.44)$$

from which (3.40) follows as the analogous statement in Proposition 3.1.

From (3.40) one obtains (3.39) just as in [11]. \diamond

Remark. Note that the condition in Proposition 3.2 that $\beta \in \mathcal{B}$ is not very restrictive. For, if some other word, say ω , appears as $\omega\omega$ in u , one may always extend the alphabet \mathcal{B} to include ω and study the corresponding trace map.

Proposition 3.2 provides in fact two pieces of information: First it shows that the Lyapunov exponent vanishes on $\mathcal{E}(\tilde{\mathcal{U}})^c$. However, this also implies that if $E \in \sigma(H_v)^c$, then $x_E^{(0)} \in \tilde{\mathcal{U}}$. This is implied by the general fact that for Schrödinger operators the Lyapunov exponent is strictly positive if E is outside the spectrum (see, e.g. [22]). This allows us to prove

Proposition 3.3. *Suppose H_v permits a trace map satisfying the assumptions of Proposition 3.2. Then $E \in \sigma(H_v)$ if and only if $\gamma(E, v) = 0$.*

Proof. To prove the proposition, set

$$\mathcal{O} \equiv \{E | \gamma(E, v) = 0\}. \quad (3.45)$$

We have just seen that $\mathcal{E}(\tilde{\mathcal{U}})^c \subset \mathcal{O}$ while in general $\mathcal{O} \subset \sigma(H_v)$. On the other hand, Lemma 3.1 shows that $\sigma(H_v) \subset (\mathcal{E}(\mathcal{U}))^c$, while by Corollary 3.1, $\mathcal{E}(\mathcal{U})^c \subset \mathcal{E}(\tilde{\mathcal{U}})^c$, so that finally we have the chain of inclusions

$$\mathcal{E}(\tilde{\mathcal{U}})^c \subset \mathcal{O} \subset \sigma(H_v) \subset \mathcal{E}(\mathcal{U})^c \subset \mathcal{E}(\tilde{\mathcal{U}})^c \quad (3.46)$$

which clearly implies the equality of all these sets and proves the proposition. \diamond

Theorem 1 is now a direct consequence of the following general theorem that was proven in [11]:

Theorem 2. [11] *Let H_v be an operator of the form (1.1), where V is a non periodic potential that takes only finitely many values. Let (Ω, T) denote the topological dynamical system where Ω is the closure of the set of translates of the sequence V_n and T the shift operator. Assume that V_n is aperiodic and (Ω, T) permits a unique ergodic T -invariant probability measure μ . Then, if $\sigma(H_v) = \{E | \gamma(E, v) = 0\}$, $\sigma(H_v)$ is supported on a set of zero Lebesgue measure. In particular, $\sigma(H_v)$ has no absolutely continuous component.*

This theorem is in fact a consequence of a lemma of Kotani [18] which states that for aperiodic potentials that take only a finite number of values, the set of energies for which the mean Lyapunov exponent (where the mean is taken over the hull Ω with respect to the T -invariant measure μ) vanishes is of Lebesgue measure zero. Using a result of Herman [23] one can then show, along the lines of a proof of Avron and Simon [24] in the case of almost periodic potentials, that under the assumption of unique ergodicity the sets on which the Lyapunov exponents for different elements in the hull vanish may differ only by sets of zero Lebesgue measure. The detailed proof of this theorem can be found in [11] and will not be reproduced here. The assumption of unique ergodicity is satisfied for substitution sequences based on primitive substitutions. The proof of this result is rather elaborate and may be found in the book by Quéffelec [1]. Therefore, Theorem 1 is proven. $\diamond \diamond$

Theorem 1 shows that for substitution sequences satisfying our hypothesis, the spectrum is manifestly different from both periodic (absolutely continuous spectrum) and random (dense pure point spectrum) potentials. However, in the examples more precise results were proven in that also the existence of eigenvalues could be excluded. In our general setup we can only exclude this possibility under a simple supplementary hypothesis:

Theorem 3. *Suppose the hypothesis of Theorem 1 are satisfied. If in addition there exists $n_0 < \infty$ s.t. $\xi^{n_0} \omega = \xi^m(\gamma_0) \xi^m(\gamma_0) \omega$, where $\gamma_0 \in \mathcal{C}$ and $\omega \in \mathcal{A}^*$ and m are arbitrary, then the spectrum of H_v is purely singular continuous and supported on a Cantor set of zero Lebesgue measure.*

Proof. The basic idea of the proof was used already in Sütő [6] to obtain the same result for the Fibonacci sequence. Namely, note that under our assumption for all $n \geq n_0$,

$$T_E^{(n)}(0) = T_E^{(n-n_0)}(\omega) T_E^{(n-n_0+m)}(\gamma_0) T_E^{(n-n_0+m)}(\gamma_0), \quad (3.47)$$

and therefore $T_E^{(n-n_0+m)}(\gamma_0)$ and $T_E^{(n-n_0+m)}(\gamma_0)^2$ are transfer matrices over $|\xi^{(n-n_0+m)}\gamma_0|$ and $2|\xi^{(n-n_0+m)}\gamma_0|$ sites, respectively. Now, (2.7) implies (see e.g. [6]) that for any normalized vector $\Psi \in \mathbb{R}^2$,

$$\frac{1}{2} \cong \max \{ \|T_E^{(n-n_0+m)}(\gamma_0)^2 \Psi\|, |\operatorname{tr} T_E^{(n-n_0+m)}(\gamma_0)| \|T_E^{(n-n_0+m)}(\gamma_0) \Psi\| \}. \quad (3.48)$$

To use (3.48), we only need the following

Lemma 3.4. *Let $\gamma_0 \in \mathcal{C}$ be any word such that the word $\gamma_0 \in \mathcal{A}^*$ contains the letter 0. Then, for all $E \in \sigma(H_v)$ there exists a sequence of integers n_i tending to infinity such that for all i , $|x_E^{(n_i)}(\beta)| \leq 2$.*

Proof. As we have stated at the beginning of this section, any letter γ_0 satisfying the assumptions of Lemma 3.4 may be used to define the set \mathcal{U} , and in each case, $\mathcal{E}(\mathcal{U})^c = \sigma(H_v)$, and thus does not depend on the chosen letter. The conclusion of the lemma is then obvious from the definition of \mathcal{U} together with the fact that the sets $\mathcal{E}(\mathcal{U}_n)$ are open. \diamond

Let now $E \in \sigma(H_v)$ and let Ψ_E be a solution of (2.1), i.e. a solution of the Schrödinger equation. Let n_i be the sequence given by Lemma 3.4. Assume that $\Psi_E(1) \neq 0$ (otherwise, of necessity, $\Psi_E(0)$ will be nonzero, and the discussion below can be repeated with n_i replaced by $-n_i$). Then

$$\|\Psi_E\|_2^2 \geq \sum_{i=1}^{\infty} \max \{ \|\Psi_E(|\xi^{n_i}\beta|)\|^2, \|\Psi_E(|2\xi^{n_i}\beta|)\|^2 \} \geq \sum_{i=1}^{\infty} \frac{1}{4} \|\Psi_E(1)\|^2 = \infty, \quad (3.49)$$

which proves that Ψ_E is not in $l^2(\mathbb{Z})$ and thus that E is not an eigenvalue. But since this holds for all energies in the spectrum, the theorem is proven. $\diamond \diamond$

Remark. The proof of Theorem 3 implies the stronger result that for all energies in the spectrum, no solution of the Schrödinger equation tends to zero at both plus and minus infinity.

Remark. The hypothesis in Theorem 3 is clearly not *necessary*. The period doubling sequence provides an example where the hypothesis does not hold but the spectrum is still singular continuous. This is also true for the Thue-Morse sequence [10, 11], where, however, an additional symmetry allows to use essentially the same argument. We feel that in all cases where the hypothesis of Theorem 1 hold, the spectrum should be singular continuous.

IV. Examples

In this final section we consider some specific examples, in fact the same ones as in [14]: the Fibonacci sequence, the Thue-Morse sequence, the period-doubling sequence, the circle sequence, the “binary” and “ternary”, “non-Pisot” sequences and finally, rather as a “counter-example,” the Rudin-Shapiro sequence.

In all examples (except Rudin–Shapiro) the alphabets \mathcal{A} will consist of at most three letters that we denote by a, b, c . For the corresponding traces (that we identify with the elements of \mathcal{B}) we will use the simplified notations

$$\begin{aligned} x &\equiv \text{tr } T_E(a), & y &\equiv \text{tr } T_E(b), & z &\equiv \text{tr } T_E(c) . \\ u &\equiv \text{tr } T_E(a)T_E(b), & v &\equiv \text{tr } T_E(b)T_E(c) , \\ w &\equiv \text{tr } T_E(a)T_E(c), & r &\equiv \text{tr } T_E(c)T_E(b)T_E(a) . \end{aligned} \quad (4.1)$$

1. *The Fibonacci Sequence.* The Fibonacci sequence is the fixpoint of the substitution ξ on two letters, a and b , defined by

$$a \rightarrow \xi(a) = ab, \quad b \rightarrow \xi(b) = a . \quad (4.2)$$

The substitution ξ is primitive, since $\xi^2(a) = aba$ and $\xi^2(b) = ab$ both contain all the letters of the alphabet. Using (2.7) the reader verifies easily that a trace map f is found as

$$x \rightarrow u, \quad y \rightarrow x, \quad u \rightarrow xu - y . \quad (4.3)$$

Thus the reduced trace map \tilde{f} is then

$$x \rightarrow u, \quad y \rightarrow x, \quad u \rightarrow xu . \quad (4.4)$$

Obviously, (4.4) may be viewed directly as the substitution ϕ , defined in Sect. 2, acting on the letters x, y, u . This substitution is semi-primitive, since, with $\mathcal{C} \equiv (x, u)$,

- (i) ϕ maps \mathcal{C} into \mathcal{C}^* and $\phi^2(x) = xu$ and $\phi^2(u) = uxu$ both contain all the letters of \mathcal{C} .
- (ii) $\phi^2(x)$ contains x and u , $\phi^2(y)$ contains u and $\phi^2(u)$ contains x and u .

Moreover, since 0 is given by a , $\xi^3 0 = abaab$ and thus contains the square of the word a .

Therefore all the hypothesis of Theorem 1 are satisfied and then the spectrum of H_v is singular and supported on a set of zero Lebesgue measure.

Moreover, $\xi^4 0 = abaababa$ begins with the square of the word aba . Now, aba is not a word in \mathcal{B} , however, following the remark after Proposition 3.2 we may enlarge \mathcal{B} by including the letter $t \equiv aba$. A simple calculation shows then that $\phi(t) = xu^2$ and this extended trace map is still semi-primitive. Thus, Theorem 3 implies that the spectrum of H_v is purely singular continuous.

This of course recovers here a result already proven in [6] and [7].

2. *The Thue–Morse Sequence.* The substitution this time is defined by [9]

$$a \rightarrow \xi(a) = ab, \quad b \rightarrow \xi(b) = ba . \quad (4.5)$$

Obviously, the substitution is primitive. Notice that both the letters a and b can be taken as “0” and that there are therefore two fixpoints $\xi^\infty(a)$ and $\xi^\infty(b)$.

Using again (2.7) with $A = B$, we can find the following trace map f :

$$\begin{aligned} x &\rightarrow u, & y &\rightarrow u , \\ u &\rightarrow xyu - x^2 - y^2 + 2 , \end{aligned} \quad (4.6)$$

and the corresponding reduced trace map \tilde{f} and the substitution ϕ are

$$x \rightarrow u, \quad y \rightarrow u, \quad u \rightarrow xyu. \quad (4.7)$$

This time, the substitution ϕ is even primitive since $\phi^2(x) = \phi^2(y) = xyu$ and $\phi^2(u) = u^2xyu$ contain all the letters of \mathcal{B} .

Finally, choosing a as 0, $\xi^2 a = abba$, which contains the square of the word b . Therefore Theorem 1 holds and thus the spectrum H_ν is singular and supported on a set of zero Lebesgue measure.

As we noticed in the last remark of chapter 3, although we cannot apply Theorem 3, the spectrum of H_ν is purely singular continuous, as was proven in [10] and [11].

3. The Period-Doubling Sequence. It is defined as the fixpoint of the primitive substitution

$$a \rightarrow \xi(a) = ab, \quad b \rightarrow \xi(b) = aa. \quad (4.8)$$

The trace map here is

$$\begin{aligned} x &\rightarrow u, & y &\rightarrow x^2 - 2, \\ u &\rightarrow x^2u - xy - u. \end{aligned} \quad (4.9)$$

ϕ is given by

$$x \rightarrow u, \quad y \rightarrow x^2, \quad u \rightarrow x^2u. \quad (4.10)$$

With $\mathcal{C} \equiv (x, u)$ one checks that it is semi-primitive, since

- (i) ϕ maps \mathcal{C} into \mathcal{C}^* and $\phi^2(x) = x^2u$ and $\phi^2(u) = u^2x^2u$.
- (ii) $\phi^2(x)$ contains x and u , $\phi^2(y)$ contains u and $\phi^2(u)$ contains x and u .

Finally, $\xi^2 0 = abaa$ contains the square of the word a and thus Theorem 1 applies. However, the hypothesis of Theorem 3 are not verified, although it was proven (through a rather cumbersome calculation) in [11] that the spectrum is singular continuous. Note however that the “inverted” sequence (obtained by setting $\xi(a) = ba$) satisfies the hypothesis of Theorem 3.

4. The Circle Sequence. The circle sequence is associated to the substitution ξ on three letters

$$\begin{aligned} a &\rightarrow \xi(a) = cac, & b &\rightarrow \xi(b) = accac, \\ c &\rightarrow \xi(c) = abcac. \end{aligned} \quad (4.11)$$

This substitution has no fixpoint, since it does not possess a letter “0,” but it has a cycle of length two and the twice iterated substitution has two fixpoints.

Using then the identities (2.7) and (2.8), we find an alphabet $\mathcal{B} \equiv (a, b, c, ab, bc, ca, abc)$, identified with $\mathcal{B} \equiv (x, y, z, u, v, w, r)$, and the following

trace map f ,

$$\begin{aligned}
 x &\rightarrow zw - x, & y &\rightarrow zw^2 - xw - z, & z &\rightarrow wr - y, \\
 u &\rightarrow (zw - x)(zw^2 - xw - z) - w, \\
 v &\rightarrow (zw^2 - xw - z)(wr - y) - yz + v, \\
 w &\rightarrow (wr - y)(zw - x) - u, \\
 r &\rightarrow (wr - y)(zw - x)((zw^2 - xw - z) - w) \\
 &\quad + w^2r - r - yw - u(zw^2 - xw - z).
 \end{aligned} \tag{4.12}$$

The reduced trace map \tilde{f} is

$$\begin{aligned}
 x &\rightarrow zw, & y &\rightarrow zw^2, & z &\rightarrow wr, \\
 u &\rightarrow z^2w^3, & v &\rightarrow zw^3r, & w &\rightarrow zw^2r, \\
 r &\rightarrow z^2w^4r.
 \end{aligned} \tag{4.13}$$

The associated substitution ϕ is again semi-primitive with $\mathcal{C} \equiv (z, w, r)$, since

- (i) ϕ maps \mathcal{C} into \mathcal{C}^* and $\phi^2(z) = zw^2rz^2w^4r$, $\phi^2(w) = wr(zw^2r)^2z^2w^4r$ and $\phi^2(r) = (wr)^2(zw^2r)^4z^2w^4r$.
- (ii) For any $\beta \in \mathcal{B}$, $\phi^2(\beta)$ contains z, w and r .

Moreover ξ^2c begin with the square of the word $ca \in \mathcal{B}$ so that both Theorem 1 and 3 apply and show that the spectrum is singular continuous in this case, too.

5. *Binary Non-Pisot Sequence.* This sequence corresponds to the substitution

$$a \rightarrow \xi(a) = ab, \quad b \rightarrow \xi(b) = aaa \tag{4.14}$$

and the trace map

$$\begin{aligned}
 x &\rightarrow u, & y &\rightarrow x^3 - 3x, \\
 u &\rightarrow x^3u - x^2y - 2xu + y
 \end{aligned} \tag{4.15}$$

with reduced trace map

$$x \rightarrow u, \quad y \rightarrow x^3, \quad u \rightarrow x^3u. \tag{4.16}$$

Here $\mathcal{C} \equiv (x, u)$ and since $\phi^2(x) = x^3u$ and $\phi^2(u) = x^4u^3$, we see that the substitution ϕ is semi-primitive. Moreover, $\xi^20 = abaaa$ contains the square of the word a , so Theorem 1 applies.

Theorem 3, however, does not apply in this case (although again, as in the case of the period doubling sequence, the inverted sequence satisfies the hypothesis of this theorem) and we do not know for sure whether the eigenvalues are present in this example.

6. *Ternary Non-Pisot Sequence.* This sequence corresponds to the substitution

$$a \rightarrow \xi(a) = c, \quad b \rightarrow \xi(b) = a, \quad c \rightarrow \xi(c) = bab. \tag{4.17}$$

As in the case of the circle sequence, this substitution does not possess a fixpoint, but a cycle of length three, whose three elements can be considered as

substitution sequences. With the alphabet $\mathcal{B} \equiv (x, y, z, u, v, w)$, we can find the trace map f

$$\begin{aligned} x &\rightarrow z, & y &\rightarrow x, & z &\rightarrow yu + x, \\ u &\rightarrow w, & v &\rightarrow u^2 - 2, & w &\rightarrow uw + w - xz, \end{aligned} \quad (4.18)$$

and the reduced trace map

$$\begin{aligned} x &\rightarrow z, & y &\rightarrow x, & z &\rightarrow yu, \\ u &\rightarrow w, & v &\rightarrow u^2, & w &\rightarrow uv. \end{aligned} \quad (4.19)$$

The substitution ϕ is semi-primitive with $\mathcal{C} \equiv (u, v, w)$ since $\phi^5(u) = wu^2uvw$, $\phi^5(v) = uvw^2uvw^2$ and $\phi^5(w) = wvw^3u^2wu^2$ and for any $\beta \in \mathcal{B}$, $\phi^3(\beta)$ contains u , v and w .

Moreover, $\xi^5 a = \xi^6 b = \xi^4 c = babacabab$ begins with the square of the word ba . Therefore, by Theorems 1 and 3, the spectrum of H_v is purely singular continuous.

7. The Rudin–Shapiro Sequence. The Rudin–Shapiro sequence [17] is defined on an alphabet of four letters. The substitution rule is

$$\begin{aligned} a &\rightarrow \xi(a) = ac, & b &\rightarrow \xi(b) = dc, \\ c &\rightarrow \xi(c) = ab, & d &\rightarrow \xi(d) = db. \end{aligned} \quad (4.20)$$

The final example serves to illustrate that even the hypothesis of Theorem 1 is not always satisfied. It has been remarked in different contexts (see [12]) that the Rudin–Shapiro sequence has quite exceptional properties and that the analysis of the spectrum of the associated operators eludes perturbative and even numerical methods.

Using the trace map computed by [20], we obtain a reduced trace map \tilde{f} on an alphabet $\mathcal{B} \equiv (x, y, z, w, s, t, q, r)$ (this trace map was obtained in [20] in a clever way in order to stay with as few traces as possible. A straightforward derivation would give a map on twelve letters which would share the same properties)

$$\begin{aligned} x &\rightarrow s, & y &\rightarrow t, & z &\rightarrow t, & w &\rightarrow s, \\ s &\rightarrow r, & t &\rightarrow q, & q &\rightarrow xwr, & r &\rightarrow yzq. \end{aligned} \quad (4.21)$$

It is easy to notice that the two alphabets $\mathcal{C}_1 \equiv (x, w, t, r)$ and $\mathcal{C}_2 \equiv (y, z, s, q)$ are mutually exchanged by the substitution ϕ associated to f . This implies that ϕ is not semi-primitive. Now, \mathcal{C}_1 and \mathcal{C}_2 are left invariant under ϕ^2 and one might hope to simply study the dynamics of the trace maps on the two sub-alphabets separately. However, the subdominant terms in the trace map (which we have not written, but see [20]) do not respect this invariance which makes it impossible to even adapt the proof of Propositions 3.1 and 3.2 to this situation. So once again, the Rudin–Shapiro sequence retains its mystery.

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