

A Review of a Work by L. Raymond: Sturmian Hamiltonians with a Large Coupling Constant—Periodic Approximations and Gap Labels



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Abstract We present a review of the work (Raymond in a constructive gap labelling for the discrete Schrödinger operator on a quasiperiodic chain (1995), [39], Raymond in *Etude algébrique de milieux quasipériodiques* (1995), [40]). The review aims at making this work more accessible and offers adaptations of some statements and proofs. In addition, this review forms an applicable framework for the complete solution of the Dry Ten Martini Problem for Sturmian Hamiltonians as appears in Band, Beckus and Loewy (Dry Ten Martini Problem for Sturmian Hamiltonians, [3]). A Sturmian Hamiltonian is a one-dimensional Schrödinger operator whose potential is a Sturmian sequence multiplied by a coupling constant, $V \in \mathbb{R}$. The spectrum of such an operator is commonly approximated by the spectra of designated periodic operators. If $V > 4$, then the spectral bands of the periodic operators exhibit a

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particular combinatorial structure. This structure provides a formula for the integrated density of states. Employing this, it is shown that if $V > 4$, then all the gaps, as predicted by the gap labeling theorem, are there.

Keywords Sturmian Hamiltonian · Spectral gap labels · Spectral tree

1 Introduction

1.1 *The Motivation for this Review*

The starting point of this paper is the unpublished work of Raymond, [39] and his PhD thesis [40] (see also [41]). The first two authors became aware of [39] via a private communication with Damanik. Band and Beckus were influenced by [39] in their joint work with Loewy [3] and found it beneficial to refer to parts of [39] in [3]. Indeed, [39] is a very stimulating work, contains some foundational results, and is referred to numerous times (see, e.g., the surveys [12–14, 26] and references within), in spite of being unpublished. We started to write the current review with three goals in mind. First, it might be worthwhile to elaborate on some of the proofs and fill in some gaps. Second, by adapting some notations and conventions, we create a unified framework toward providing the complete solution for the Dry Ten Martini Problem for Sturmian Hamiltonians, [2, 3]. Finally, we felt that the whole community might benefit from having a published version of Raymond’s work upon reaching its thirtieth anniversary. Hence, we joined forces to produce the current review, with Raymond joining as well after this review was already initiated. While this review was in final stages of preparation, we became aware that a similar publication is planned in [38], as part of the book series initiated by Baake and Grimm [6, 7].

In this review, we make the connection to [39] as transparent as possible. In particular, throughout the review we clarify as much as possible where we merely rephrase statements from [39] and where we elaborate or bring new statements and terminology. When writing the current review, we were trying to provide an appropriate balance between two objectives. On the one hand, our desire is to reflect the original work [39] with no substantial changes. On the other hand, at times we felt that the exposition may profit by including adaptations based on later papers and recent progress in the field.

We should emphasize that the current review covers only the first five sections of [39] that form the starting point for resolving the Dry Ten Martini Problem for Sturmian Hamiltonians in [3]. We do not treat here the last section of [39] about the Hausdorff dimension of the Fibonacci Hamiltonian. This part in [39] led to further progress in the study of the fractal dimensions of the spectrum of Sturmian Hamiltonians, see, e.g., [15, 20, 24, 28, 34]. Reviewing this part of [39] is not included here since the focus is on the study of the integrated density of states and the gap labels.

1.2 A Short Historical Review

Let us start by introducing the model. We consider bounded linear operators $H_{\alpha,V} : \ell^2(\mathbb{Z}) \rightarrow \ell^2(\mathbb{Z})$, given by

$$(H_{\alpha,V}\psi)(n) := \psi(n+1) + \psi(n-1) + V\chi_{[1-\alpha,1)}(n\alpha \bmod 1)\psi(n), \quad (1.1)$$

where $V \in \mathbb{R}$ is the *coupling constant* and $\chi_{[1-\alpha,1)}$ is the characteristic function of the interval $[1-\alpha, 1)$. Whenever $\alpha \in \mathbb{R} \setminus \mathbb{Q}$, the operator $H_{\alpha,V}$ is aperiodic (in the sense that its potential sequence is not periodic) and it is known as a *Sturmian Hamiltonian*.

We provide a short summary on the developments for the spectral theory of Sturmian Hamiltonians and refer the reader to the surveys [12–14, 26] and references therein for more details. This class of operators serves as the guiding example for one-dimensional quasicrystals and was introduced in [29, 37]. This model is also called *Kohmoto model* and a plot of the associated spectra, as they vary with α —called the *Kohmoto butterfly*—can be found in Fig. 1.

A first mathematical analysis of the so-called Fibonacci Hamiltonian $H_{\alpha,V}$ with $\alpha = \frac{\sqrt{5}-1}{2}$ was developed in [10]. Shortly after it was proven that the Fibonacci Hamiltonian has Cantor spectrum of Lebesgue measure zero and the spectral measure is purely singular continuous, [44, 45]. For all Sturmian Hamiltonians (i.e., all $\alpha \notin \mathbb{Q}$

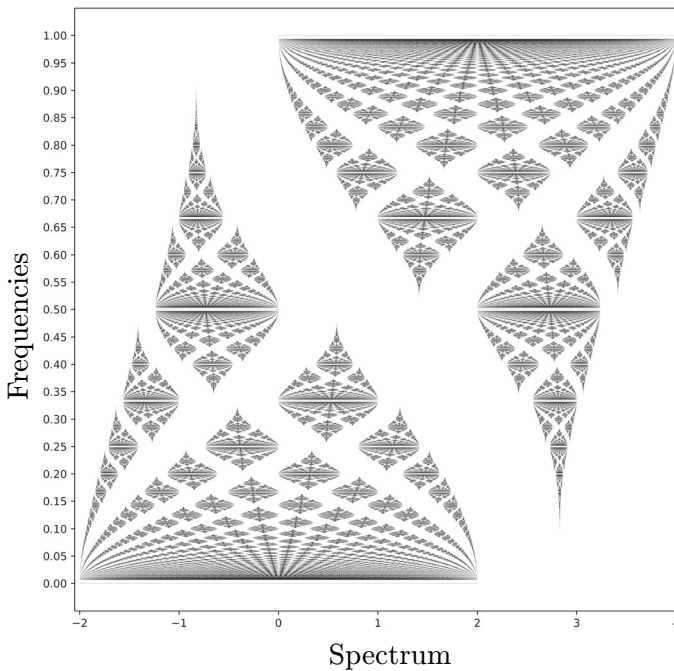


Fig. 1 The Kohmoto butterfly for $V = 2$

and $V \neq 0$), Cantor spectrum of Lebesgue measure zero was proven in [8]. This result was generalized in [30] to a large class of one-dimensional dynamical systems. The absence of point spectrum and upper bounds on the growth of solutions for Sturmian Hamiltonians were thoroughly studied as well [21–23].

Influenced by these results, one may ask whether all the spectral gaps that are predicted by the gap labeling theorem [1, 4] appear. This is the so-called Dry Ten Martini Problem for Sturmian Hamiltonians. Such a question was originally asked by Kac in 1981 for the almost Mathieu operator (“are all gaps there?”), see [42]. For large enough coupling constant, $V > 4$, it was proven in [39] that all gaps are there, and this is reviewed in the current paper. For the Fibonacci Hamiltonian and small enough coupling V , it was proven in [18] that all spectral gaps are there. This result was extended in [35] for $\alpha \in [0, 1] \setminus \mathbb{Q}$ with eventually periodic continued fraction expansion and small enough coupling constant. In a remarkable study of the Fibonacci Hamiltonian [20], it was proven that all gaps are there for all $V \neq 0$ and $\alpha = \frac{\sqrt{5}-1}{2}$. Finally, a complete solution of the Dry Ten Martini Problem for Sturmian Hamiltonians for all $\alpha \in [0, 1] \setminus \mathbb{Q}$ and all $V \neq 0$ is provided in [3]. Moreover, the hierarchical structure of the periodic approximations spectra (initiated in [39]) was extended in [3] to all $V \neq 0$.

This hierarchical structure also laid the ground to estimate the Hausdorff dimension for the Fibonacci Hamiltonian in [39]. It influenced the study of the fractal dimension and the transport exponent for Sturmian Hamiltonians during the last decades, see, e.g., [11, 15, 19, 20, 24, 28, 33, 34].

Organization of the paper. The paper is structured as follows. Section 2 discusses the Sturmian sequences and their periodic mechanical words. In addition, we introduce there a designated space of finite continued fraction expansions following the lines of [3]. In Sect. 3, we present the standard Floquet–Bloch theory via transfer matrices and the discriminant. Various useful identities of the discriminants are presented there. Section 4 describes the spectra of the periodic approximations and their special combinatorial structure—first in general and then specializing for the case $V > 4$. Section 5 applies the aforementioned combinatorial structure for the study of the integrated density of states and the gap labeling for $V > 4$.

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2 The Sturmian Potential

This section is dedicated to studying the Sturmian sequence $\chi_{[1-\alpha,1)}(n\alpha \bmod 1)$, which serves as the potential of the Sturmian Hamiltonian (1.1). In particular, we will consider rational values of α , which give rise to periodic sequences and periodic Hamiltonians. Most of the content of this section does not appear in [39] and our main motivation for including it here is to use already in the current review some tools and notations which are essential for [3].

2.1 The Space \mathcal{C} of Finite Continued Fraction Expansions

Every irrational number $\alpha \in \mathbb{R} \setminus \mathbb{Q}$ has a unique continued fraction expansion [27], i.e.:

$$\alpha = c_0 + \frac{1}{c_1 + \frac{1}{c_2 + \frac{1}{\ddots}}},$$

where $c_0 \in \mathbb{Z}$ and $c_k \in \mathbb{N}$ for $k \geq 1$ and the sequence (c_0, c_1, c_2, \dots) is unique. If $\alpha \in \mathbb{Q}$, then there is a finite sequence (c_0, c_1, \dots, c_k) such that

$$\alpha = c_0 + \frac{1}{c_1 + \frac{1}{\ddots + \frac{1}{c_k}}},$$

and we refer to (c_0, c_1, \dots, c_k) as a finite continued fraction expansion of α . However, the sequence (c_0, c_1, \dots, c_k) is not unique for a rational α , see [27, Chap I.4] and Remark 2.1. Since we are only interested in $\alpha \in [0, 1]$, we always have $c_0 = 0$. In the current paper, we modify the conventional notation of continued fraction expansions in two aspects:

- We add an artificial digit $c_{-1} = 0$ to each finite continued fraction expansion $(0, c_1, \dots, c_k)$ and represent it by the string of “*digits*” $[0, 0, c_1, \dots, c_k]$.
- We allow the last digit c_k of a string $[0, 0, c_1, \dots, c_k]$ to attain also the values 0 and -1 , namely, $c_k \in \mathbb{N}_{-1} := \mathbb{N} \cup \{-1, 0\}$.

Summarizing the above, we defined the formal space of *finite continued fraction expansions* to be

$$\mathcal{C} := \{[0], [0, 0]\} \cup \bigcup_{k \in \mathbb{N}} \{[0, 0, c_1, \dots, c_k] : c_1, \dots, c_{k-1} \in \mathbb{N}, c_k \in \mathbb{N}_{-1}\}.$$

The purpose of these deviations from the conventional notation is mainly to describe the different types of the spectral bands in Sect. 4.2. These types depend on the particular choice of $\mathbf{c} \in \mathcal{C}$ and not only on the rational number which is represented by the continued fraction (more details appear in Sect. 4.2 and in [3, Proposition 2.10]).

For $\mathbf{c} = [0, c_0, c_1, \dots, c_k] \in \mathcal{C}$ and $m \in \mathbb{N}_{-1}$, we will use the notation

$$[\mathbf{c}, m] := [0, c_0, c_1, \dots, c_k, m] \in \mathcal{C},$$

whenever it is defined. We use frequently in this work the condition $[\mathbf{c}, m] \in \mathcal{C}$. The constraints this condition imposes are: if $\mathbf{c} = [0]$, then $m = 0$ and if $k \in \mathbb{N}$, then $c_k \geq 1$.

We connect the set of continued fractions with rational numbers by introducing the evaluation map $\varphi : \mathcal{C} \rightarrow \mathbb{R} \cup \{\infty\}$. It is defined for all $\mathbf{c} \in \mathcal{C} \setminus \{[0], [0, 0, -1]\}$ by

$$\varphi([0, c_0, c_1, \dots, c_k]) := \begin{cases} \varphi([0, c_0, c_1, \dots, c_{k-2}, c_{k-1} - 1]), & k \geq 2 \text{ and } c_k = -1, \\ \varphi([0, c_0, c_1, \dots, c_{k-2}]), & k \in \mathbb{N} \text{ and } c_k = 0, \\ c_0 + \frac{1}{c_1 + \frac{1}{\ddots + \frac{1}{c_k}}}, & \text{otherwise.} \end{cases} \quad (2.1)$$

In addition to that we set $\varphi([0]) := \infty$ and $\varphi([0, 0, -1]) = -1$. The first line in the right-hand side of (2.1) is equivalent to substituting $c_k = -1$ in the continued fraction expansion. The second line is more delicate; if one allows taking $c_k \in \mathbb{R}$ then one gets

$$\lim_{c_k \rightarrow 0} \left(c_0 + \frac{1}{c_1 + \frac{1}{\ddots + \frac{1}{c_k}}} \right) = c_0 + \frac{1}{c_1 + \frac{1}{\ddots + \frac{1}{c_{k-2}}}},$$

which is the rationale standing behind the definition $\varphi([0, c_0, c_1, \dots, c_{k-2}, c_{k-1}, 0]) := \varphi([0, c_0, c_1, \dots, c_{k-2}])$ in (2.1).

Remark 2.1 From the definition of the map φ , we get $\text{Im}(\varphi) \subseteq (\mathbb{Q} \cap [0, 1]) \cup \{-1\} \cup \{\infty\}$. A basic yet important observation is that the map φ is not injective. This may be seen already from its definition in (2.1). In addition,

$$\varphi([0, c_0, c_1, \dots, c_{k-2}, c_{k-1}, c_k, 1]) = \varphi([0, c_0, c_1, \dots, c_{k-2}, c_{k-1}, c_k + 1]),$$

which is a common dual representation within continued fraction expansions [27, Chap I.4]. Furthermore, one can check that

$$\varphi(\mathbf{c}) = \infty \quad \Leftrightarrow \quad \mathbf{c} \in \{[0], [0, 0, 0], [0, 0, 1, -1]\}.$$

The motivation behind using continued fraction expansions is for approximating irrational $\alpha \in [0, 1] \setminus \mathbb{Q}$ by rational values, which allows to approximate aperiodic Hamiltonians (1.1) by periodic ones. Specifically, given $\alpha \in [0, 1] \setminus \mathbb{Q}$ with

$$\alpha = c_0 + \frac{1}{c_1 + \frac{1}{c_2 + \frac{1}{\ddots}}}, \quad (2.2)$$

we define for each $k \in \mathbb{N}$,

$$\mathbf{c}_k := [0, 0, c_1, \dots, c_k] \quad \text{and} \quad \alpha_k := \varphi(\mathbf{c}_k).$$

The values α_k offer an optimal way to approximate α in the sense $\lim_{k \rightarrow \infty} \alpha_k = \alpha$, and thus we refer to α_k as the k -th convergent of α [27, Chap. I.3].

We further denote $\frac{p_k}{q_k} := \alpha_k$, where $p_k, q_k \in \mathbb{N}$ are chosen to be coprime. It is useful to extend this notation so that it includes also the values $k \in \{-1, 0\}$. This is done by setting

$$\begin{aligned} \alpha_{-1} &:= \varphi([0]) = \infty, & p_{-1} &= 1, & q_{-1} &= 0, \\ \alpha_0 &:= \varphi([0, 0]) = 0, & p_0 &= 0, & q_0 &= 1. \end{aligned}$$

Note that for $k = -1$, we adopt the formal convention, $\alpha_{-1} = \frac{p_{-1}}{q_{-1}} = \infty$. The reason for introducing p_{-1}, p_0, q_{-1} and q_0 is given by the following recursive formulas [27, Theorem 1]: for $k \in \mathbb{N}_0$

$$p_{k+1} = c_{k+1}p_k + p_{k-1} \quad \text{and} \quad q_{k+1} = c_{k+1}q_k + q_{k-1}. \quad (2.3)$$

Remark 2.2 It is beneficial to make the analogy between the notations introduced above and the notations in [39]. The notation (k, p) , appearing first in [39, Proposition 2.2], is replaced in this review by $[0, 0, c_1, \dots, c_{k-1}, p] = [\mathbf{c}_{k-1}, p]$. We do so, since we find in [3] that it is essential to keep track of all numbers in the continued fraction expansion simultaneously and consider values of $\mathbf{c} \in \mathcal{C}$ which correspond to different $\alpha \notin \mathbb{Q}$. This matter is not raised in [39], where it is sufficient to fix a single $\alpha \notin \mathbb{Q}$ and for that the notation (k, p) is adequate.

2.2 Sturmian Words and Mechanical Words

We present here a brief introduction to Sturmian words and mechanical words. For elaborate surveys, see [5, 31].

We start by denoting for $\alpha \in [0, 1]$ and $n \in \mathbb{Z}$,

$$\omega_\alpha(n) := \chi_{[1-\alpha, 1)}(n\alpha \bmod 1). \quad (2.4)$$

Another equivalent representation of the sequence $\omega_\alpha \in \{0, 1\}^{\mathbb{Z}}$ is the following.

Lemma 2.3 ([8, 39], Lemma 1, Definition 2.1) *Let $\alpha \in [0, 1]$ and $n \in \mathbb{Z}$. Then*

$$\omega_\alpha(n) = \lfloor (n+1)\alpha \rfloor - \lfloor n\alpha \rfloor, \quad (2.5)$$

where $\lfloor \cdot \rfloor$ is the floor function.

Proof First, observe that $\lfloor \alpha(n+1) \rfloor - \lfloor \alpha n \rfloor \in \{0, 1\}$, for all $n \in \mathbb{Z}$. Using that the claim follows from

$$\begin{aligned} \omega_\alpha(n) = 1 &\iff n\alpha \bmod 1 \in [1-\alpha, 1) \\ &\iff \exists m \in \mathbb{Z} : n\alpha \in [m+1-\alpha, m+1) \\ &\iff \lfloor \alpha(n+1) \rfloor - \lfloor \alpha n \rfloor = 1. \end{aligned} \quad \square$$

We use the notation ω_α for both rational and irrational values of α . The infinite words defined by $\lfloor \alpha(n+1) \rfloor - \lfloor \alpha n \rfloor$ are also called *(lower) mechanical words (with slope α)* [31, Sect. 2.1.2]. If $\alpha = \frac{p}{q} \in [0, 1] \cap \mathbb{Q}$, then it is elementary to see that ω_α is q -periodic, i.e., $\omega_\alpha(n+q) = \omega_\alpha(n)$ for all $n \in \mathbb{Z}$. If $\alpha \notin \mathbb{Q}$ then ω_α is called a Sturmian sequence, which is not a periodic word. In this case, it is useful to study the (q_k) -periodic words ω_{α_k} as approximations of ω_α where $\alpha_k = \frac{p_k}{q_k}$ are the k th convergents of α and p_k, q_k are coprime.

We have seen in (2.3) that there is a recursive formula which connects the period lengths, q_k , for three subsequent k values. We show next that the periods themselves (i.e., the finite sub-words of length q_k) are also connected via a recursive relation. We denote these periods by $W_k \in \{0, 1\}^{q_k}$, setting

$$W_k(i) := \omega_{\alpha_k}(i), \quad 0 \leq i \leq q_k - 1 \quad (2.6)$$

and claiming the following.

Lemma 2.4 *The periods of the mechanical words satisfy the following:*

$$W_0 = 0, \quad W_1 = \underbrace{0 \dots 0}_{c_1-1} 1.$$

If $k \geq 2$ then

$$W_k = \begin{cases} W_{k-2} W_{k-1}^{c_k}, & k \equiv 0 \pmod{2}, \\ W_{k-1}^{c_k} W_{k-2}, & k \equiv 1 \pmod{2}, \end{cases}$$

where the power means a concatenation of words.

In addition, for $k \geq 1$, these periods appear as the prefix of the infinite Sturmian word ω_α in the following sense:

- If $k \equiv 0 \pmod{2}$ then $\omega_\alpha(i) = W_k(i)$ for all $0 \leq i \leq q_k - 1$.
- If $k \equiv 1 \pmod{2}$ then $\omega_\alpha(i) = W_k(i)$ for all $0 \leq i \leq q_k - 2$.

In fact, it will be shown in the following sections that we care of the words W_k only up to a cyclic shift. In this sense, the expressions $W_{k-2}W_{k-1}^{c_k}$ and $W_{k-1}^{c_k}W_{k-2}$ are the same. Therefore, in the literature (and, in particular, in [39, Eq. (2)]) only the expression $W_{k-1}^{c_k}W_{k-2}$ is used. Indeed, W_k equals to $W_{k-1}^{c_k}W_{k-2}$ up to a possible cyclic shift is proven and used in various works, see, e.g., [8], [22, Proposition 2.2] and [12, Theorem 2.15]. Another difference between the common viewpoint and ours is that usually the periods W_k of the mechanical words $\omega_{\alpha k}$ are compared to the Sturmian sequence ω_α , whereas we wish to compare between the various periods to themselves, W_k , W_{k-1} , and W_{k-2} .

We decided to supplement the discussion in the current review by treating the precise sub-word W_k , as it is defined in (2.6), and not only up to cyclic shift. We employ this exact representation in Sect. 7 when defining the finite-dimensional Hamiltonian matrices (7.1) for the Floquet–Bloch theory. These matrices also play a substantial role in [3]. For these reasons we have Lemma 2.4 as written here (and not only up to a cyclic shift) and its proof. Statements which are similar to Lemma 2.4 can be also found in [32, Eq. (2.8)] and [31, Problem 2.2.10].

The reader is referred to Sect. 6 for the proof of Lemma 2.4 and related results.

3 Transfer Matrices and the Discriminant

In this section, we study the spectrum of the operator $H_{\alpha,V}$ (1.1) while our main focus lies on rational $\alpha \in [0, 1]$. In this work, we use the rational approximations α_k to study the spectrum of $H_{\alpha,V}$ for $\alpha \in [0, 1] \setminus \mathbb{Q}$. If $\alpha = \frac{p}{q} \in [0, 1]$ is rational, then ω_α is q -periodic. Hence, the spectrum of $H_{\alpha,V}$ is given by Floquet–Bloch theory using transfer matrices and the discriminant, as is described in the following. We note that there is an equivalent approach to Floquet–Bloch theory by employing $q \times q$ Hamiltonian matrices which depend on the Bloch parameter. This equivalent approach (and its connections to transfer matrices) is described in Sect. 7 and extensively used in [3].

3.1 The Spectrum of Periodic Operators Via Transfer Matrices and the Discriminant

We briefly present here some basic Floquet–Bloch theory using the transfer matrix formalism. We keep the exposition as short as possible and mainly intend to set the notation and the tools to be used in the sequel. Two good sources for a more thorough introduction to the one-dimensional discrete Floquet–Bloch theory are [43, Chap 5] and [46, Chap. 7].

Let $V \in \mathbb{R}$ and $\alpha \in [0, 1]$. The difference equations associated to $H_{\alpha,V}$ are

$$Eu(n) = u(n-1) + u(n+1) + V\omega_\alpha(n)u(n), \quad E \in \mathbb{R}, n \in \mathbb{Z}. \quad (3.1)$$

Solutions of this equation are studied via the so-called one-step transfer matrices

$$A_\alpha(n)(E, V) := \begin{pmatrix} E - V\omega_\alpha(n) & -1 \\ 1 & 0 \end{pmatrix}, \quad E \in \mathbb{R}, n \in \mathbb{Z}.$$

Writing the difference equations in a matrix form, we obtain the following.

Lemma 3.1 *Let $V \in \mathbb{R}$, $\alpha \in [0, 1]$, $u : \mathbb{Z} \rightarrow \mathbb{C}$ and $E \in \mathbb{R}$ be such that Eqs. (3.1) are satisfied for all $n \in \mathbb{Z}$. Then we have for all $n \in \mathbb{Z}$*

$$A_\alpha(n)(E, V) \begin{pmatrix} u(n) \\ u(n-1) \end{pmatrix} = \begin{pmatrix} u(n+1) \\ u(n) \end{pmatrix} \quad \text{and} \quad \det(A_\alpha(n)(E, V)) = 1.$$

Proof This follows by a short computation. \square

Let $\mathbf{c} \in \mathcal{C}$ with $\frac{p}{q} := \varphi(\mathbf{c}) \in [0, 1]$ with p, q coprime. We observed in the previous section that the potential ω_α is q -periodic for rational $\alpha = \frac{p}{q}$. Thus, it is advantageous to define the (q -step) transfer matrix

$$M_{\mathbf{c}} := A_{\frac{p}{q}}(q-1) \cdot A_{\frac{p}{q}}(q-2) \dots A_{\frac{p}{q}}(1) \cdot A_{\frac{p}{q}}(0) \quad (3.2)$$

and get the following immediate implication.

Lemma 3.2 *Let $V \in \mathbb{R}$, $\mathbf{c} \in \mathcal{C}$ with $\frac{p}{q} := \varphi(\mathbf{c}) \in [0, 1]$. Then*

$$M_{\mathbf{c}}(E, V) \begin{pmatrix} u(0) \\ u(-1) \end{pmatrix} = \begin{pmatrix} u(q) \\ u(q-1) \end{pmatrix}$$

holds for all $u : \mathbb{Z} \rightarrow \mathbb{C}$ and $E \in \mathbb{R}$ satisfying (3.1). In addition, $\det M_{\mathbf{c}} = 1$.

Proof This is an immediate consequence of Lemma 3.1. \square

Lemma 3.2 extends to $\mathbf{c} = [0, 0, -1]$ for which $\varphi(\mathbf{c}) = -1$. To do so, we set $\frac{p}{q} = \frac{-1}{1}$ and apply the definition of the mechanical word from Lemma 2.3 to get for all $n \in \mathbb{Z}$,

$$\omega_{-1}(n) := \lfloor (n+1)(-1) \rfloor - \lfloor n(-1) \rfloor = -1,$$

and

$$A_{-1}(n)(E, V) = \begin{pmatrix} E + V & -1 \\ 1 & 0 \end{pmatrix} = M_{[0,0,-1]}(E, V). \quad (3.3)$$

We continue by using the recursive structure of the Sturmian words, as expressed in Lemma 2.4, in order to provide the recursive relations between the transfer matrices.

Lemma 3.3 *Let $E \in \mathbb{R}$ and $V \in \mathbb{R}$. Denote*

$$M_{[0]}(E, V) := \begin{pmatrix} 1 & -V \\ 0 & 1 \end{pmatrix},$$

and let $\mathbf{c} = [0, 0, c_1, \dots, c_k] \in \mathcal{C}$ with $\varphi(\mathbf{c}) \in [0, 1] \cup \{-1\}$.

(a) If $\mathbf{c} = [0, 0]$, then

$$M_{[0,0]}(E, V) = \begin{pmatrix} E & -1 \\ 1 & 0 \end{pmatrix}.$$

(b) If $k \in \mathbb{N}$ and $c_k \in \mathbb{N}_0$, then

$$M_{\mathbf{c}}(E, V) = \begin{cases} M_{[0,0,c_1,\dots,c_{k-1}]}(E, V)^{c_k} \cdot M_{[0,0,c_1,\dots,c_{k-2}]}(E, V), & k \equiv 0 \pmod{2}, \\ M_{[0,0,c_1,\dots,c_{k-2}]}(E, V) \cdot M_{[0,0,c_1,\dots,c_{k-1}]}(E, V)^{c_k}, & k \equiv 1 \pmod{2}. \end{cases} \quad (3.4)$$

(c) If $k \in \mathbb{N}$ and $c_k \in \mathbb{N}_{-1}$, then

$$\text{tr}(M_{\mathbf{c}}) = \text{tr}(M_{[0,0,c_1,\dots,c_{k-2}]} \cdot M_{[0,0,c_1,\dots,c_{k-1}]}^{c_k}). \quad (3.5)$$

Remark

(a) We clarify the lower recursive relations in Lemma 3.3 by explicitly writing

$$M_{[0,0,c_1]} = M_{[0]} \cdot M_{[0,0]}^{c_1} \quad \text{and} \quad M_{[0,0,c_1,c_2]} = M_{[0,0,c_1]}^{c_2} \cdot M_{[0,0]}(E, V).$$

(b) In addition, we note that (3.4) does not hold for $c_k = -1$ (or rather, should be appropriately modified), whereas (3.5) does hold also for all $c_k \in \mathbb{N}_{-1}$. This property of the trace is important and will be used in the next subsection.

Proof For $k = 0$, we get $\mathbf{c} = [0, 0]$ and since $\omega_{\varphi([0,0])} = \omega_0 = 0^\infty$ we have $q_0 = 1$ and

$$M_{[0,0]} = A_{\frac{p_0}{q_0}}(0) = \begin{pmatrix} E & -1 \\ 1 & 0 \end{pmatrix},$$

proving (a).

Next, we prove (b). If $k = 1$, then $\mathbf{c} = [0, 0, c_1]$ with $c_1 \in \mathbb{N}$, as otherwise (i.e., if $c_1 = 0$) $\varphi(\mathbf{c}) = \infty$. Hence, $\varphi(\mathbf{c}) = \frac{1}{c_1}$ and Lemma 2.4 implies

$$\omega_{\frac{1}{c_1}}^\perp(0) \omega_{\frac{1}{c_1}}^\perp(1) \dots \omega_{\frac{1}{c_1}}^\perp(c_1 - 2) \omega_{\mathbf{c}}(c_1 - 1) = 00 \dots 01.$$

Using the definition of the transfer matrix, (3.2), we get

$$\begin{aligned}
 M_{[0,0,c_1]} &= A_{\frac{1}{c_1}}(c_1 - 1) \cdot A_{\frac{1}{c_1}}(c_1 - 2) \dots A_{\frac{1}{c_1}}(1) \cdot A_{\frac{1}{c_1}}(0) \\
 &= \begin{pmatrix} E - V & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} E & -1 \\ 1 & 0 \end{pmatrix}^{c_1-1} \\
 &= \begin{pmatrix} 1 - V & \\ 0 & 1 \end{pmatrix} \begin{pmatrix} E & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} E & -1 \\ 1 & 0 \end{pmatrix}^{c_1-1} \\
 &= M_{[0]} \cdot M_{[0,0]}^{c_1},
 \end{aligned}$$

which verifies the statement for $k = 1$ and $c_k \in \mathbb{N}$. Note that the case $k = 1$ and $c_k = 0$ results in $\mathbf{c} = [0, 0, 0]$ satisfying $\varphi(\mathbf{c}) = \infty$ which is excluded by assumption. If $k \geq 2$ and $c_k \notin \{-1, 0\}$, then (b) follows from Lemma 2.4.

Now, let $k \geq 2$ and $c_k = 0$. We have $\mathbf{c} = [0, 0, c_1, \dots, c_{k-2}, c_{k-1}, 0]$ and by definition of the evaluation map, we get $\varphi(\mathbf{c}) = \varphi([0, 0, c_1, \dots, c_{k-2}])$. Thus, $M_{\mathbf{c}}(E, V) = M_{[0,0,c_1,\dots,c_{k-2}]}(E, V)$ follows since $M_{\mathbf{c}}$ only depends on the evaluation $\varphi(\mathbf{c})$. In particular, (3.4) holds also for $c_k = 0$ (regardless of the parity of k).

It is left to prove (3.5). As a matter of fact, the cyclic property of the trace yields that (3.5) is a direct consequence of (3.4) if $c_k \neq -1$.

If $c_k = -1$ we have $\mathbf{c} = [0, 0, c_1, \dots, c_{k-1}, -1]$ and $\varphi(\mathbf{c}) = \varphi([0, 0, c_1, \dots, c_{k-1} - 1])$ and by definition $M_{\mathbf{c}} = M_{[0,0,c_1,\dots,c_{k-1}-1]}$. If $k \geq 2$ we get

$$\begin{aligned}
 tr(M_{\mathbf{c}}) &= tr(M_{[0,0,c_1,\dots,c_{k-1}-1]}) \\
 &= tr(M_{[0,0,c_1,\dots,c_{k-3}]} \cdot M_{[0,0,c_1,\dots,c_{k-2}]}^{c_{k-1}-1}) \\
 &= tr((M_{[0,0,c_1,\dots,c_{k-3}]} \cdot M_{[0,0,c_1,\dots,c_{k-2}]}^{c_{k-1}}) \cdot M_{[0,0,c_1,\dots,c_{k-2}]}^{-1}) \\
 &= tr(M_{[0,0,c_1,\dots,c_{k-1}]} \cdot M_{[0,0,c_1,\dots,c_{k-2}]}^{-1}) \\
 &= tr(M_{[0,0,c_1,\dots,c_{k-2}]} \cdot M_{[0,0,c_1,\dots,c_{k-1}]}^{-1}),
 \end{aligned}$$

where in the second and fourth equalities we used (3.4) together with the cyclic property of the trace (which allows not to distinguish between even and odd k 's) and in the last equality we used that $tr(M) = tr(M^{-1})$ whenever $\det M = 1$ (and this holds for transfer matrices by Lemma 3.1). All is left is to check the case $k = 1$ and $c_k = -1$. In this case, $\mathbf{c} = [0, 0, -1]$, $\varphi(\mathbf{c}) = -1$ and a straightforward computation invoking (3.3) gives

$$tr(M_{[0]} M_{[0,0]}^{-1}) = V + E = tr(M_{[0,0,-1]}).$$

□

By standard Floquet–Bloch theory (applied to one-dimensional Jacobi operators), the spectrum of $H_{\frac{p}{q}, V}$ (for $\frac{p}{q} = \varphi(\mathbf{c})$) may be described by the trace of $M_{\mathbf{c}}$. Therefore, define the discriminant $t_{\mathbf{c}}$ for $\mathbf{c} \in \mathcal{C}$ by

$$t_{\mathbf{c}}(E, V) := \text{tr}(M_{\mathbf{c}}(E, V))$$

and

$$\sigma_{\mathbf{c}}(V) := t_{\mathbf{c}}(\cdot, V)^{-1}([-2, 2]).$$

Example 3.4 Observe that if $\varphi(\mathbf{c}) = \infty$, then $t_{\mathbf{c}}(E, V) = 2$ and so $\sigma_{\mathbf{c}}(V) = \mathbb{R}$ hold. If $\varphi(\mathbf{c}) = -1$, then (3.3) leads to $t_{[0,0,-1]}(E, V) = E + V$ and so $\sigma_{[0,0,-1]}(V) = [-2 - V, 2 - V]$ for all $V \in \mathbb{R}$.

If $\varphi(\mathbf{c}) \neq \infty$, we bring here a summary of useful properties which may be found, for example, in [43, Sect. 5.4], [46, Sect. 7.1].

Proposition 3.5 *Let $\mathbf{c} \in \mathcal{C}$ with $\varphi(\mathbf{c}) \notin \{-1, \infty\}$ and $V \in \mathbb{R}$.*

Then the following properties hold:

- (a) $\sigma_{\mathbf{c}}(V) = \sigma(H_{\varphi(\mathbf{c}), V})$.
- (b) Denoting $\frac{p}{q} = \varphi(\mathbf{c})$, the set $t_{\mathbf{c}}(\cdot, V)^{-1}((-2, 2))$ consists of exactly q open intervals.
- (c) The discriminant $t_{\mathbf{c}}$ is monotone on each connected component of $t_{\mathbf{c}}(\cdot, V)^{-1}((-2, 2))$.

The connected components $t_{\mathbf{c}}(\cdot, V)^{-1}((-2, 2))$ mentioned in Proposition 3.5 are the interior of the so-called *spectral bands* of $\sigma_{\mathbf{c}}(V)$. The spectral bands are closed intervals whose edge points are given by $t_{\mathbf{c}}(\cdot, V)^{-1}(\{-2, 2\})$. In general, it is possible that different spectral bands overlap at their endpoint. However, this is not the case for the approximations of the Sturmian Hamiltonian if $V \neq 0$, see Proposition 4.1.

Remark We were trying to keep the notation here close to the one in [39] and, in particular, use the notations M and t for the transfer matrix and its trace (discriminant). Nevertheless, we deviate in the subscript notation, using $M_{\mathbf{c}}$ instead of M_k and $t_{\mathbf{c}}$ instead of $t_{(k,p)}$. The reasons for this change are exactly the ones which are specified in Remark 2.2.

3.2 Algebraic Identities of the Transfer Matrices and Their Traces

In this subsection, we develop some identities for the traces $t_{\mathbf{c}}$. These identities will be used in the following sections to derive spectral properties of the periodic operators $H_{\varphi(\mathbf{c}), V}$. Some of these identities can be found in [8, 39]. However, we use here a slightly different notation (to fit [3]) and, in particular, use the mechanical word sequences $\omega_{\varphi(\mathbf{c})}$ for all values of $\mathbf{c} \in \mathcal{C}$, rather than a single fixed Sturmian

sequence ω_α which is the approach used in [8, 39]. For the sake of a self-contained presentation, we provide here complete proofs of all the relevant identities.

We start by noting a basic property of the discriminant $t_{\mathbf{c}} = \text{tr}(M_{\mathbf{c}})$: even though it is a function of \mathbf{c} , it depends only on the value $\varphi(\mathbf{c})$. This fundamental property deserves an explicit mention here, as it is substantially used in the sequel.

Lemma 3.6 *Let $\mathbf{c}, \tilde{\mathbf{c}} \in \mathcal{C}$ be such that $\varphi(\mathbf{c}) = \varphi(\tilde{\mathbf{c}})$, then*

$$t_{\mathbf{c}}(\cdot, V) = t_{\tilde{\mathbf{c}}}(\cdot, V) \quad \text{and} \quad \sigma_{\mathbf{c}}(V) = \sigma_{\tilde{\mathbf{c}}}(V) \quad \text{for all } V \in \mathbb{R}.$$

Proof This property is immediate from the definition of $M_{\mathbf{c}}$, (3.2), which depends purely on the value of $\varphi(\mathbf{c})$, if $\varphi(\mathbf{c}) \neq \infty$. For $\varphi(\mathbf{c}) = \infty$, the matrix $M_{\mathbf{c}}$ does depend on $\mathbf{c} \in \{[0], [0, 0, 0], [0, 0, 1 - 1]\}$. However, a short computation gives $t_{\mathbf{c}}(E, V) = 2$ if $\varphi(\mathbf{c}) = \infty$. The statement $\sigma_{\mathbf{c}}(V) = \sigma_{\tilde{\mathbf{c}}}(V)$ follows directly from the equality of the traces. \square

For the sake of representation, we write $t_{\mathbf{c}}$ instead of $t_{\mathbf{c}}(E, V)$. As an immediate corollary, we get

Corollary 3.7 *Let $[0, c_0, c_1, \dots, c_k] \in \mathcal{C}$ with $c_k \in \mathbb{N}$. Then the following identities hold:*

$$\begin{aligned} t_{[0, c_0, \dots, c_{k-1}, c_k, 0]} &= t_{[0, c_0, \dots, c_{k-1}]} \\ t_{[0, c_0, \dots, c_{k-1}, c_k, -1]} &= t_{[0, c_0, \dots, c_{k-1}, c_k - 1]} \\ t_{[0, c_0, \dots, c_{k-1}, c_k, 1]} &= t_{[0, c_0, \dots, c_{k-1}, c_k + 1]}. \end{aligned}$$

Proof This is an implication of Lemma 3.6 together with the identities

$$\varphi([\mathbf{c}, 0]) = \varphi([0, c_0, \dots, c_{k-1}]), \quad \varphi([\mathbf{c}, -1]) = \varphi([0, c_0, \dots, c_{k-1}, c_k - 1]),$$

and $\varphi([\mathbf{c}, 1]) = \varphi([0, c_0, \dots, c_{k-1}, c_k + 1])$ for $\mathbf{c} = [0, c_0, \dots, c_k]$. \square

Lemma 3.8 ([39, Proposition 2.2]) *Let $\mathbf{c} \in \mathcal{C}$ and $m \in \mathbb{N}_0$ such that $[\mathbf{c}, m] \in \mathcal{C}$. Then*

$$t_{[\mathbf{c}, m+1]} = t_{\mathbf{c}} t_{[\mathbf{c}, m]} - t_{[\mathbf{c}, m-1]}.$$

Proof Let $\mathbf{c}' \in \mathcal{C}$ and $c_k \in \mathbb{N}_0$ be such that $\mathbf{c} = [\mathbf{c}', c_k]$. Observe that $A^2 = \text{tr}(A)A - \det(A)\mathbf{1}_2$ for complex 2×2 matrices (this is actually a special case of Cayley–Hamilton theorem). In particular, we will use this identity for the transfer matrices, for which $\det(M_{\mathbf{c}}) = 1$ by Lemma 3.1. With this at hand we get

$$\begin{aligned}
t_{[c,m+1]} &= t_{[c',c_k,m+1]} = tr(M_{[c',c_k,m+1]}) \\
&= tr(M_{c'} M_c^{m+1}) \\
&= tr(M_{c'} M_c^{m-1} M_c^2) \\
&= tr(M_{c'} M_c^{m-1} [tr(M_c) M_c - \det(M_c) \mathbf{1}_2]) \\
&= tr(M_c) tr(M_{c'} M_c^m) - tr(M_{c'} M_c^{m-1}) \\
&= tr(M_c) tr(M_{[c,m]}) - tr(M_{[c,m-1]}) \\
&= t_c t_{[c,m]} - t_{[c,m-1]},
\end{aligned}$$

where in the second and sixth lines we used (3.5) of Lemma 3.3. \square

Next, we aim at generalizing Lemma 3.8. To do so, we introduce the *dilated Chebyshev polynomials of the second kind* $S_l : \mathbb{R} \rightarrow \mathbb{R}$ (see [36, Eq. (18.1.3)]). These polynomials are inductively defined by

$$S_{-1}(x) := 0, \quad S_0(x) := 1, \quad S_l(x) = x S_{l-1}(x) - S_{l-2}(x). \quad (3.6)$$

Section 8 contains an elaborate account on these polynomials, their connection to the “usual” Chebyshev polynomials of the second kind and various useful identities which are used in this review as well as in [3].

Lemma 3.9 ([39, Proposition 2.2]) *Let $c \in \mathcal{C}$ and $m \geq l \geq -1$ such that $[c, m] \in \mathcal{C}$, then*

$$t_{[c,m+1]} = S_{l+1}(t_c) t_{[c,m-l]} - S_l(t_c) t_{[c,m-l-1]}.$$

Proof We fix $m \in \mathbb{N}_{-1}$ and prove the statement by induction over $l \in \mathbb{N}_{-1}$. For $l = -1$, we use Lemma 3.8 to get

$$S_0(t_c) t_{[c,m-l]} - S_{-1}(t_c) t_{[c,m-l-1]} = 1 \cdot t_{[c,m+1]} + 0 \cdot t_{[c,m]} = t_{[c,m+1]}.$$

Now assume the statement is correct for $m > l \geq -1$. We then get

$$\begin{aligned}
t_{[c,m+1]} &= S_{l+1}(t_c) t_{[c,m-l]} - S_l(t_c) t_{[c,m-l-1]} \\
&= S_{l+1}(t_c) [t_c t_{[c,m-l-1]} - t_{[c,m-l-2]}] - S_l(t_c) t_{[c,m-l-1]} \\
&= [t_c S_{l+1}(t_c) - S_l(t_c)] t_{[c,m-l-1]} - S_{l+1}(t_c) t_{[c,m-l-2]} \\
&= S_{l+2}(t_c) t_{[c,m-(l+1)]} - S_{l+1}(t_c) t_{[c,m-(l+1)-1]},
\end{aligned}$$

where we used Lemma 3.8 in the second equality, and the Chebyshev polynomial recursion in the last equality. \square

In the following, an extra parameter $\ell \in \{-1, 0\}$ is introduced. Later in this review so-called spectral bands I_c in σ_c of backward type A and B are introduced that are defined by adding to c the digit 0 if I_c is backward type A and -1 if I_c is backward type B , see Definition 4.10.

Corollary 3.10 *Let $\mathbf{c} \in \mathcal{C}$ and $m \in \mathbb{N}$ be such that $[\mathbf{c}, m] \in \mathcal{C}$. For $\ell \in \{-1, 0\}$, we have*

$$t_{[\mathbf{c}, m]} = S_{m-\ell-1}(t_{\mathbf{c}})t_{[\mathbf{c}, 1+\ell]} - S_{m-\ell-2}(t_{\mathbf{c}})t_{[\mathbf{c}, \ell]}.$$

Proof This is a direct consequence of Lemma 3.9. \square

We proceed to apply this corollary to get another useful identity involving Chebyshev polynomials and the traces.

Lemma 3.11 *Let $\mathbf{c} \in \mathcal{C}$ and $m \in \mathbb{N}$ be such that $[\mathbf{c}, m] \in \mathcal{C}$. For any $\xi \in \{0, 1\}$ and $\ell \in \{-1, 0\}$, we have*

$$S_{m-1-\ell}(t_{\mathbf{c}}) [t_{[\mathbf{c}, m-1]} + (-1)^\xi t_{[\mathbf{c}, 1+\ell]}] = [S_{m-2-\ell}(t_{\mathbf{c}}) + (-1)^\xi] [t_{[\mathbf{c}, m]} + (-1)^\xi t_{[\mathbf{c}, \ell]}].$$

Proof First, we use twice the recursion relation for the Chebyshev polynomials to get

$$\begin{aligned} S_l(x)S_{l-2}(x) - S_{l-1}(x)^2 &= xS_{l-1}(x)S_{l-2}(x) - S_{l-1}(x)^2 - S_{l-2}(x)^2 \\ &= S_{l-1}(x)S_{l-3}(x) - S_{l-2}(x)^2. \end{aligned}$$

In particular, we get that this expression is independent of l and therefore

$$S_l(x)S_{l-2}(x) - S_{l-1}(x)^2 = S_1(x)S_{-1}(x) - S_0(x)^2 = -1.$$

Using this identity, Lemma 3.9 and Corollary 3.10, the lemma follows by straightforward computation. For example, for $\ell = -1$,

$$\begin{aligned} &S_m(t_{\mathbf{c}}) [t_{[\mathbf{c}, m-1]} + (-1)^\xi t_{[\mathbf{c}, 0]}] \\ &= S_m(t_{\mathbf{c}}) [S_{m-1}(t_{\mathbf{c}})t_{[\mathbf{c}, 0]} - S_{m-2}(t_{\mathbf{c}})t_{[\mathbf{c}, -1]} + (-1)^\xi t_{[\mathbf{c}, 0]}] \\ &= S_m(t_{\mathbf{c}})S_{m-1}(t_{\mathbf{c}})t_{[\mathbf{c}, 0]} - S_m(t_{\mathbf{c}})S_{m-2}(t_{\mathbf{c}})t_{[\mathbf{c}, -1]} + (-1)^\xi S_m(t_{\mathbf{c}})t_{[\mathbf{c}, 0]} \\ &= S_m(t_{\mathbf{c}})S_{m-1}(t_{\mathbf{c}})t_{[\mathbf{c}, 0]} - [S_{m-1}^2(t_{\mathbf{c}}) - 1]t_{[\mathbf{c}, -1]} + (-1)^\xi S_m(t_{\mathbf{c}})t_{[\mathbf{c}, 0]} \\ &= S_m(t_{\mathbf{c}})t_{[\mathbf{c}, 0]} [S_{m-1}(t_{\mathbf{c}}) + (-1)^\xi] - [S_{m-1}^2(t_{\mathbf{c}}) - 1]t_{[\mathbf{c}, -1]} \\ &= [S_{m-1}(t_{\mathbf{c}}) + (-1)^\xi] [S_m(t_{\mathbf{c}})t_{[\mathbf{c}, 0]} - (S_{m-1}(t_{\mathbf{c}}) + (-1)^{\xi+1})t_{[\mathbf{c}, -1]}] \\ &= [S_{m-1}(t_{\mathbf{c}}) + (-1)^\xi] [S_m(t_{\mathbf{c}})t_{[\mathbf{c}, 0]} - S_{m-1}(t_{\mathbf{c}})t_{[\mathbf{c}, -1]} + (-1)^\xi t_{[\mathbf{c}, -1]}] \\ &= [S_{m-1}(t_{\mathbf{c}}) + (-1)^\xi] [t_{[\mathbf{c}, m]} + (-1)^\xi t_{[\mathbf{c}, -1]}]. \end{aligned}$$

The statement for $\ell = 0$ follows the same lines except that the case $m = 1$ needs to be treated separately (since we used Corollary 3.10 moving from the first to the second line, which cannot be applied if $\ell = 0$ and $m = 1$). \square

3.3 The Fricke–Vogt Invariant

The Fricke–Vogt invariant serves an important role in the spectral analysis of Sturmian Hamiltonians. We review here this well-known part of the theory, and rephrase it according to our convention to use the space \mathcal{C} .

Denote by $[\cdot, \cdot]$ the matrix commutator $[A, B] := AB - BA$. Note that $\text{tr}([A, B]) = 0$, as tr is linear and $\text{tr}(AB) = \text{tr}(BA)$.

Lemma 3.12 ([39, Proposition 2.3]) *Let $V \in \mathbb{R}$, $\mathbf{c} = [c_{-1}, c_0, \dots, c_k] \in \mathcal{C}$ with $k \in \mathbb{N}_{-1}$ and $[\mathbf{c}, m, n] \in \mathcal{C}$ with $m \in \mathbb{N}_0$ and $n \in \mathbb{N}_{-1}$. Then*

$$[M_{[\mathbf{c}, m]}, M_{\mathbf{c}} M_{[\mathbf{c}, m]}^n]^2 = V^2 \mathbf{1}_2,$$

where $\mathbf{1}_2$ is the 2×2 identity matrix.

Proof Denote $A := [M_{[\mathbf{c}, m]}, M_{\mathbf{c}} M_{[\mathbf{c}, m]}^n]$. As for each 2×2 matrix (e.g., as a special case of Cayley–Hamilton theorem) we have

$$A^2 = \text{tr}(A)A - \det(A)\mathbf{1}_2 = -\det(A)\mathbf{1}_2,$$

where in the second equality we used that $\text{tr}(A) = 0$. Hence, to validate the statement we need to show $\det(A) = -V^2$. Computing the determinant gives

$$\begin{aligned} \det(A) &= \det(M_{[\mathbf{c}, m]} M_{\mathbf{c}} M_{[\mathbf{c}, m]}^n - M_{\mathbf{c}} M_{[\mathbf{c}, m]}^n M_{[\mathbf{c}, m]}) \\ &= \det(M_{[\mathbf{c}, m]} M_{\mathbf{c}} - M_{\mathbf{c}} M_{[\mathbf{c}, m]}) \det(M_{[\mathbf{c}, m]}^n)^n \\ &= \det([M_{[\mathbf{c}, m]}, M_{\mathbf{c}}]), \end{aligned}$$

where we used that the determinant of a transfer matrix is one by Lemma 3.2. To finish the proof, we use induction over $k \in \mathbb{N}_{-1}$ to show $\det([M_{[\mathbf{c}, m]}, M_{\mathbf{c}}]) = -V^2$ (for any $[\mathbf{c}, m] \in \mathcal{C}$ and $\mathbf{c} = [c_{-1}, c_0, \dots, c_k]$). For the induction base, we observe

$$\begin{aligned} [M_{[0,0]}, M_{[0]}] &= \begin{pmatrix} E & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & -V \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} 1 & -V \\ 0 & 1 \end{pmatrix} \begin{pmatrix} E & -1 \\ 1 & 0 \end{pmatrix} \\ &= \begin{pmatrix} E - VE & -1 \\ 1 & -V \end{pmatrix} - \begin{pmatrix} E - V & -1 \\ 1 & 0 \end{pmatrix} \\ &= \begin{pmatrix} V & -VE \\ 0 & -V \end{pmatrix}, \end{aligned}$$

and indeed $\det([M_{[0,0]}, M_{[0]}]) = -V^2$. For the induction step, suppose the statement is true for $k \in \mathbb{N}_{-1}$. Note that for 2×2 -matrices B and C , we have $[B, C] = -[C, B]$ and $\det(-B) = \det(B)$. Thus, the previous identity on the determinant of the commutator yields

$$\begin{aligned}
\det \left(\left[M_{[\mathbf{c}, c_{k+1}, m]}, M_{[\mathbf{c}, c_{k+1}]} \right] \right) &= \det \left(\left[M_{[\mathbf{c}, c_{k+1}]}, M_{[\mathbf{c}, c_{k+1}, m]} \right] \right) \\
&= \det \left(\left[M_{[\mathbf{c}, c_{k+1}]}, M_{\mathbf{c}} M_{[\mathbf{c}, c_{k+1}]}^m \right] \right) \\
&= \det \left(\left[M_{[\mathbf{c}, c_{k+1}]}, M_{\mathbf{c}} \right] \right) = -V^2,
\end{aligned}$$

where in the second equality we used (3.4) of Lemma 3.3 assuming k is odd. If k is even, as similar computation leads to the result. \square

Proposition 3.13 ([39, Proposition 2.3], Fricke–Vogt Invariant) *Let $V \in \mathbb{R}$, $\mathbf{c} \in \mathcal{C}$ and $m \in \mathbb{N}_0$ such that $[\mathbf{c}, m-1] \in \mathcal{C}$, then*

$$t_{\mathbf{c}}^2 + t_{[\mathbf{c}, m]}^2 + t_{[\mathbf{c}, m-1]}^2 - t_{\mathbf{c}} t_{[\mathbf{c}, m]} t_{[\mathbf{c}, m-1]} = 4 + V^2.$$

To prove this proposition we use the following algebraic identity.

Lemma 3.14 *Let A, B be two real 2×2 matrices such that $\det(A) = 1$. Then*

$$\text{tr}(AB) = \text{tr}(A)\text{tr}(B) - \text{tr}(A^{-1}B).$$

Proof Since A is a 2×2 matrix with $\det(A) = 1$, we conclude $A + A^{-1} = \text{tr}(A)\mathbf{1}_2$. Hence, $\text{tr}(AB) = \text{tr}(\text{tr}(A)B - A^{-1}B) = \text{tr}(A)\text{tr}(B) - \text{tr}(A^{-1}B)$. \square

Proof of Proposition 3.13 Let $\mathbf{c}' \in \mathcal{C}$ and $c_k \in \mathbb{N}_0$ be such that $\mathbf{c} = [\mathbf{c}', c_k]$. Denoting $A := [M_{\mathbf{c}}, M_{\mathbf{c}'} M_{\mathbf{c}}^m]$ and applying Lemma 3.12 yields

$$\text{tr}(A^2) = \text{tr}(V^2 \mathbf{1}_2) = 2V^2.$$

On the other hand, a direct computation of $\text{tr}(A^2)$ gives

$$\begin{aligned}
\text{tr}(A^2) &= \text{tr}((M_{\mathbf{c}} M_{\mathbf{c}'} M_{\mathbf{c}}^m - M_{\mathbf{c}'} M_{\mathbf{c}}^{m+1})^2) \\
&= \text{tr}((M_{\mathbf{c}} M_{\mathbf{c}'} M_{\mathbf{c}}^m)^2) + \text{tr}((M_{\mathbf{c}'} M_{\mathbf{c}}^{m+1})^2) - 2\text{tr}(M_{\mathbf{c}} M_{\mathbf{c}'} M_{\mathbf{c}}^m M_{\mathbf{c}'} M_{\mathbf{c}}^{m+1}) \\
&= 2\text{tr}((M_{\mathbf{c}'} M_{\mathbf{c}}^{m+1})^2) - 2\text{tr}(M_{\mathbf{c}'} M_{\mathbf{c}}^m M_{\mathbf{c}'} M_{\mathbf{c}}^{m+2}).
\end{aligned}$$

For the first term we use the identity $B^2 = \text{tr}(B)B - \det(B)\mathbf{1}_2$ for the 2×2 -matrix $B = M_{\mathbf{c}'} M_{\mathbf{c}}^{m+1}$ and then Lemmas 3.3(c), 3.3(c) and 3.8 lead to

$$\begin{aligned}
\text{tr}((M_{\mathbf{c}'} M_{\mathbf{c}}^{m+1})^2) &= (\text{tr}(M_{\mathbf{c}'} M_{\mathbf{c}}^{m+1}))^2 - 2 \\
&= t_{[\mathbf{c}, m+1]}^2 - 2 \\
&= (t_{\mathbf{c}} t_{[\mathbf{c}, m]} - t_{[\mathbf{c}, m-1]})^2 - 2 \\
&= t_{\mathbf{c}}^2 t_{[\mathbf{c}, m]}^2 + t_{[\mathbf{c}, m-1]}^2 - 2t_{\mathbf{c}} t_{[\mathbf{c}, m]} t_{[\mathbf{c}, m-1]} - 2.
\end{aligned}$$

For the second term, we apply Lemma 3.14 and Lemma 3.3 (c) to get

$$\begin{aligned}
 \text{tr}(M_{\mathbf{c}'} M_{\mathbf{c}}^m M_{\mathbf{c}'} M_{\mathbf{c}}^{m+2}) &= \text{tr}(M_{\mathbf{c}'} M_{\mathbf{c}}^m) \text{tr}(M_{\mathbf{c}'} M_{\mathbf{c}}^{m+2}) - \text{tr}((M_{\mathbf{c}'} M_{\mathbf{c}}^m)^{-1} M_{\mathbf{c}'} M_{\mathbf{c}}^{m+2}) \\
 &= t_{[\mathbf{c}, m]} t_{[\mathbf{c}, m+2]} - \text{tr}(M_{\mathbf{c}}^2) \\
 &= t_{[\mathbf{c}, m]} t_{[\mathbf{c}, m+2]} - t_{\mathbf{c}}^2 + 2 \\
 &= t_{[\mathbf{c}, m]} (t_{\mathbf{c}} t_{[\mathbf{c}, m+1]} - t_{[\mathbf{c}, m]}) - t_{\mathbf{c}}^2 + 2 \\
 &= t_{\mathbf{c}} t_{[\mathbf{c}, m]} t_{[\mathbf{c}, m+1]} - t_{[\mathbf{c}, m]}^2 - t_{\mathbf{c}}^2 + 2 \\
 &= t_{\mathbf{c}} t_{[\mathbf{c}, m]} (t_{\mathbf{c}} t_{[\mathbf{c}, m]} - t_{[\mathbf{c}, m-1]}) - t_{[\mathbf{c}, m]}^2 - t_{\mathbf{c}}^2 + 2 \\
 &= t_{\mathbf{c}}^2 t_{[\mathbf{c}, m]}^2 - t_{\mathbf{c}} t_{[\mathbf{c}, m]} t_{[\mathbf{c}, m-1]} - t_{[\mathbf{c}, m]}^2 - t_{\mathbf{c}}^2 + 2,
 \end{aligned}$$

where in the third equality we used the identity $B^2 = \text{tr}(B)B - \det(B)\mathbf{1}_2$ with $B = M_{\mathbf{c}}$, and in the fourth and sixth equalities we used Lemma 3.8.

Combining the identities above provides the statement of the proposition. \square

4 The Spectra of Periodic Approximations of Sturmian Hamiltonians

We start applying the tools from the previous section in order to study the spectral bands of the periodic approximations of the Sturmian Hamiltonian, as is done in [39, Sect. 3.1]. We start by providing general results for all Sturmian Hamiltonians (Sect. 4.1) and then restrict to $V > 4$ where further analysis may be obtained (Sect. 4.2).

4.1 Basic Spectral Properties for all $V \neq 0$

We provide basic properties on the spectrum of a periodic approximation of a Sturmian Hamiltonians, i.e., $H_{q, V}^{\frac{p}{q}}$. To do so, we mainly use the transfer matrices and the discriminant, as was introduced in the previous section. The results in this subsection appeared already in [8, 10, 44]. Since the results here apply for all $V \neq 0$, we tend to omit (only in this subsection) the notation V from the proofs.

The following proposition is a refinement of Proposition 3.5 for the operators $H_{q, V}^{\frac{p}{q}}$. Its first part appears in [39, Proposition 3.1.(i)].

Proposition 4.1 *Let $V \neq 0$ and $\mathbf{c} \in \mathcal{C}$ with $\frac{p}{q} := \varphi(\mathbf{c}) \neq \infty$ and p and q coprime. Then the following assertions hold:*

(a) *The spectrum $\sigma_{\mathbf{c}}(V) = \sigma(H_{q, V}^{\frac{p}{q}})$ consists of exactly q connected components which are closed intervals.*

As usual, we call these intervals, the spectral bands of $H_{q, V}^{\frac{p}{q}}$ (or of $\sigma(H_{q, V}^{\frac{p}{q}})$).

(b) *The restriction of the discriminant $t_{\mathbf{c}}$ to each of the spectral bands is strictly monotone.*

Proof We need to prove only the first part of the proposition, as the second part is classical (see, e.g., [43, Theorem 5.4.2]). By [43, Theorem 5.4.2] the spectrum of a q -periodic Jacobi operator (such as $H_{q,V}^{\mathbf{c}}$) consists of q closed intervals, which might overlap only at their boundaries. Assume by contradiction that E is such a point where two intervals overlap. By [43, Theorem 5.4.3] this implies that $M_{\mathbf{c}}(E) = \pm 1_2$, for $\mathbf{c} \in \mathcal{C}$ such that $\varphi(\mathbf{c}) = \frac{p}{q}$. Substituting this in Lemma 3.12 gives $V^2 1_2 = [M_{[\mathbf{c},m]}, M_{\mathbf{c}} M_{[\mathbf{c},m]}^n]^2 = 0$, for any $m, n \in \mathbb{N}$. Hence, we get $V = 0$ and a contradiction. \square

Next, we rephrase a statement from [8, Proposition 4] and immediately apply it to connect the spectra $\sigma_{\mathbf{c}}$.

Lemma 4.2 *Let $V \neq 0$ and $\mathbf{c} = [0, c_0, c_1, \dots, c_k] \in \mathcal{C}$. Let $E \in \mathbb{R}$ and $i < k$. If*

$$|t_{[0,c_0,c_1,\dots,c_{i-2}]}(E)| > 2 \quad \text{and} \quad |t_{[0,c_0,c_1,\dots,c_{i-1}]}(E)| > 2$$

then there exists $C > 1$ such that for all $i \leq j \leq k$, $|t_{[0,c_0,c_1,\dots,c_j]}(E)| > 2C^{q_j}$, where $\varphi([0, c_0, c_1, \dots, c_j]) = \frac{p_j}{q_j}$ with p_j, q_j coprime.

Proof This follows from [8, Proposition 4] by fixing an $\alpha \in [0, 1] \setminus \mathbb{Q}$ such that the first digits of the continuous fraction expansion of α coincide with c_0, c_1, \dots, c_k . \square

Lemma 4.3 ([39, Proposition 3.1,(ii)] spectral monotonicity property) *Let $V \neq 0$ and let $\mathbf{c} = [0, c_0, c_1, \dots, c_k] \in \mathcal{C}$ with $\varphi(\mathbf{c}) \geq 0$ and $k \in \mathbb{N}_0$. Then*

$$\sigma_{\mathbf{c}}(V) \subseteq \sigma_{[0,c_0,c_1,\dots,c_{k-2}]}(V) \cup \sigma_{[0,c_0,c_1,\dots,c_{k-1}]}(V).$$

In addition, if $[\mathbf{c}, -1] \in \mathcal{C}$, then

$$\sigma_{\mathbf{c}}(V) \subseteq \sigma_{[\mathbf{c},0]}(V) \cup \sigma_{[\mathbf{c},-1]}(V).$$

Proof We start by proving the first inclusion. If $E \notin \sigma_{[0,c_0,c_1,\dots,c_{k-2}]} \cup \sigma_{[0,c_0,c_1,\dots,c_{k-1}]}$, then Proposition 3.5 implies

$$|t_{[0,c_0,c_1,\dots,c_{k-2}]}(E)| > 2 \quad \text{and} \quad |t_{[0,c_0,c_1,\dots,c_{k-1}]}(E)| > 2.$$

Thus, Lemma 4.2 leads to $|t_{\mathbf{c}}(E)| > 2$ and by Proposition 3.5, $E \notin \sigma_{\mathbf{c}}$, which proves the first inclusion.

To prove the second inclusion, note first that if $k = 0$ and $\mathbf{c} = [0, 0]$, then the inclusion is trivial as $\sigma_{[\mathbf{c},0]} = \sigma_{[0]} = \mathbb{R}$. Suppose now $k \geq 1$. Then the condition $[\mathbf{c}, -1] \in \mathcal{C}$ implies that $c_k \geq 1$ (in particular $c_k \notin \{-1, 0\}$). We assume first that $c_k > 1$. Then, by Corollary 3.7, $t_{\mathbf{c}} = t_{[0,c_0,c_1,\dots,c_{k-1},1]}$ and therefore $\sigma_{\mathbf{c}} = \sigma_{[0,c_0,c_1,\dots,c_{k-1},1]}$.

Applying the first part of the lemma on $\tilde{\mathbf{c}} = [0, c_0, c_1, \dots, c_k - 1, 1]$ gives

$$\sigma_{\mathbf{c}} = \sigma_{[0, c_0, c_1, \dots, c_k - 1, 1]} \subseteq \sigma_{[0, c_0, c_1, \dots, c_{k-1}]} \cup \sigma_{[0, c_0, c_1, \dots, c_k - 1]},$$

and this yields the second part of the lemma since $t_{[\mathbf{c}, 0]} = t_{[0, c_0, c_1, \dots, c_{k-1}]}$ and $t_{[\mathbf{c}, -1]} = t_{[0, c_0, c_1, \dots, c_k - 1]}$ by Corollary 3.7 and Proposition 3.5. To complete the proof assume that $c_k = 1$. In this case $t_{[\mathbf{c}, 0]} = t_{[0, c_0, c_1, \dots, c_{k-1}]}$ and $t_{[\mathbf{c}, -1]} = t_{[0, c_0, c_1, \dots, c_{k-2}]}$ (the latter is by applying twice Corollary 3.7) and once again the second part of the lemma follows from the first. \square

We end by connecting the spectrum of an aperiodic Sturmian Hamiltonian, $H_{\alpha, V}$, with $\alpha \notin \mathbb{Q}$ with the spectra of periodic operators which approximate it. To do so, we apply the following result from [8].

Proposition 4.4 ([8]) *Let $\alpha \in [0, 1] \setminus \mathbb{Q}$ with infinite continued fraction expansion $(c_i)_{i=0}^\infty$. Then*

$$\sigma(H_{\alpha, V}) = \left\{ E \in \mathbb{R} : \{t_{[0, c_0, c_1, \dots, c_k]}(E)\}_{k \in \mathbb{N}} \text{ is a bounded sequence} \right\}.$$

Proof This is proven in [8]. \square

Corollary 4.5 *Let $\alpha \in (0, 1) \setminus \mathbb{Q}$ with infinite continued fraction expansion $(c_i)_{i=0}^\infty$. Then we get for all $k \in \mathbb{N}$*

$$\sigma(H_{\alpha, V}) \subseteq \sigma_{[0, 0, c_1, \dots, c_k]}(V) \cup \sigma_{[0, 0, c_1, \dots, c_{k+1}]}(V).$$

Proof Let $E \in \sigma(H_{\alpha, V})$ and assume by contradiction that there is some $k \in \mathbb{N}$ such that $E \notin \sigma_{[0, 0, c_1, \dots, c_k]}(V) \cup \sigma_{[0, 0, c_1, \dots, c_{k+1}]}(V)$. By Proposition 3.5, $|t_{[0, 0, c_1, \dots, c_k]}(E)| > 2$ and $|t_{[0, 0, c_1, \dots, c_{k+1}]}(E)| > 2$. Applying Lemma 4.2 we get that there exists $C > 1$ such that

$$|t_{[0, 0, c_1, \dots, c_n]}(E)| > C^{q_n} \quad \text{for all } n \in \mathbb{N}.$$

In particular $\{t_{[0, 0, c_1, \dots, c_n]}(E)\}_{k \in \mathbb{N}}$ is an unbounded sequence, but this contradicts $E \in \sigma(H_{\alpha, V})$ by Proposition 4.4. \square

Both Lemma 4.3 and Corollary 4.5 provide monotonicity statements of the spectra. In addition to those, we also have the following spectral convergence result.

Proposition 4.6 *Let $V \in \mathbb{R}$ and $\alpha \notin \mathbb{Q}$ with infinite continued fraction expansion $(c_i)_{i=0}^\infty$. For $k \in \mathbb{N}_0$, set $\mathbf{c}_k = [0, 0, c_1, \dots, c_k] \in \mathcal{C}$. Then*

$$\sigma(H_{\alpha, V}) = \lim_{k \rightarrow \infty} \sigma_{[\mathbf{c}_k, 1]}(V) = \lim_{k \rightarrow \infty} \sigma_{\mathbf{c}_k}(V) = \bigcap_{k \in \mathbb{N}_0} (\sigma_{\mathbf{c}_k}(V) \cup \sigma_{[\mathbf{c}_k, 1]}(V)).$$

Proof By [9, Theorem 1], the spectral map $[0, 1] \ni \beta \mapsto \sigma(H_{\beta, V})$ is continuous at all irrational $\beta \in [0, 1]$ and for all $V \in \mathbb{R}$. Observe that $\lim_{k \rightarrow \infty} \varphi(\mathbf{c}_k) = \lim_{k \rightarrow \infty} \varphi([\mathbf{c}_k, 1]) = \alpha$ where φ is the evaluation map. Thus,

$$\sigma(H_{\alpha, V}) = \lim_{k \rightarrow \infty} \sigma_{[\mathbf{c}_k, 1]}(V) = \lim_{k \rightarrow \infty} \sigma_{\mathbf{c}_k}(V)$$

follows using $\alpha \notin \mathbb{Q}$ and $\sigma_{\mathbf{c}}(V) = \sigma(H_{\varphi(\mathbf{c}), V})$ for $\mathbf{c} \in \mathcal{C}$ proven in Proposition 3.5.

Set $\Lambda_k(V) := \sigma_{\mathbf{c}_k}(V) \cup \sigma_{[\mathbf{c}_k, 1]}(V)$ for $k \in \mathbb{N}_0$ and $V \in \mathbb{R}$. Lemma 4.3 and Corollary 4.5 imply $\sigma(H_{\alpha, V}) \subseteq \Lambda_{k+1}(V) \subseteq \Lambda_k(V)$. Thus, $\sigma(H_{\alpha, V}) \subseteq \bigcap_{k \in \mathbb{N}_0} \Lambda_k(V)$ follows. By the convergence of $\sigma_{[\mathbf{c}_k, 1]}(V)$ and $\sigma_{\mathbf{c}_k}(V)$, we conclude that $\{\Lambda_k(V)\}_{k \in \mathbb{N}_0}$ converge monotonically in the Hausdorff metric to $\sigma(H_{\alpha, V})$. Thus, if $E \notin \sigma(H_{\alpha, V})$, then there is an $\varepsilon > 0$ such that $B_\varepsilon(E) := \{E' \in \mathbb{R} : |E - E'| < \varepsilon\}$ does not intersect $\sigma(H_{\alpha, V})$. Then the Hausdorff convergence of $\{\Lambda_k(V)\}_{k \in \mathbb{N}_0}$ to $\sigma(H_{\alpha, V})$ implies that there is a $k_0 \in \mathbb{N}_0$ such that $B_{\varepsilon/2}(E) \cap \Lambda_k(V) = \emptyset$ for all $k \geq k_0$. Hence, $E \notin \bigcap_{k \in \mathbb{N}_0} \Lambda_k(V)$ is derived proving $\bigcap_{k \in \mathbb{N}_0} \Lambda_k(V) = \sigma(H_{\alpha, V})$. \square

4.2 Spectral Bands Structure for Large Coupling Constant, $V > 4$

From this point on until the end of the paper, we specialize our discussion for the case $V > 4$. Under this assumption, one can prove quite a few useful connections between the periodic spectra, $\{\sigma_{\mathbf{c}}\}_{\mathbf{c} \in \mathcal{C}}$.

We start with the three-intersection-property. This observation can essentially be found in [10] for the Fibonacci Hamiltonian and was generalized in [39, Proposition 3.1.(iii)]. This property starts failing if $|V| \leq 4$ and this is one major obstacle to treat the small coupling regime.

Proposition 4.7 ([10, 39]) *Let $V > 4$, $\mathbf{c} \in \mathcal{C}$ and $m \in \mathbb{N}_0$ such that $[\mathbf{c}, m-1] \in \mathcal{C}$. Then*

$$\sigma_{\mathbf{c}}(V) \cap \sigma_{[\mathbf{c}, m]}(V) \cap \sigma_{[\mathbf{c}, m-1]}(V) = \emptyset.$$

Proof Assume by contradiction that there is some $E \in \sigma_{\mathbf{c}}(V) \cap \sigma_{[\mathbf{c}, m]}(V) \cap \sigma_{[\mathbf{c}, m-1]}(V)$. By Proposition 3.5, we obtain

$$|t_{\mathbf{c}}(E)|, |t_{[\mathbf{c}, m]}(E)|, |t_{[\mathbf{c}, m-1]}(E)| \leq 2.$$

Substituting this in Proposition 3.13, $V > 4$ yields

$$20 \geq t_{\mathbf{c}}^2(E) + t_{[\mathbf{c}, m]}^2(E) + t_{[\mathbf{c}, m-1]}^2(E) - t_{\mathbf{c}}(E)t_{[\mathbf{c}, m]}(E)t_{[\mathbf{c}, m-1]}(E) = 4 + V^2 > 20,$$

a contradiction. \square

Corollary 4.8 *Let $V > 4$, and $\mathbf{c} \in \mathcal{C}$ such that $[\mathbf{c}, -1] \in \mathcal{C}$. If $E \in \sigma_{\mathbf{c}}(V)$, then either*

$$E \in \sigma_{[\mathbf{c}, 0]}(V) \text{ or } E \in \sigma_{[\mathbf{c}, -1]}(V),$$

but not both.

Proof Assume $E \in \sigma_{\mathbf{c}}(V)$. By Lemma 4.3, we get $E \in \sigma_{[\mathbf{c}, 0]}(V) \cup \sigma_{[\mathbf{c}, -1]}(V)$. Now, apply Proposition 4.7 with $m = 0$ and get that either $E \in \sigma_{[\mathbf{c}, 0]}(V)$ or $E \in \sigma_{[\mathbf{c}, -1]}(V)$, but not both. \square

Proposition 4.9 *Let $V > 4$, and $\mathbf{c} \in \mathcal{C}$ such that $[\mathbf{c}, -1] \in \mathcal{C}$. If $I \subseteq \sigma_{\mathbf{c}}(V)$ is a spectral band, then I is either contained in a spectral band of $\sigma_{[\mathbf{c}, 0]}(V)$ or in a spectral band of $\sigma_{[\mathbf{c}, -1]}(V)$, but not in both.*

Proof Since I is a spectral band, we conclude that I is closed and connected. Now both $I \cap \sigma_{[\mathbf{c}, 0]}(V)$ and $I \cap \sigma_{[\mathbf{c}, -1]}(V)$ are closed too and according to Corollary 4.8, we have the following disjoint union $I = (I \cap \sigma_{[\mathbf{c}, 0]}(V)) \sqcup (I \cap \sigma_{[\mathbf{c}, -1]}(V))$. Since I is connected, one of the closed sets $I \cap \sigma_{[\mathbf{c}, 0]}(V)$ and $I \cap \sigma_{[\mathbf{c}, -1]}(V)$ must be empty and the other equals to I . Hence, I is contained in either $\sigma_{[\mathbf{c}, 0]}(V)$ or $\sigma_{[\mathbf{c}, -1]}(V)$. Using the same argument we may conclude that I is contained in a single connected component (spectral band) of $\sigma_{[\mathbf{c}, 0]}(V)$ or $\sigma_{[\mathbf{c}, -1]}(V)$. \square

Proposition 4.9 motivates a classification of the spectral bands into two types. We start employing such a dichotomy of the spectral bands and see that it leads to a hierarchical structure of the spectral bands from different spectra, $\sigma_{\mathbf{c}}$. This structure is developed and described in detail in the rest of this section.

Let $I = [a, b]$ and $J = [c, d]$ be two closed intervals. We say that I is *strictly included* in J and denote $I \subseteq_{\text{str}} J$ if $c < a$ and $b < d$. Note that this implies the (weaker) inclusion $I \subseteq J$.

Definition 4.10

Let $V \in \mathbb{R}$ and $\mathbf{c} \in \mathcal{C}$ be such that $\varphi(\mathbf{c}) \in [0, 1]$ and $[\mathbf{c}, 0], [\mathbf{c}, -1] \in \mathcal{C}$. A spectral band $I(V)$ of $\sigma_{\mathbf{c}}(V)$ is called

- *backward type A*
if there exists a spectral band $J(V)$ in $\sigma_{[\mathbf{c}, 0]}(V)$ such that $I(V) \subseteq_{\text{str}} J(V)$.
- *weak backward type A*
if there exists a spectral band $J(V)$ in $\sigma_{[\mathbf{c}, 0]}(V)$ such that $I(V) \subseteq J(V)$.
- *backward type B*
if there exists a spectral band $J(V)$ in $\sigma_{[\mathbf{c}, -1]}(V)$ such that $I(V) \subseteq_{\text{str}} J(V)$.
- *weak backward type B*
if there exists a spectral band $J(V)$ in $\sigma_{[\mathbf{c}, -1]}(V)$ such that $I(V) \subseteq J(V)$.

Remark In [39, Definition 3.2], a spectral band of weak backward type A is called a type III band, and a spectral band of weak backward type B is called a type II band. After that, the notations A and B (for such bands) also appeared in the literature, see, e.g., [15, 20, 28]. We prefer to use here (and also in [3]) the notations A, B for visual reasons and to distinguish those from the notation G introduced in the sequel for spectral gaps. In addition, only the notions of weak backward types appear in [39, Definition 3.2] (though not in this name). We introduce here also the stronger notion of (non-weak) backward types and use them to prove slightly stronger statements, since those are needed in order to obtain further results for $V < 4$ in [3].

In [39, Definition 3.2] also the notion of type I gap is introduced being a spectral band $I(V)$ in $\sigma_{[c,1]}(V)$ that is contained in $\sigma_{[c,1,-1]}(V)$ (so a weak backward B band). By Proposition 4.9, $I(V) \cap \sigma_c(V) = \emptyset$ and so $I(V)$ is contained in a spectral gap of $\sigma_c(V)$. As mentioned before, we omit this terminology here but when coding the spectrum in Sect. 5.2 the label G is rather used. These bands are a placeholder for the corresponding B band one level higher, confer Definition 5.3.

Using Definition 4.10 and Proposition 4.9 we conclude the following.

Corollary 4.11 *For all $V > 4$ and $\mathbf{c} \in \mathcal{C}$ with $\varphi(\mathbf{c}) \in [0, 1]$, every spectral band in $\sigma_c(V)$ is either of weak backward type A or weak backward type B , but not both.*

Proof This is just a reformulation of Proposition 4.9. □

We note that according to Definition 4.10, whether a spectral band is a (weak) backward type A or B (or not at all) depends on the value of V . We see later (Theorem 4.22) that as long as $V > 4$, the type of a spectral band does not depend on the value of V . This statement is generalized in [3, Theorem 2.15] for all $V \neq 0$. Note that there is no use to consider the backward type properties for $V = 0$, as in this case all spectra of all operators $H_{\alpha,V}$ are equal to $[-2, 2]$.

If $\mathbf{c} \in \mathcal{C}$ with $\varphi(\mathbf{c}) \in (0, 1)$ and $[\mathbf{c}, 0], [\mathbf{c}, -1] \in \mathcal{C}$, then there are $c_1, c_2, \dots, c_k \in \mathbb{N}$ for some $k \in \mathbb{N}$ such that either $\mathbf{c} = [0, 0, c_1, \dots, c_k + 1]$ or $\mathbf{c} = [0, 0, c_1, \dots, c_k, 1]$. Indeed, the rational number $\varphi(\mathbf{c})$ has exactly two different continued fraction expansion [27, Chap I.4]. Then the weak backward type of a spectral band in σ_c depends on the chosen representation. More precisely, a straightforward computation using Corollary 3.7 (see details in [3, Proposition 2.10]) yields

- $I(V)$ is of weak backward type A in $\sigma_{[0,0,c_1,\dots,c_k+1]}(V)$ if and only if $I(V)$ is of weak backward type B in $\sigma_{[0,0,c_1,\dots,c_k,1]}(V)$ and
- $I(V)$ is of weak backward type B in $\sigma_{[0,0,c_1,\dots,c_k+1]}(V)$ if and only if $I(V)$ is of weak backward type A in $\sigma_{[0,0,c_1,\dots,c_k,1]}(V)$.

We note that this duality does not show up in [39]. There one considers a fixed $\alpha \in [0, 1] \setminus \mathbb{Q}$ with a fixed infinite continued fraction expansion $(\tilde{c}_k)_{k \in \mathbb{N}_0}$ and rational number $\alpha_k = \varphi([0, 0, \tilde{c}_1, \dots, \tilde{c}_k])$. Hence, α_k has a unique finite continued fraction expansion. Here and in [3], we consider all elements of \mathcal{C} and this is why this duality is evident.

We demonstrate the classification of spectral bands to weak backward types, by explicitly computing a few spectral bands in the following.

Example 4.12 According to Example 3.4 we have for $V \in \mathbb{R}$,

$$\sigma_{[0]}(V) = \sigma_{[0,0,0]}(V) = \sigma_{[0,0,1,-1]}(V) = \mathbb{R} \quad \text{and} \quad \sigma_{[0,0,-1]}(V) = [-2 - V, 2 - V].$$

We examine $\sigma_{[0,0]}(V) = [-2, 2]$ and wish to determine its backward type. To do so we need to examine $\sigma_{[0,0,0]}(V) = \mathbb{R}$ and $\sigma_{[0,0,-1]}(V) = [-2 - V, 2 - V]$. By Definition 4.10, we see that for all $V \neq 0$ the spectral band $I_{[0,0]}(V) := [-2, 2]$ is of backward type *A* but not of weak backward type *B*.

A few additional spectra are

$$\sigma_{[0,0,1]}(V) = [-2 + V, 2 + V] \quad \text{and} \quad \sigma_{[0,0,1,0]}(V) = \sigma_{[0,0]}(V) = [-2, 2].$$

Given these spectra, one sees that for all $V \neq 0$, the spectral band $I_{[0,0,1]}(V) := [-2 + V, 2 + V]$ of $\sigma_{[0,0,1]}(V)$ is of backward type *B* but not of weak backward type *A*.

The spectral bands considered in this example are actually of a well-defined backward type and not just *weak* backward type. This is stronger than what is currently proved in Corollary 4.11. This stronger version indeed holds, in general, for all spectral bands as we prove in Theorem 4.22.

Next, we extend the classification of spectral bands into types by adding forward types to the backward type (later we show that they are actually the same).

Let $I = [a, b]$ and $J = [c, d]$ be two closed intervals. We say that I is *to the left* of J (or J is *to the right* of I) and denote $I \prec J$ if $a < c$ and $b < d$. Moreover, we say I is *strictly to the left* of J (or J is *strictly to the right* of I) and denote $I \prec_{\text{str}} J$ if $b < c$. Observe that $I \prec_{\text{str}} J$ holds if and only if $I \prec J$ and $I \cap J = \emptyset$.

Definition 4.13 Let $V \in \mathbb{R} \setminus \{0\}$. Let $\mathbf{c} \in \mathcal{C}$ and $m \in \mathbb{N}$ be such that $[\mathbf{c}, m] \in \mathcal{C}$. A spectral band $I_{\mathbf{c}}(V)$ of $\sigma_{\mathbf{c}}(V)$ is called of *m-forward type A* with $M = m - 1$ (respectively, *m-forward type B* with $M = m$) if the following holds.

(A) There exist M spectral bands of $\sigma_{[\mathbf{c},m]}(V)$ (denoted $I_{[\mathbf{c},m]}^1(V), \dots, I_{[\mathbf{c},m]}^M(V)$) which satisfy

(A1) $I_{[\mathbf{c},m]}^i(V) \subseteq_{\text{str}} I_{\mathbf{c}}(V)$ for all $1 \leq i \leq M$.

In particular, these bands are of backward type *A*.

(A2) $I_{[\mathbf{c},m]}^i(V)$ is not of weak backward type *B* for all $1 \leq i \leq M$.

(B) For each $n \in \mathbb{N}$, there exist $M + 1$ spectral bands of $\sigma_{[\mathbf{c},m,n]}(V)$ (denoted $I_{[\mathbf{c},m,n]}^1(V), \dots, I_{[\mathbf{c},m,n]}^{M+1}(V)$) which satisfy

(B1) $I_{[c,m,n]}^j(V) \subseteq_{\text{str}} I_{[c,m,n-1]}^j(V)$ for all $1 \leq j \leq M+1$, where $I_{[c,m,0]}^j(V) := I_c^j(V)$.

In particular, these bands are of backward type B .

(B2) $I_{[c,m,n]}^j(V)$ is not of weak backward type A for all $1 \leq j \leq M+1$.

(I) For each $n \in \mathbb{N}$, we have

$$I_{[c,m,n]}^1(V) < I_{[c,m]}^1(V) < I_{[c,m,n]}^2(V) < I_{[c,m]}^2(V) \dots < I_{[c,m]}^M(V) < I_{[c,m,n]}^{M+1}(V).$$

We say $I_c(V)$ satisfies the stronger interlacing property if (I) is replaced by

$$I_{[c,m,n]}^1(V) <_{\text{str}} I_{[c,m]}^1(V) <_{\text{str}} I_{[c,m,n]}^2(V) <_{\text{str}} \dots <_{\text{str}} I_{[c,m]}^M(V) <_{\text{str}} I_{[c,m,n]}^{M+1}(V). \quad (I_{\text{str}})$$

Remark Definition 4.13 rephrases the content of [39, Lemma 3.3]. A few notes should be made about the similarities and differences of both. First, as is commonly done in this review, we use the notation $c \in \mathcal{C}$ rather than (k, p) as in [39]. Second, we state the lemma from [39] as a definition here, since in [3] we need to keep the separation between backward types and forwards type for the sake of some of the proofs (even if at the end we realize that both concepts are equivalent). Third, Definition 4.13 introduces a slightly stronger notion of forward type than the one which appears explicitly¹ in [39, Lemma 3.3]; the strengthening is by using everywhere the strict inclusion \subseteq_{str} rather than \subseteq and also by having in (B1) $I_{[c,m,n]}^j(V) \subseteq_{\text{str}} I_{[c,m,n-1]}^j(V)$ for all $n \in \mathbb{N}$ rather than just $I_{[c,m,n]}^j(V) \subseteq_{\text{str}} I_c^j(V)$. This strengthening is crucial in [3], and that is why we choose to deviate from the original exposition in [39, Lemma 3.3].

Our next task is to show that indeed each spectral band has a well-defined forward type as in Definition 4.13. Actually, we will see that if a spectral band is of weak backward type A (respectively, B) then it is also of m -forward type A (respectively, B) for all $m \in \mathbb{N}$. This will be stated in Proposition 4.18. But before doing so, we need to prove two preparatory lemmas (Lemmas 4.14 and 4.16).

Lemma 4.14 *Let $V > 4$. Let $c \in \mathcal{C}$ and $m \in \mathbb{N}$ be such that $[c, m] \in \mathcal{C}$. Let $I_c(V)$ be a spectral band in $\sigma_c(V)$ of weak backward type A with $M = m - 1$ (respectively, of weak backward type B with $M = m$). Then the following holds (compare with Definition 4.13):*

¹ In the original paper [39], the strict inclusion and strict order were implicitly assumed without an explicit proof.

- (a) *There exist exactly M spectral bands of $\sigma_{[c,m]}(V)$ (denoted $I_{[c,m]}^1(V), \dots, I_{[c,m]}^M(V)$) which are contained in $I_c(V)$. These spectral bands satisfy properties (A1) and (A2) from Definition 4.13.*
- (b) *There exist exactly $M + 1$ spectral bands of $\sigma_{[c,m,1]}(V)$ (denoted $I_{[c,m,1]}^1(V), \dots, I_{[c,m,1]}^{M+1}(V)$) which are contained in $I_c(V)$. These spectral bands satisfy*
- (1) *$I_{[c,m,1]}^j(V) \subseteq I_c(V)$, for all $1 \leq j \leq M + 1$. In particular, these bands are of weak backward type B.*
 - (2) *$I_{[c,m,1]}^j(V)$ is not of weak backward type A for all $1 \leq j \leq M + 1$.*
- (c) *The following interlacing property holds:*

$$I_{[c,m,1]}^1(V) <_{\text{str}} I_{[c,m]}^1(V) <_{\text{str}} I_{[c,m,1]}^2(V) <_{\text{str}} I_{[c,m]}^2(V) \dots <_{\text{str}} I_{[c,m]}^M(V) <_{\text{str}} I_{[c,m,1]}^{M+1}(V).$$

Remark We can colloquially phrase Lemma 4.14 as follows: if the spectral band $I_c(V)$ is of a weak backward type A (or B), then for all $m \in \mathbb{N}$ it is “partially” m -forward type A or B, correspondingly. By “partially” we mean that $I_c(V)$ fully satisfies properties (A1) and (A2) (in Definition 4.13), but it satisfies properties (B1), (B2) and the strong interlacing (I_{str}) only for $n = 1$ and property (B1) is satisfied only in its weak version, i.e., that all $I_{[c,m,1]}^j$ are of weak backward type B. Another difference between Lemma 4.14 and Definition 4.13 (m -forward type) goes in the other direction: in this lemma we state that the spectral bands $\{I_{[c,m]}^i\}_{i=1}^M$ and $\{I_{[c,m,n]}^j\}_{j=1}^{M+1}$ are unique, which is not part of Definition 4.13.

Proof First, we fix the value of $V > 4$ throughout the proof, but for brevity we omit V from the various notations (for example, writing just I and σ_c). We fix the following auxiliary variable:

$$\delta_B := \begin{cases} 0, & I \text{ is of backward type A,} \\ 1, & I \text{ is of backward type B,} \end{cases}$$

which allows us to prove the lemma simultaneously for both these cases. Note that with this notation $M = m - 1 + \delta_B$, for the value M which is introduced in the statement.

We introduce two other notations which will help throughout the proof. Given $c \in \mathcal{C}$ and a spectral band $I_c \subseteq \sigma_c$, we know by Proposition 3.5 that $t_c(I_c) = [-2, 2]$ and $t_c|_{I_c}$ is strictly monotone. Hence, for each $x \in [-2, 2]$ we may denote by $E_c^{I_c}(x)$ the unique value in I_c such that $t_c(E_c^{I_c}(x)) = x$.

The proof consists of four steps, which we briefly summarize before going into the details. To obtain the candidates for the spectral bands $I_{[c,m]}^i$ in property (A) and the spectral bands $I_{[c,m,1]}^j$ in property (B), we indicate specific energy values $\{A_i\}_{i=1}^M$

and $\{B_i\}_{i=1}^{M+1}$ in I and find the spectral bands of $\sigma_{[c,m]}$ and $\sigma_{[c,m,1]}$ which contain these values. This forms the first two steps of the proof. The third step would be to prove property (I) by observing the order between the aforementioned energy values $\{A_i\}_{i=1}^M$ and $\{B_i\}_{i=1}^{M+1}$. The last step is to show that there are no other spectral bands in $\sigma_{[c,m]}$ and $\sigma_{[c,m,1]}$ which satisfy those properties, implying the uniqueness which is mentioned in (A) and (B).

Step 1: Defining the spectral bands $\{I_{[c,m]}^i\}_{i=1}^M$ and proving (A2) and partially (A1): Define $A_i := E_c^{I_c}(2 \cos(\frac{i\pi}{m+\delta_B}))$ for $i = 1, \dots, m-1+\delta_B = M$ satisfying $t_c(A_i) = 2 \cos(\frac{i\pi}{m+\delta_B})$. We use these values to define spectral bands in $\sigma_{[c,m]}$, and show later that those are exactly $\{I_{[c,m]}^i\}_{i=1}^M$ from Definition 4.13(A). Corollary 3.10 (applied for $\ell = -\delta_B$) implies

$$t_{[c,m]}(A_i) = S_{m-1+\delta_B}(t_c(A_i))t_{[c,1-\delta_B]}(A_i) - S_{m-2+\delta_B}(t_c(A_i))t_{[c,-\delta_B]}(A_i).$$

The dilated Chebyshev polynomials satisfy $S_l(2 \cos \theta) = \frac{\sin((l+1)\theta)}{\sin \theta}$, see Lemma 8.3. Using this and $t_c(A_i) = 2 \cos(\frac{i\pi}{m+\delta_B})$, we evaluate the dilated Chebyshev polynomials which appear in the last equation:

$$S_{m-1+\delta_B}(t_c(A_i)) = S_{m-1+\delta_B}\left(2 \cos\left(\frac{i\pi}{m+\delta_B}\right)\right) = \frac{\sin\left((m+\delta_B)\frac{i\pi}{m+\delta_B}\right)}{\sin\left(\frac{i\pi}{m+\delta_B}\right)} = 0,$$

and

$$\begin{aligned} S_{m-2+\delta_B}(t_c(A_i)) &= S_{m-2+\delta_B}\left(2 \cos\left(\frac{i\pi}{m+\delta_B}\right)\right) \\ &= \frac{\sin\left((m-1+\delta_B)\frac{i\pi}{m+\delta_B}\right)}{\sin\left(\frac{i\pi}{m+\delta_B}\right)} \\ &= \frac{\sin\left(i\pi - \frac{i\pi}{m+\delta_B}\right)}{\sin\left(\frac{i\pi}{m+\delta_B}\right)} \\ &= \frac{\sin(i\pi) \cos\left(\frac{i\pi}{m+\delta_B}\right) - \cos(i\pi) \sin\left(\frac{i\pi}{m+\delta_B}\right)}{\sin\left(\frac{i\pi}{m+\delta_B}\right)} \\ &= -\cos(i\pi) = (-1)^{i+1}. \end{aligned}$$

Combining the computations above gives

$$t_{[c,m]}(A_i) = (-1)^i t_{[c,-\delta_B]}(A_i).$$

Since I_c has a well-defined weak backward type (either A or B), by the definition of δ_B we get that $|t_{[c,-\delta_B]}|_{I_c} \leq 2$. Since $A_i \in I_c$, the equation above implies $|t_{[c,m]}(A_i)| \leq 2$. This means that $\{A_i\}_{i=1}^M \subseteq \sigma_{[c,m]}$. Hence, for each $1 \leq i \leq M$ we may denote by $I_{[c,m]}^i$ the spectral band in $\sigma_{[c,m]}$ which contains A_i . At this point, we note that it could be that different $A_{i_0} \neq A_{i_1}$ give rise to the same spectral bands $I_{[c,m]}^{i_0}$ and $I_{[c,m]}^{i_1}$. However, we prove below in step 3 that $A_{i_0} \neq A_{i_1}$ implies $I_{[c,m]}^{i_0} \neq I_{[c,m]}^{i_1}$.

We show now that for each i the spectral band $I_{[c,m]}^i$ is of weak backward type A and not of weak backward type B . By Corollary 4.8, we have that either $A_i \in \sigma_{[c,m,0]} = \sigma_c$ or $A_i \in \sigma_{[c,m,-1]}$. Since $A_i \in I_c \subseteq \sigma_c$ we get that $A_i \notin \sigma_{[c,m,-1]}$. By Proposition 4.9, we have that $I_{[c,m]}^i$ is either contained in a spectral band of $\sigma_{[c,m,0]}$ or of $\sigma_{[c,m,-1]}$. But, since $A_i \notin \sigma_{[c,m,-1]}$ the former option holds and we get that $I_{[c,m]}^i$ is contained in I_c . In particular $I_{[c,m]}^i$ is of weak backward type A and not of weak backward type B . This shows property (A2), but it does not yet show property (A1) since we only proved that $I_{[c,m]}^i$ is of weak backward type A . We will complete the proof of property (A1) in step 3, where we also prove that $A_{i_0} \neq A_{i_1}$ implies $I_{[c,m]}^{i_0} \neq I_{[c,m]}^{i_1}$ and that they satisfy (A1).

Step 2: Defining the spectral bands $\{I_{[c,m,1]}^j\}_{j=1}^{M+1}$:

We proceed similar as in step 1. Define $B_j := E_c^{I_c}(2 \cos(\frac{j\pi}{m+\delta_B+1}))$ for $j = 1, \dots, m + \delta_B = M + 1$ satisfying $t_c(B_j) = 2 \cos(\frac{j\pi}{m+\delta_B+1})$. Similar to the previous step in the proof, we will now use these values to define spectral bands in $\sigma_{[c,m,1]}$. Corollaries 3.7 and 3.10 (applied for $\ell = -\delta_B$) lead to

$$\begin{aligned} t_{[c,m,1]}(B_j) &= t_{[c,m+1]}(B_j) \\ &= S_{m+\delta_B}(t_c(B_j))t_{[c,1-\delta_B]}(B_j) - S_{m+\delta_B-1}(t_c(B_j))t_{[c,-\delta_B]}(B_j). \end{aligned}$$

The dilated Chebyshev polynomials satisfy $S_\ell(2 \cos \theta) = \frac{\sin((\ell+1)\theta)}{\sin \theta}$, see Lemma 8.3. Using this and $t_c(B_j) = 2 \cos(\frac{j\pi}{m+\delta_B+1})$, we evaluate the dilated Chebyshev polynomials which appear in the last equation:

$$S_{m+\delta_B}(t_c(B_j)) = S_{m+\delta_B}\left(2 \cos\left(\frac{j\pi}{m+\delta_B+1}\right)\right) = \frac{\sin\left((m+\delta_B+1)\frac{j\pi}{m+\delta_B+1}\right)}{\sin\left(\frac{j\pi}{m+\delta_B+1}\right)} = 0,$$

and

$$\begin{aligned}
S_{m+\delta_B-1}(t_{\mathbf{c}}(B_j)) &= S_{m+\delta_B-1}\left(2\cos\left(\frac{j\pi}{m+\delta_B+1}\right)\right) \\
&= \frac{\sin\left((m+\delta_B)\frac{j\pi}{m+\delta_B+1}\right)}{\sin\left(\frac{j\pi}{m+\delta_B+1}\right)} \\
&= \frac{\sin\left(j\pi - \frac{j\pi}{m+\delta_B+1}\right)}{\sin\left(\frac{j\pi}{m+\delta_B+1}\right)} \\
&= \frac{\sin(j\pi)\cos\left(\frac{j\pi}{m+\delta_B+1}\right) - \cos(j\pi)\sin\left(\frac{j\pi}{m+\delta_B+1}\right)}{\sin\left(\frac{j\pi}{m+\delta_B+1}\right)} \\
&= -\cos(j\pi) = (-1)^{j+1}.
\end{aligned}$$

Combining the computations above gives

$$t_{[\mathbf{c},m,1]}(B_j) = (-1)^j t_{[\mathbf{c},-\delta_B]}(B_j).$$

Since $I_{\mathbf{c}}$ has a well-defined weak backward type (either A or B), by the definition of δ_B we get that $|t_{[\mathbf{c},-\delta_B]}|_{I_{\mathbf{c}}} \leq 2$. Since $B_j \in I_{\mathbf{c}}$, the equation above implies $|t_{[\mathbf{c},m,1]}(B_j)| \leq 2$. This means that $\{B_j\}_{j=1}^{M+1} \subseteq \sigma_{[\mathbf{c},m,1]}$. Hence, for each $1 \leq j \leq M+1$ we may denote by $I_{[\mathbf{c},m,1]}^j$ the spectral band in $\sigma_{[\mathbf{c},m,1]}$ which contains B_j . Now, similar to the argument in step 1, we deduce that each $I_{[\mathbf{c},m,1]}^j$ is of weak backward type B and not of weak backward type A .

We note that just as in the previous step, we should still prove that $I_{[\mathbf{c},m,1]}^{j_0} \neq I_{[\mathbf{c},m,1]}^{j_1}$ if $j_0 \neq j_1$.

Step 3: Band interlacing: As mentioned before, the interlacing follows by the corresponding interlacing of $\{A_i\}_{i=1}^M$ and $\{B_j\}_{j=1}^{M+1}$. The interlacing of $\{A_i\}_{i=1}^M$ and $\{B_j\}_{j=1}^{M+1}$ results from the interlacing of the zeros of two successive dilated Chebyshev polynomials, as these belong to a family of orthogonal polynomials. Writing this explicitly, we note that $0 < \frac{j}{M+2} < \frac{j}{M+1} < \frac{j+1}{M+2} < \pi$, for all $1 \leq j \leq M$, so that the sets $\{\frac{i}{M+1}\}_{i=1}^M, \{\frac{j}{M+2}\}_{j=1}^{M+1}$ interlace. The sets $\{A_i\}_{i=1}^M, \{B_j\}_{j=1}^{M+1}$ are obtained as a monotone function acting on these sets and hence also interlace. Indeed, to see this recall that $A_i := E_{\mathbf{c}}^{I_{\mathbf{c}}}(2\cos(\pi\frac{i}{M+1}))$, $B_j := E_{\mathbf{c}}^{I_{\mathbf{c}}}(2\cos(\pi\frac{j}{M+2}))$ and note the strict monotonicity of the cosine on $[0, \pi]$ and the strict monotonicity of $t_{\mathbf{c}}$ on $I_{\mathbf{c}}$ together with $E_{\mathbf{c}}^{I_{\mathbf{c}}} = (t_{\mathbf{c}}|_{I_{\mathbf{c}}})^{-1}$.

Hence, we get that either

$$B_1 < A_1 < B_2 < \dots < A_M < B_{M+1}, \quad (4.1)$$

or

$$B_1 > A_1 > B_2 > \cdots > A_M > B_{M+1}. \quad (4.2)$$

Whether (4.1) is used or (4.2) is determined by $\text{sign}(t'_c|_{I_c})$ which is indeed constant (see Proposition 3.5). We now draw a few conclusions from this interlacing. In the previous two steps we have seen that $\{A_i\}_{i=1}^M \subseteq \sigma_c \cap \sigma_{[c,m]}$ and $\{B_j\}_{j=1}^M \subseteq \sigma_c \cap \sigma_{[c,m,1]}$. Applying Proposition 4.7 with $c' = [c, m, 1]$, $m' = 0$ yields $\sigma_c(V) \cap \sigma_{[c,m]}(V) \cap \sigma_{[c,m,1]}(V) = \emptyset$ (as always, for $V > 4$). We get, in particular, that for all i , $A_i \notin \sigma_{[c,m,1]}$ and all j , $B_j \notin \sigma_{[c,m]}$. We use this to observe that for some $i_0 \neq i_1$, the spectral band $I_{[c,m]}^{i_0} \subseteq \sigma_{[c,m]}$ contains A_{i_0} , the spectral band $I_{[c,m]}^{i_1} \subseteq \sigma_{[c,m]}$ contains A_{i_1} , and by the interlacing ((4.1) and (4.2)) there is some point $B_j \notin \sigma_{[c,m]}$ between A_{i_0} and A_{i_1} . This means, in particular, that all the spectral bands $\{I_{[c,m]}^i\}_{i=1}^M$, defined in step 1, are distinct. In exactly the same manner we conclude that all the spectral bands $\{I_{[c,m,1]}^j\}_{j=1}^{M+1}$, defined in step 2, are distinct. By Proposition 4.7, $I_{[c,m]}^i \cap I_{[c,m,1]}^j = \emptyset$ holds for all i, j since both are contained in $\sigma_c(V)$. Thus, the desired strong interlacing property (I_{str}) of Definition 4.13 follows for $n = 1$. We should just note that if the interlacing of the sets $\{A_i\}_{i=1}^M, \{B_j\}_{j=1}^{M+1}$ is as in (4.2), we should reshuffle the indices in order to get the interlacing as in (4.1). Namely, we permute the indices of $\{A_i\}_{i=1}^M$ by $1 \leftrightarrow M, 2 \leftrightarrow M-1, \dots$, and permute the indices of $\{B_j\}_{j=1}^{M+1}$ by $1 \leftrightarrow M+1, 2 \leftrightarrow M$, and so on. Obviously, this affects the indices of the spectral bands $\{I_{[c,m]}^i\}_{i=1}^M$ and $\{I_{[c,m,1]}^j\}_{j=1}^{M+1}$, and we get the strong interlacing property of Definition 4.13, (I_{str}) for $n = 1$.

Using the interlacing property we may also deduce that the spectral bands $I_{[c,m]}^i$ are of backward type A. We already obtained in step 1 that they are of weak backward type A. But, thanks to the interlacing property there is another spectral band to the left and to the right of each $I_{[c,m]}^i$ which is also included in I_c . Hence, each $I_{[c,m]}^i$ is strictly included in I_c and it is of backward type A. Thus, $\{I_{[c,m]}^i\}_{i=1}^M$ satisfy also (A1).

Step 4: Uniqueness of the bands: We show now that the spectral bands $\{I_{[c,m]}^i\}_{i=1}^M$ are the only spectral bands of $\sigma_{[c,m]}$ which are contained in I_c and that $\{I_{[c,m,1]}^j\}_{j=1}^{M+1}$ are the only spectral bands of $\sigma_{[c,m,1]}$ which are contained in I_c .

Let $J \subseteq \sigma_{[c,m]}$ such that $J \subseteq I_c$. We will show that $A_i \in J$ for some $1 \leq i \leq M$ and conclude that $J = I_{[c,m]}^i$, which proves the uniqueness in property (A).

Due to Corollary 4.11, I_c has a well-defined weak backward type (either A or B). By definition of δ_B , we therefore get that $I_c \subseteq \sigma_c \cap \sigma_{[c, -\delta_B]}$. Hence, also $J \subseteq \sigma_c \cap \sigma_{[c, -\delta_B]}$. Then Proposition 4.7 implies $\sigma_c(V) \cap \sigma_{[c, 1-\delta_B]}(V) \cap \sigma_{[c, -\delta_B]}(V) = \emptyset$ for $V > 4$ and so we conclude $J \cap \sigma_{[c, 1-\delta_B]} = \emptyset$. Thus, Proposition 3.5 leads to $|t_{[c, 1-\delta_B]}(E)| > 2$ for all $E \in J$. Similarly, we have $\sigma_c(V) \cap \sigma_{[c, m-1]}(V) \cap \sigma_{[c,m]}(V) = \emptyset$ for $V > 4$ by Proposition 4.7 and so $J \subseteq \sigma_c \cap \sigma_{[c,m]}$. Thus, $|t_{[c, m-1]}(E)| > 2$ follows for all $E \in J$.

Since $t_{[c, 1-\delta_B]}$ and $t_{[c, m-1]}$ are continuous in E , the signs of $t_{[c, 1-\delta_B]}(E)$ and $t_{[c, m-1]}(E)$ are constant for all $E \in J$ by the previous considerations. Thus, we can choose an $\xi \in \{0, 1\}$ such that

$$t_{[c, m-1]}(E) + (-1)^\xi t_{[c, 1-\delta_B]}(E) \neq 0 \quad \text{for all } E \in J.$$

Since $J \subseteq I_c \subseteq \sigma_{[c, -\delta_B]}$, we have $|t_{[c, -\delta_B]}(E)| \leq 2$ for all $E \in J$. In addition, $|t_{[c, m]}(E)| = 2$ if E is the left or right edge of J . Note that the sign of $t_{[c, m]}(E)$ changes if E is the left, respectively, the right edge of J . Therefore, by the intermediate value theorem there exists $E_0 \in J$ such that

$$t_{[c, m]}(E_0) + (-1)^\xi t_{[c, -\delta_B]}(E_0) = 0.$$

Then Lemma 3.11 (applied for $\ell = -\delta_B$) gives

$$\begin{aligned} & S_{m-1+\delta_B}(t_c(E_0)) \left[\underbrace{t_{[c, m-1]}(E_0) + (-1)^\xi t_{[c, 1-\delta_B]}(E_0)}_{\neq 0 \text{ as } E_0 \in J} \right] \\ &= \left[S_{m-2+\delta_B}(t_c(E_0)) + (-1)^\xi \right] \left[\underbrace{t_{[c, m]}(E_0) + (-1)^\xi t_{[c, -\delta_B]}(E_0)}_{=0} \right]. \end{aligned}$$

We conclude $S_{m-1+\delta_B}(t_c(E_0)) = 0$ for $E_0 \in J \subseteq I$.

Since by definition of the dilated Chebyshev polynomials $S_0 \equiv 1$, we get $m-1+\delta_B \neq 0$. Hence $m-1+\delta_B \geq 1$ and we conclude $|t_c(E_0)| < 2$, since dilated Chebyshev polynomials do not vanish outside $(-2, 2)$, see Lemma 8.2(f). Therefore, there exists some $\theta \in (0, \pi)$ such that $t_c(E_0) = 2 \cos \theta$ and

$$0 = S_{m-1+\delta_B}(2 \cos \theta) = \frac{\sin((m+\delta_B)\theta)}{\sin \theta},$$

where we used Lemma 8.3 in the last equality. We conclude that $\theta = \frac{i\pi}{m+\delta_B}$ for some $1 \leq i \leq m-1+\delta_B$. Therefore, $t_c(E_0) = 2 \cos\left(\frac{i\pi}{m+\delta_B}\right)$ or, equivalently, $E_0 = E_c^I(2 \cos(\frac{i\pi}{m+\delta_B}))$. But this is exactly the definition of A_i in the beginning of the proof, and so $E_0 = A_i$. Thus, $J = I_{[c, m]}^i$ follows proving the uniqueness in (a).

In order to show the uniqueness for the spectral bands $\left\{ I_{[c, m, 1]}^j \right\}_{j=1}^{M+1}$, we repeat the arguments above, mainly replacing m with $m+1$ and using $\sigma_{[c, m, 1]} = \sigma_{[c, m+1]}$ and $\sigma_{[c, m, 1, -1]} = \sigma_{[c, m, 0]}$ by Lemma 3.6. Briefly, if we assume that J is a spectral band of $\sigma_{[c, m, 1]}$ such that $J \subseteq I$, we are able to conclude that there exists $1 \leq j \leq m+\delta_B$ such that $E_0 := 2 \cos\left(\frac{j\pi}{m+1+\delta_B}\right) \in J$. Thus, $E_0 = B_j$ for some $1 \leq j \leq m+\delta_B$

follows where $\{B_j\}_{j=1}^{m+\delta_B}$ where defined in step 2. Hence, $J = I_{[c,m,1]}^j$ follows proving the uniqueness in (b). \square

In the course of proving Lemma 4.14, we have gained some information regarding the location of the spectral bands $I_{[c,m]}^i$. We state this here as a separate corollary, since it is useful in a proof which appears in [3, Eq. (7.11)].

Corollary 4.15 *Let $V > 4$, $c \in \mathcal{C}$ and $m \in \mathbb{N}$ be such that $[c, m] \in \mathcal{C}$. If $I_c(V)$ is a spectral band in $\sigma_c(V)$ of weak backward type B . There exist unique $\{E_i\}_{i=1}^m \subseteq I_c$ such that*

$$t_c(E_i) = 2 \cos \left(\frac{i\pi}{m+1} \right) \cdot \text{sign}(t_c(L(I_c))),$$

where $L(I_c)$ is the left edge of I_c . In addition, for all $1 \leq i \leq m$, $E_i \in I_{[c,m]}^i$, where $I_{[c,m]}^i$ are the spectral bands from Lemma 4.14 (also Definition 4.13).

In order to upgrade Lemma 4.14(b) to the spectral bands $\{I_{[c,m,n]}^j\}_{j=1}^{M+1}$ (as required in (B) in Definition 4.13), the following lemma is used.

Lemma 4.16 *Let $V > 4$. Let $n \in \mathbb{N}$, $[c', n] \in \mathcal{C}$ and I be a spectral band in $\sigma_{[c',n]}$ of weak backward type B . Then there is a unique spectral band J in $\sigma_{[c',n+1]}$ such that $J \subseteq_{\text{str}} I$. In particular, J is of backward type B .*

Proof The proof of this lemma follows from Lemma 4.14. Let $I \subseteq \sigma_{[c',n]}$ be a spectral band of backward type B . Applying Lemma 4.14 for $c := [c', n]$ gives that there exists a unique spectral band $J \subseteq \sigma_{[c',n,1]}$ such that $J \subseteq_{\text{str}} I$. Equivalently, J is a spectral band of backward type A when J is considered a spectral band of $\sigma_{[c',n,1]}$. Nevertheless, since $\sigma_{[c',n,1]} = \sigma_{[c',n+1]}$, we may consider J as a spectral band of $\sigma_{[c',n+1]}$ since $\sigma_{[c',n,1,0]} = \sigma_{[c',n+1,-1]}$ by Lemma 3.6. Thus, J is of backward type B as a spectral band of $\sigma_{[c',n+1]}$ for the same reason, since $J \subseteq_{\text{str}} I$. \square

Lemma 4.16 implies that every spectral band of backward type B of $\sigma_{[c,n]}$ contains another (unique) spectral band of backward type B of $\sigma_{[c,n+1]}$. This construction continues indefinitely by recursion, and hence we call it the *tower property*.

Corollary 4.17 (Tower property) *Let $V > 4$, $[c', 1] \in \mathcal{C}$ and $I_{[c',1]}$ be a spectral band of $\sigma_{[c',1]}(V)$ of weak backward type B . Then there are unique spectral bands $I_{[c',n]}$ in $\sigma_{[c',n]}(V)$ of backward type B for all $n \geq 2$ such that $I_{[c',j+1]} \subseteq_{\text{str}} I_{[c',j]}$ for all $j \in \mathbb{N}$.*

Proof This follows directly from an induction over $n \geq 2$ and Lemma 4.16. \square

Proposition 4.18 *Let $V > 4$ and $c \in \mathcal{C}$ with $[c, m] \in \mathcal{C}$ for all $m \in \mathbb{N}$. Let $I_c(V)$ be a spectral band in $\sigma_c(V)$ of weak backward type A (respectively, weak backward type B). Then $I_c(V)$ is of m -forward type A (respectively, m -forward type B) for all $m \in \mathbb{N}$. In addition,*

- (a) The spectral bands $\{I_{[\mathbf{c},m]}^i(V)\}_{i=1}^M$ mentioned in the m -forward definition (Definition 4.13) are the only spectral bands in $\sigma_{[\mathbf{c},m]}(V)$ which are included in $I_{\mathbf{c}}(V)$.
- (b) The spectral bands $\{I_{[\mathbf{c},m,n]}^j(V)\}_{j=1}^{M+1}$ mentioned in the m -forward definition (Definition 4.13) are the only spectral bands in $\sigma_{[\mathbf{c},m,n]}(V)$ which satisfy properties (B1) and (B2) (in Definition 4.13).
- (c) The strong interlacing property (I_{str}) holds.

Proof As before, we omit all the V dependencies here but note that the proof relies on various results using $V > 4$. Combining Lemma 4.14 with Lemma 4.16 implies the existence and uniqueness of the spectral bands $\{I_{[\mathbf{c},m]}^i\}_{i=1}^M$ and $\{I_{[\mathbf{c},m,1]}^j\}_{j=1}^{M+1}$, and these spectral bands satisfy properties (A1), (A2) and (I_{str}), see Definition 4.13. Let $1 \leq j \leq M+1$. Then Corollary 4.17 (applied for $\mathbf{c}' = [\mathbf{c}, m]$) asserts that for all $n \in \mathbb{N}$, there exist a unique spectral band $I_{[\mathbf{c},m,n]}^j$ such that

$$I_{[\mathbf{c},m,n]}^j \subseteq_{\text{str}} I_{[\mathbf{c},m,n-1]}^j \subseteq_{\text{str}} \dots \subseteq_{\text{str}} I_{[\mathbf{c},m,1]}^j \subseteq I_{\mathbf{c}}.$$

By construction $I_{[\mathbf{c},m,n]}^j$ is of backward type B for all $n > 1$ and not of weak backward type A by Corollary 4.11. Thus, for all $n > 1$, the spectral bands $\{I_{[\mathbf{c},m,n]}^j\}_{j=1}^{M+1}$ satisfy properties (B1) and (B2). All that is left to show is $I_{[\mathbf{c},m,1]}^j \subseteq_{\text{str}} I_{\mathbf{c}}$ for all $1 \leq j \leq M+1$.

Let $E_- < E_+$ be chosen such that $I_{\mathbf{c}} = [E_-, E_+]$. Thus, $|t_{\mathbf{c}}(E_{\pm})| = 2$ holds by Proposition 3.5. In addition, Lemma 4.14 implies $I_{[\mathbf{c},m,1]}^1 \prec_{\text{str}} \dots \prec_{\text{str}} I_{[\mathbf{c},m,1]}^{M+1}$ and $I_{[\mathbf{c},m,1]}^j \subseteq I_{\mathbf{c}}$. Therefore, it is sufficient to prove $|t_{[\mathbf{c},m,1]}(E_{\pm})| > 2$ in order to conclude that $I_{[\mathbf{c},m,1]}^j \subseteq_{\text{str}} I_{\mathbf{c}}$ for all $1 \leq j \leq M+1$.

As $|t_{\mathbf{c}}(E_{\pm})| = 2$, Lemma 8.2 implies $|S_{l+1}(t_{\mathbf{c}}(E_{\pm}))| = l+2$. Thus, applying Lemma 3.9 and the reversed triangle inequality gives that for $m \geq l \geq -1$,

$$\begin{aligned} |t_{[\mathbf{c},m,1]}(E_{\pm})| &= |t_{[\mathbf{c},m+1]}(E_{\pm})| \\ &= |S_{l+1}(t_{\mathbf{c}}(E_{\pm})) t_{[\mathbf{c},m-l]}(E_{\pm}) - S_l(t_{\mathbf{c}}(E_{\pm})) t_{[\mathbf{c},m-l-1]}(E_{\pm})| \\ &\geq (l+2)|t_{[\mathbf{c},m-l]}(E_{\pm})| - (l+1)|t_{[\mathbf{c},m-l-1]}(E_{\pm})|. \end{aligned} \tag{4.3}$$

We continue estimating the previous term by a suitable choice of l depending whether $I_{\mathbf{c}}(V)$ is of weak backward type A or B .

If $I_{\mathbf{c}}(V)$ is of weak backward type A , set $l = m-1$. Note that $I_{\mathbf{c}}(V) \subseteq \sigma_{[\mathbf{c},0]}(V)$ (since we assume now that $I_{\mathbf{c}}(V)$ is of weak backward type A) and therefore $|t_{[\mathbf{c},0]}(E_{\pm})| \leq 2$. Then $E_{\pm} \subseteq \sigma_{\mathbf{c}}(V) \cap \sigma_{[\mathbf{c},0]}(V)$ leads to $E_{\pm} \notin \sigma_{[\mathbf{c},1]}(V)$ by Proposition 4.7 and $V > 4$. Thus, $|t_{[\mathbf{c},1]}(E_{\pm})| > 2$ is concluded from Proposition 3.5. Substituting $|t_{[\mathbf{c},0]}(E_{\pm})| \leq 2$ and $|t_{[\mathbf{c},1]}(E_{\pm})| > 2$ in Eq. (4.3) gives

$$|t_{[c,m,1]}(E_{\pm})| \geq (m+1)|t_{[c,1]}(E_{\pm}) - m|t_{[c,0]}(E_{\pm})| > 2$$

finishing the proof in this case.

If $I_c(V)$ is of weak backward type B , set $l = m$ and note that $|t_{[c,-1]}(E_{\pm})| \leq 2$. In addition, $|t_{[c,0]}(E_{\pm})| > 2$ holds as $E_{\pm} \in I_c(V)$ and $I_c(V)$ is not of weak backward type A by Corollary 4.11 and $V > 4$. Then Equation (4.3) leads to

$$|t_{[c,m,1]}(E_{\pm})| \geq (m+2)|t_{[c,0]}(E_{\pm})| - (m+1)|t_{[c,-1]}(E_{\pm})| > 2$$

finishing the proof. \square

Proposition 4.18 is comparable to [39, Lemma 3.3]. Nevertheless, Proposition 4.18 is slightly stronger in three aspects: using everywhere the strict inclusion \subseteq_{str} rather than \subseteq ; stating the properties for all $m, n \in \mathbb{N}$; and also by having in (B1) $I_{[c,m,n]}^j(V) \subseteq_{\text{str}} I_{[c,m,n-1]}^j(V)$ for all $n \in \mathbb{N}$ rather than just $I_{[c,m,n]}^j(V) \subseteq_{\text{str}} I_c^j(V)$. This strengthening is crucial in [3], and that is why we choose to deviate from the original exposition in [39, Lemma 3.3].

Proposition 4.18 shows the implication between (weak) backward type and forward type. Therefore, we are motivated to include both in one definition (Definition 4.19) and to prove their equivalence if $V > 4$, see Theorem 4.22.

Definition 4.19 Let $V > 4$ and $m \in \mathbb{N}$. Let $c \in \mathcal{C}$ such that $[c, m] \in \mathcal{C}$. A spectral band I_c of $\sigma_c(V)$ is called of

- *type A* if I_c is of backward type A and it is also of m -forward type A for all $m \in \mathbb{N}$.
- *type B* if I_c is of backward type B and it is also of m -forward type B for all $m \in \mathbb{N}$.

Before proving the main theorem—that each spectral band is of type A or B , we provide a useful corollary of Proposition 4.18 for which the following example is a warm up.

Example 4.20 Let $V > 4$. Then a short computation yields that $\sigma_{[0,0]}(V) = [-2, 2] =: I_{[0,0]}(V)$ is of backward type A and $\sigma_{[0,0,1]}(V) = [-2 + V, 2 + V] =: K_{[0,0,1]}(V)$ is of backward type B , see also Example 4.12. Thus, Proposition 4.18 implies that $I_{[0,0]}(V)$ is of type A and $K_{[0,0,1]}(V)$ is of type B . Moreover, Proposition 4.18 and Lemma 4.16 imply for all $n \geq 2$ that there are $\{I_{[0,0,n]}^i(V)\}_{i=1}^{n-1}$ of type A and one spectral band $K_{[0,0,n]}(V)$ of type B such that

$$\sigma_{[0,0,n]} = \bigcup_{i=1}^{n-1} I_{[0,0,n]}^i(V) \cup K_{[0,0,n]}(V), \quad K_{[0,0,l]}(V) \subseteq_{\text{str}} K_{[0,0,l-1]}(V) \text{ for } 2 \leq l \leq n,$$

and

$$I_{[0,0,n]}^1(V) \prec_{\text{str}} I_{[0,0,n]}^2(V) \prec_{\text{str}} \dots \prec_{\text{str}} I_{[0,0,n]}^{n-1}(V) \prec_{\text{str}} K_{[0,0,n]}(V).$$

The structure is sketched in Fig. 2.

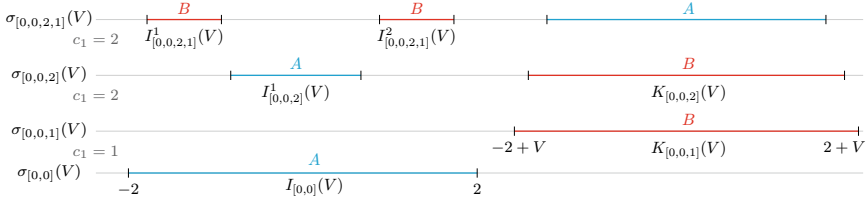


Fig. 2 The first spectral bands defined in Example 4.20

Corollary 4.21 *Let $V > 4$ and $\mathbf{c}' = [0, c_0, c_1, \dots, c_k] \in \mathcal{C}$ be such that $c_k \geq 1$ if $k \geq 1$ and $\varphi(\mathbf{c}') \in [0, 1]$. Consider a spectral band J in $\sigma_{\mathbf{c}'}(V)$.*

(a) *If J is of weak backward type A, then J is of backward type A and either*

- $J = [-2, 2]$ and $\varphi(\mathbf{c}') = 0$, or
- *there is a unique spectral band $I_{\mathbf{c}}$ in $\sigma_{\mathbf{c}}(V)$ with $\mathbf{c} = [0, c_0, c_1, \dots, c_{k-1}]$ and a $1 \leq i \leq M$ (where $M = c_k - 1$ if $I_{\mathbf{c}}$ is of type A and $M = c_k$ if $I_{\mathbf{c}}$ is of type B) such that $J = I_{[\mathbf{c}, m]}^i$ with $m = c_k$ where the latter is the unique i th spectral band associated with $I_{\mathbf{c}}$ defined in (A).*

(b) *If J is of weak backward type B, then J is of backward type B and either*

- $J = K_{[0,0,n]}$ from Example 4.20, $\varphi(\mathbf{c}) = \frac{1}{n}$ and $k = 1$, or
- *there is a unique spectral band $I_{\mathbf{c}}$ in $\sigma_{\mathbf{c}}(V)$ with $\mathbf{c} = [0, c_0, c_1, \dots, c_{k-2}]$ and a $1 \leq j \leq M + 1$ (where $M = c_{k-1} - 1$ if $I_{\mathbf{c}}$ is of type A and $M = c_{k-1}$ if $I_{\mathbf{c}}$ is of type B) such that $J = I_{[\mathbf{c}, m, n]}^j$ with $m = c_{k-1}$, $n = c_k$ where the latter is the unique j th spectral band associated with $I_{\mathbf{c}}$ defined in (B).*

In addition, there is a unique spectral band $I_{[\mathbf{c}, c_{k-1}, 1]}$ in $\sigma_{[\mathbf{c}, c_{k-1}, 1]}(V)$ of type B such that either $J = I_{[\mathbf{c}, c_{k-1}, 1]}^j$ (if $c_k = 1$) or $J \subseteq_{\text{str}} I_{[\mathbf{c}, c_{k-1}, 1]}^j$ (if $c_k > 1$).

Proof Define $\mathbf{c} = [0, c_0, c_1, \dots, c_{k-1}]$.

(a) Let $J \subseteq \sigma_{\mathbf{c}'}(V)$ be of weak backward type A. Note first that $\sigma_{[0,0]}(V) = [-2, 2]$, where the corresponding spectral band is of type A, see Example 4.20. If $\varphi(\mathbf{c}') \in [0, 1]$, we conclude $k \geq 1$ and $\varphi([\mathbf{c}', 0]) = \varphi(\mathbf{c}) \geq 0$. Then there is a spectral band $I_{\mathbf{c}} \subseteq \sigma_{\mathbf{c}}(V)$ with $J \subseteq I_{\mathbf{c}}$. By Corollary 4.11, $I_{\mathbf{c}}$ is either of weak backward type A or B. Thus, Proposition 4.18(a) implies the statement and, in particular, the uniqueness of the bands $\{I_{[\mathbf{c}, m]}^i(V)\}_{i=1}^M$ for $m = c_k$.

(b) If $k = 0$, then $\mathbf{c}' = [0, 0]$ and the spectral band in $\sigma_{[0,0]}(V)$ is of type A, see Example 4.20. If $k = 1$, then $\mathbf{c}' = [0, 0, n]$ with $n \geq 1$ by assumption. Thus, the only spectral band $J \subseteq \sigma_{\mathbf{c}'}(V)$ of weak backward type B is the spectral band $K_{[0,0,n]}$ described in Example 4.20. Hence, $J = K_{[0,0,n]}$ follows satisfying $K_{[0,0,n]} \subseteq K_{[0,0,1]} = [-2 + V, 2 + V] = \sigma_{[0,0,1]}(V)$, where $K_{[0,0,1]}$ is of type B. Note that $K_{[0,0,n]} \subseteq_{\text{str}} K_{[0,0,1]}$ if $n > 1$ and else $K_{[0,0,n]} = K_{[0,0,1]}$.

Next, we treat the case $k \geq 2$ with $c_k \geq 1$. If $c_k = 1$, then $\sigma_{[\mathbf{c}', -1]}(V) = \sigma_{\mathbf{c}}(V)$ holds by Lemma 3.6. Thus, there is a spectral band $I_{\mathbf{c}} \subseteq \sigma_{\mathbf{c}}(V)$ such that $J \subseteq_{\text{str}} I_{\mathbf{c}}$. Set

$m = c_{k-1}$. Observe that J is a spectral band in $\sigma_{[c, m, 1]}(V)$. Thus, Proposition 4.18(b) implies $J = I_{[c, m, c_1]}^j$ for some $1 \leq j \leq M + 1$.

If $c_k \geq 2$, then $\sigma_{[c', -1]}(V) = \sigma_{[c, c_{k-1}, c_k - 1]}(V)$ where $c_k - 1 \geq 1$. Thus, there is a spectral band $J_{c_k - 1}$ in $\sigma_{[c, c_{k-1}, c_k - 1]}(V) = \sigma_{[c', -1]}(V)$ with $J \subseteq J_{c_k - 1}$. Since $V > 4$, Corollary 4.11 asserts that $J_{c_k - 1}$ is either of weak backward type A or B . We claim that $J_{c_k - 1}$ is of weak backward type B . Therefore assume toward contradiction that $J_{c_k - 1}$ is of weak backward type A . Then $J_{c_k - 1} \subseteq \sigma_{[c, c_{k-1}, c_k - 1, 0]}(V) = \sigma_{[c', 0]}(V)$ follows. Thus, $J \subseteq \sigma_{c'}(V)$, $J \subseteq \sigma_{[c', 0]}(V)$, and $J \subseteq \sigma_{[c', -1]}(V)$ while $J \neq \emptyset$, contradicting Proposition 4.7 using $V > 4$. Hence, $J_{c_k - 1}$ is of weak backward type B . Thus, we can inductively conclude that there are spectral bands J_l in $\sigma_{[c, c_{k-1}, l]}(V)$ of weak backward type B for all $1 \leq l \leq c_k - 1$ such that

$$J \subseteq J_{c_k - 1} \subseteq J_{c_k - 2} \subseteq \dots \subseteq J_1.$$

Since $J_1 \subseteq \sigma_{[c, c_{k-1}, 1]}(V)$ is of weak backward type B , J_1 is included in a spectral band I_c in $\sigma_c(V)$. Set $m = c_{k-1}$ and $n = c_k$. Observe that J is a spectral band in $\sigma_{[c, m, n]}(V)$ and I_c is either of weak backward type A or B . Thus, Proposition 4.18(b) implies $J = I_{[c, m, n]}^j$ for some $1 \leq j \leq M + 1$. In particular, $J = I_{[c, c_{k-1}, 1]}^j$ if $n = c_k = 1$ and $J \subseteq_{\text{str}} I_{[c, c_{k-1}, 1]}^j$ if $n = c_k > 1$. \square

Theorem 4.22 *For all $V > 4$ and $c \in \mathcal{C}$ with $[c, m] \in \mathcal{C}$ for all $m \in \mathbb{N}$, every spectral band in $\sigma_c(V)$ is either of type A or B and its type is independent of the value of $V > 4$. In addition, for every spectral band $I_c(V)$ in $\sigma_c(V)$ and all $m, n \in \mathbb{N}$, the spectral bands $\{I_{[c, m]}^i(V)\}_{i=1}^M$ and $\{I_{[c, m, n]}^j(V)\}_{j=1}^{M+1}$ mentioned in the m -forward definition (Definition 4.13) are unique and the strong interlacing property (I_{str}) holds.*

Remark Theorem 4.22 collects all the previous statements of this section. This result is comparable to [39, Lemma 3.3], as was discussed before. The independence of the spectral band type in the value of $V > 4$ was not explicitly mentioned in [39, Lemma 3.3]. Showing this is based on combining a continuity argument and the three intersection property (Proposition 4.7). Further discussions on the role of this independence may be found in [3].

Proof Let $V > 4$ and $c \in \mathcal{C}$ be such that $[c, m] \in \mathcal{C}$ for all $m \in \mathbb{N}$. Let $I_c(V)$ be a spectral band in $\sigma_c(V)$. By Corollary 4.11, we have that $I_c(V)$ has a well-defined weak backward type (either A or B) for all $V > 4$. Suppose $I_c(V)$ is of weak backward type A (respectively, B). Then Proposition 4.18 implies that $I_c(V)$ is of m -forward type A (respectively, m -forward type B) for all $m \in \mathbb{N}$. In addition, Corollary 4.21 asserts that $I_c(V)$ is also of backward type A (respectively, B). Hence, $I_c(V)$ is of type A (respectively, B).

According to the previous considerations, $I_c(V)$ is either of type A or B for each $V > 4$. We explain now why this type is independent on the value of V (as long as $V > 4$). Therefore observe that it suffices to prove that if $I_c(V_0)$ is of type A (respectively, B) for one $V_0 > 4$, then $I_c(V)$ is of type A (respectively, B) for all $V > 4$. Assume toward contradiction this is not the case. Then there is a $V_0 > 4$ and

a sequence $\{V_n\}_{n \in \mathbb{N}} \subseteq (4, \infty)$ such that $\lim_{n \rightarrow \infty} V_n = V_0$ and the type of $I_c(V_0)$ is different to the type $I_c(V_n)$ for all $n \in \mathbb{N}$. Without loss of generality assume $I_c(V_0)$ is of type A and $I_c(V_n)$ is of type B for all $n \in \mathbb{N}$ (the other case is treated similarly). In particular, $I_c(V_0) \subseteq \sigma_{[c,0]}(V_0)$ and $I_c(V_n) \subseteq \sigma_{[c,-1]}(V_n)$ for all $n \in \mathbb{N}$. In order to continue, we need the following observations.

Let $c' \in \mathcal{C}$. For $V \in \mathbb{R}$, the preimage $t_{c'}(\cdot, V)^{-1}(\{\pm 2\})$ coincides with the edges of the spectral bands, confer the discussion at Proposition 3.5. Thus, if $J(V) = [a(V), b(V)]$ is a spectral band of $\sigma_{c'}(V)$, then $|t_{c'}(a(V), V)| = 2 = |t_{c'}(b(V), V)|$. From the definition of $t_{c'}$, it is immediate that $(4, \infty) \ni V \mapsto a(V) \in \mathbb{R}$ and $(4, \infty) \ni V \mapsto b(V) \in \mathbb{R}$ are continuous. Note that indeed these edges are continuous on $V \in \mathbb{R} \setminus \{0\}$, see also a discussion in [3, cor. 3.2]. Thus, $(4, \infty) \ni V \mapsto \sigma_{c'}(V)$ is also continuous (as a finite union of intervals with continuous edges) in the Hausdorff metric.

Let $I_c(V) = [a(V), b(V)]$. By assumption, we have $a(V_0) \in I_c(V_0) \subseteq \sigma_{[c,0]}(V_0)$ and $a(V_n) \in I_c(V_n) \subseteq \sigma_{[c,-1]}(V_n)$ for all $n \in \mathbb{N}$. By continuity of $V \mapsto a(V)$, $V \mapsto \sigma_{[c,0]}(V)$ and $V \mapsto \sigma_{[c,-1]}(V)$, we conclude

$$\sigma_{[c,0]}(V_0) \ni a(V_0) = \lim_{n \rightarrow \infty} a(V_n) \in \lim_{n \rightarrow \infty} \sigma_{[c,-1]}(V_n) = \sigma_{[c,-1]}(V_0).$$

Thus, $a(V_0) \in \sigma_c(V_0) \cap \sigma_{[c,0]}(V_0) \cap \sigma_{[c,-1]}(V_0)$ follows contradicting Proposition 4.7 and $V > 4$. \square

5 The Integrated Density of State for Sturmian Hamiltonian

A Sturmian Hamiltonian, $H_{\alpha,V}$ with $\alpha \notin \mathbb{Q}$ gives rise to periodic Hamiltonians $H_{q,V}^p$ whose spectra converge to $\sigma(H_{\alpha,V})$ (Proposition 4.6). The spectra of these periodic operators exhibit a special structure, as is described in the previous section and summarized in Theorem 4.22. We employ it in this section in order to study the integrated density of states of $H_{\alpha,V}$ for $V > 4$.

5.1 A Light Introduction to the Integrated Density of States and Its Gap Labels

We briefly introduce the integrated density of states for the Sturmian Hamiltonian, $H_{\alpha,V}$. First, restricting $H_{\alpha,V}$ to $\ell^2(\{1, \dots, n\})$, we obtain a Hermitian $n \times n$ matrix, denoted by $H_{\alpha,V}|_{[1,n]}$. We denote its set of n eigenvalues by $\sigma(H_{\alpha,V}|_{[1,n]})$ and use it to define

$$N_{\alpha,V}(E) := \lim_{n \rightarrow \infty} \frac{\#\left\{\lambda \in \sigma\left(H_{\alpha,V}|_{[1,n]}\right) : \lambda \leq E\right\}}{n}. \quad (5.1)$$

The limit in (5.1) is known to exist for all $\alpha \in [0, 1] \setminus \mathbb{Q}$, $V \in \mathbb{R}$ and $E \in \mathbb{R}$, see, e.g., [16, 25, 42]. The function $E \mapsto N_{\alpha, V}(E)$ is called the integrated density of states (IDS) of $H_{\alpha, V}$. There are a few equivalent ways to define the IDS in our case. Here, we choose the way which is computationally the most convenient within the framework developed in this paper. This definition of the IDS is common in the physics literature. Within the mathematics literature, it is also known by the name the integrated (normalized) empirical spectral distribution. Two fundamental properties of the IDS in our setting are

(IDS1) The IDS $N_{\alpha, V} : \mathbb{R} \rightarrow [0, 1]$ is a monotone, non-decreasing, and a continuous function.

(IDS2) We have $E \in \mathbb{R} \setminus \sigma(H_{\alpha, V})$ if and only if there exists an $\varepsilon > 0$ such that the restriction $N_{\alpha, V}$ is constant on $(E - \varepsilon, E + \varepsilon)$.

In particular, we have that the IDS is constant on the spectral gaps, i.e., on the connected components of $\mathbb{R} \setminus \sigma(H_{\alpha, V})$. The values that the IDS attains at the gaps are also called the gap labels. The gap labeling theory is a general theory [1, 4, 17], which predicts the set of all possible gap labels of an operator. Applying the gap labeling theory to $H_{\alpha, V}$ leads to the following assertion.

Proposition 5.1 *For all $\alpha \in [0, 1] \setminus \mathbb{Q}$ and $V \in \mathbb{R} \setminus \{0\}$,*

$$\{N_{\alpha, V}(E) : E \in \mathbb{R} \setminus \sigma(H_{\alpha, V})\} \subseteq \{l\alpha \bmod 1 : l \in \mathbb{Z}\} \cup \{1\}.$$

The question which was raised by Mark Kac (though in the context of the almost Mathieu operator) is whether there is an equality above, or in his words, “Are all gaps there?”. Since then this problem was given the name “The Dry Ten Martini Problem” [42]. It is shown in Theorem 5.25 that there is indeed equality if $V > 4$ (in [3] this result is extended to all $V \neq 0$).

As a first step toward the proof of Theorem 5.25, we show how the definition of the IDS in (5.1) may be restated in terms of the spectral bands of the periodic approximations $H_{\frac{p_k}{q_k}, V}$, as presented previously. Therefore, note that $\{E\} = [E, E]$ is an interval and so we can use the notation $I \prec_{\text{str}} \{E\}$ for another interval I .

Proposition 5.2 *Let $V \in \mathbb{R} \setminus \{0\}$ and $\alpha \in [0, 1] \setminus \mathbb{Q}$ with continued fraction expansion $(c_k)_{k=0}^\infty$. Consider its convergents $\varphi([0, c_0, \dots, c_k]) = \frac{p_k}{q_k}$, $k \in \mathbb{N}$ with p_k, q_k coprime. Then for all $E \in \mathbb{R}$, we have*

$$N_{\alpha, V}(E) = \lim_{k \rightarrow \infty} \frac{\#\{I : I \text{ is a spectral band of } \sigma(H_{\frac{p_k}{q_k}, V}) \text{ with } I \prec_{\text{str}} \{E\}\}}{q_k}. \quad (5.2)$$

Proof We start by noting that the words $(\omega_\alpha(1), \dots, \omega_\alpha(q_k))$ and $(\omega_{\frac{p_k}{q_k}}(1), \dots, \omega_{\frac{p_k}{q_k}}(q_k))$ are equal up to a cyclic shift. This can be deduced, for example, by combining Lemma 2.4 with [31, Proposition 2.2.24] (using that our words W_k are the words s_k in [31, Proposition 2.2.24] up to a cyclic shift). This means that the

matrices $H_{\alpha,V}|_{[1,q_k]}$ and $H_{\frac{p_k}{q_k},V}|_{[1,q_k]}$ are unitarily equivalent (since their diagonals are equal up to a cyclic shift). Using this observation and passing to the subsequence $n_k := q_k$, $k \in \mathbb{N}$, in the limit of (5.1) yields

$$\begin{aligned} N_{\alpha,V}(E) &= \lim_{k \rightarrow \infty} \frac{\#\left\{\lambda \in \sigma\left(H_{\alpha,V}|_{[1,q_k]}\right) : \lambda \leq E\right\}}{q_k} \\ &= \lim_{k \rightarrow \infty} \frac{\#\left\{\lambda \in \sigma\left(H_{\frac{p_k}{q_k},V}|_{[1,q_k]}\right) : \lambda \leq E\right\}}{q_k}. \end{aligned}$$

At this point the reader is referred to Sect. 7 and, in particular, Proposition 7.1 where the Floquet–Bloch theory is summarized. Assigning to each $H_{\frac{p_k}{q_k},V}$ a $q_k \times q_k$ -Hermitian matrix $H_{\mathbf{c}_k,V}(\theta)$ with $\theta \in [0, \pi]$, the union (over $\theta \in [0, \pi]$) of these matrices eigenvalues equals to $\sigma_{\mathbf{c}_k}(V) = \sigma(H_{\frac{p_k}{q_k},V})$, see Proposition 7.1. From now on, set $\theta = 0$. The matrices $H_{\frac{p_k}{q_k},V}|_{[1,q_k]}$ and $H_{\mathbf{c}_k,V}(0)$ differ by a matrix of rank two using Eq. (7.1). Hence, the counting functions $\#\left\{\lambda \in \sigma\left(H_{\frac{p_k}{q_k},V}|_{[1,q_k]}\right) : \lambda \leq E\right\}$ and $\#\left\{\lambda \in \sigma\left(H_{\mathbf{c}_k,V}(0)\right) : \lambda \leq E\right\}$ differ by at most two.² Hence, we may replace the numerator in the limit above to get

$$N_{\alpha,V}(E) = \lim_{k \rightarrow \infty} \frac{\#\left\{\lambda \in \sigma\left(H_{\mathbf{c}_k,V}(0)\right) : \lambda \leq E\right\}}{q_k}.$$

According to Proposition 7.1 and, in particular, Eq. (7.3), $H_{\mathbf{c}_k,V}(0)$ has exactly one eigenvalue in each spectral band $\sigma_{\mathbf{c}_k}(V)$. Thus, the number of spectral bands I in $\sigma_{\mathbf{c}_k}(V) = \sigma(H_{\frac{p_k}{q_k},V})$ satisfying $I \prec_{\text{str}} \{E\}$ differs at most by one from $\#\left\{\lambda \in \sigma\left(H_{\mathbf{c}_k,V}(0)\right) : \lambda \leq E\right\}$. Hence, (5.2) follows. \square

Remark The equivalence between (5.1) and (5.2) was conjectured in [10, Sect. 5]. An explanation of this equivalence is given at the end of Section 2 in [39]. The proof above contains an elaborated argument.³

² To be more precise, the difference is a traceless matrix of rank two. By appropriately applying perturbation theory one can show that this results in at most a difference of one in the eigenvalue counting, see, e.g., [3, Corollary III.2].

³ The denominators in (5.1) and (5.2) may differ by one, even if E is in a spectral gap, as opposed to what is written in [39]. This was also pointed out to LR by Mark Embree. However, this does not affect the value to which the limit converges.

5.2 Symbolic Representation (Coding) of the Periodic Spectra

Fix $\alpha \notin \mathbb{Q}$ and consider the spectrum $\sigma(H_{\alpha,V})$ for $V > 4$. We use the spectra of periodic operators to provide covers of $\sigma(H_{\alpha,V})$ allowing us to represent the IDS as a power series, see Eq. (5.5) in Sect. 5.3. Toward this we define.

Definition 5.3 For $\mathbf{c} \in \mathcal{C}$ with $[\mathbf{c}, 1] \in \mathcal{C}$ we define the level $L_{\mathbf{c},V}$ by

$$L_{\mathbf{c},V} := \left\{ I : \begin{array}{l} I \text{ is a spectral band of } \sigma_{\mathbf{c}}(V) \text{ of type } A \text{ or } B \text{ or} \\ I \text{ is a spectral band of } \sigma_{[\mathbf{c},1]}(V) \text{ of type } B \end{array} \right\}.$$

We equip the set $L_{\mathbf{c},V}$ with the order relation \prec_{str} , i.e., $[a, b] \prec_{\text{str}} [c, d]$ if $b < c$, which was already introduced before Definition 4.13. This is in fact a total order relation on $L_{\mathbf{c},V}$ if $V > 4$, as is shown next in Lemma 5.4.

Let us first consider some examples. The lowest level is $L_{[0,0],V} = \{[-2, 2], [V - 2, V + 2]\}$. Observe that if $V > 4$, then $[-2, 2] \prec_{\text{str}} [V - 2, V + 2]$. A sketch of $L_{[0,0],V}$ and other sets can be found in Fig. 3. Observe that $L_{[0,0],V}$ and $L_{[0,0,1],V}$ both contain the interval $[-2 + V, 2 + V]$. Thus, these sets $L_{[0,0],V}$ and $L_{[0,0,1],V}$ are not disjoint, in general.

Lemma 5.4 Let $V > 4$ and $\mathbf{c}, [\mathbf{c}, 1] \in \mathcal{C}$. Then, for all $I, I' \in L_{\mathbf{c},V}$, we either have $I = I'$ or $I \cap I' = \emptyset$. In particular, $(L_{\mathbf{c},V}, \prec_{\text{str}})$ is totally ordered.

Proof Let $I, I' \in L_{\mathbf{c},V}$. We only need to show that $I \cap I' = \emptyset$, since then either $I \prec_{\text{str}} I'$ or $I' \prec_{\text{str}} I$ follows. If I, I' are both spectral bands of $\sigma_{\mathbf{c}}(V)$, respectively, $\sigma_{[\mathbf{c},1]}(V)$, then $I \cap I' = \emptyset$ as they are disjoint connected components of the same spectrum, see Proposition 4.1. Otherwise, assume $I \subseteq \sigma_{\mathbf{c}}(V)$ and $I' \subseteq \sigma_{[\mathbf{c},1]}(V)$. Then I' is necessarily of type B and, in particular, (by the backward type B property)

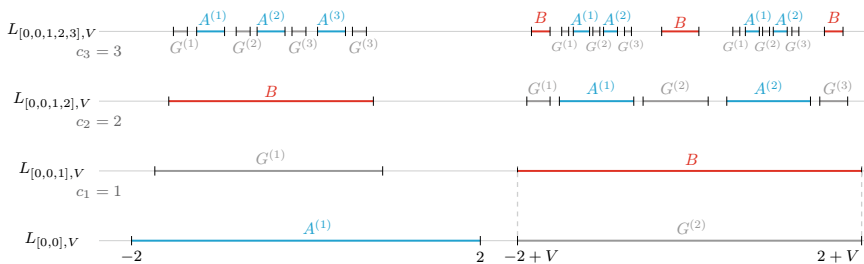


Fig. 3 Visualization of the sets $L_{\mathbf{c},V}$ for some $\mathbf{c} \in \mathcal{C}$. A label $A^{(i)}$, B or $G^{(i)}$ is assigned to each spectral band. This label assignment describes the coding map b_V from Proposition 5.8 for this particular case

there exists a spectral band $J' \subseteq \sigma_{[\mathbf{c}, 1, -1]}(V)$ such that $I' \subseteq J'$. But $\sigma_{[\mathbf{c}, 1, -1]}(V) = \sigma_{[\mathbf{c}, 0]}(V)$ and by Proposition 4.7 we have

$$\sigma_{\mathbf{c}}(V) \cap \sigma_{[\mathbf{c}, 1]}(V) \cap \sigma_{[\mathbf{c}, 0]}(V) = \emptyset,$$

so that $I \cap I' = I \cap J' \cap I' = \emptyset$. \square

Let $\alpha \in [0, 1] \setminus \mathbb{Q}$ with continued fraction expansion given by $(c_k)_{k=0}^\infty$. Define the finite continued fraction expansions $\mathbf{c}_k := [0, c_0, c_1, \dots, c_k] \in \mathcal{C}$ for $k \in \mathbb{N}_0$. In the following, we say $L_{\mathbf{c}_k, V}$ is a cover of a set $A \subseteq \mathbb{R}$ if $A \subseteq \bigcup_{I \in L_{\mathbf{c}_k, V}} I$.

Lemma 5.5 *Let $V > 4$ and $\alpha \in [0, 1] \setminus \mathbb{Q}$ with continued fraction expansion $(c_k)_{k=0}^\infty$ and $\mathbf{c}_k := [0, c_0, c_1, \dots, c_k] \in \mathcal{C}$ for $k \in \mathbb{N}_0$. Then the following holds.*

- (a) *For all $k \in \mathbb{N}_0$, $L_{\mathbf{c}_k, V}$ is a cover of $L_{\mathbf{c}_{k+1}, V}$.*
- (b) *For all $k \in \mathbb{N}_0$, $L_{\mathbf{c}_k, V}$ is a cover of $\sigma(H_{\alpha, V})$.*
- (c) *For all $k \in \mathbb{N}_0$, $\Lambda_k(V) := \sigma_{\mathbf{c}_k}(V) \cup \sigma_{[\mathbf{c}_k, 1]}(V) = \bigcup_{I \in L_{\mathbf{c}_k, V}} I$. Furthermore, $\lim_{k \rightarrow \infty} \bigcup_{I \in L_{\mathbf{c}_k, V}} I = \bigcap_{k \in \mathbb{N}_0} \Lambda_k(V) = \sigma(H_{\alpha, V})$ where the limit is taken in the Hausdorff metric.*

Proof If $I \subseteq \sigma_{[\mathbf{c}_{k+1}, 1]}(V)$ is of type B , then it is contained in $\sigma_{[\mathbf{c}_{k+1}, 1, -1]}(V) = \sigma_{\mathbf{c}_k}(V)$ using Lemma 3.6 and Corollary 3.7. Thus, $L_{\mathbf{c}_k, V}$ covers I and so $L_{\mathbf{c}_k, V}$ is a cover of all spectral bands in $\sigma_{[\mathbf{c}_{k+1}, 1]}(V)$ of type B . If $I \subseteq \sigma_{\mathbf{c}_{k+1}}(V)$ is of type A , then it is contained in $\sigma_{[\mathbf{c}_{k+1}, 0]}(V) = \sigma_{\mathbf{c}_k}(V)$ using Lemma 3.6 and Corollary 3.7. Thus, $L_{\mathbf{c}_k, V}$ covers I . If $I \subseteq \sigma_{\mathbf{c}_{k+1}}(V)$ is of type B , then Corollary 4.21(b) implies that there is a $J \subseteq \sigma_{[\mathbf{c}_k, 1]}(V)$ of type B with $I \subseteq J$. Thus, $L_{\mathbf{c}_k, V}$ covers I as well. Combined with the previous considerations, we obtain that $L_{\mathbf{c}_k, V}$ is a cover of $\sigma_{\mathbf{c}_{k+1}}(V)$ and all spectral bands in $\sigma_{[\mathbf{c}_{k+1}, 1]}(V)$ of type B , namely, $L_{\mathbf{c}_k, V}$ is a cover of $L_{\mathbf{c}_{k+1}, V}$. Thus, (a) is proven.

Having this, (b) follows from Proposition 4.6.

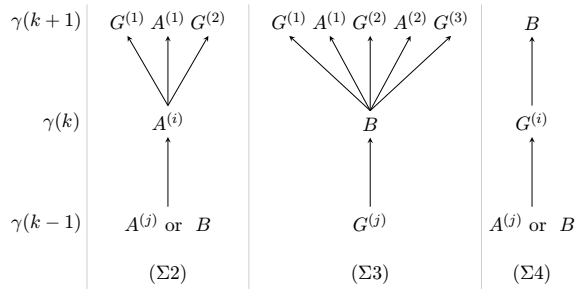
By definition, we have $\bigcup_{I \in L_{\mathbf{c}_k, V}} I \subseteq \Lambda_k(V)$. Moreover, every spectral band of $\sigma_{[\mathbf{c}_k, 1]}(V)$ of type A is contained in $\sigma_{\mathbf{c}_k}(V)$. Thus, $\bigcup_{I \in L_{\mathbf{c}_k, V}} I = \Lambda_k(V)$ and now (c) follows from Proposition 4.6. \square

By the first part of the last lemma, every spectral band of $L_{\mathbf{c}_{k+1}, V}$ is contained in a unique spectral band of $L_{\mathbf{c}_k, V}$. We may use this in order to construct a symbolic representation (coding) of each spectral band in level $L_{\mathbf{c}_k, V}$ in terms of the spectral bands in all previous levels in which it is recursively included.

Definition 5.6 Let $\alpha \in [0, 1] \setminus \mathbb{Q}$ with continued fraction expansion $(c_k)_{k=0}^\infty$ and $\mathbf{c}_k := [0, c_0, c_1, \dots, c_k] \in \mathcal{C}$ for $k \in \mathbb{N}_0$. Consider the countable alphabet $\mathcal{A} := \{A^{(i)} : i \in \mathbb{N}\} \cup \{G^{(i)} : i \in \mathbb{N}\} \cup \{B\}$. A (finite or infinite) *spectral- α -code* is either a finite sequence $\gamma = (\gamma(0), \gamma(1), \dots, \gamma(k)) \in \mathcal{A}^{k+1}$ or an infinite sequence $\gamma = (\gamma(0), \gamma(1), \dots) \in \mathcal{A}^{\mathbb{N}_0}$ satisfying the following:

$$(\Sigma 1) \quad \gamma(0) \in \{A^{(1)}, G^{(2)}\}.$$

Fig. 4 Visualization of the properties $(\Sigma 2)$, $(\Sigma 3)$, $(\Sigma 4)$ with $c_{k+1} = 2$. Each figure shows the possible descendants $\gamma(k+1)$ of $\gamma(k)$ as well as from which element in \mathcal{A} , the element $\gamma(k)$ could come from



(Σ2) If $\gamma(j) \in \{A^{(i)} : i \in \mathbb{N}\}$ then $\gamma(j+1) \in \{A^{(i)} : 1 \leq i \leq c_{j+1} - 1\} \cup \{G^{(i)} : 1 \leq i \leq c_{j+1}\}$.

(Σ3) If $\gamma(j) = B$ then $\gamma(j+1) \in \{A^{(i)} : 1 \leq i \leq c_{j+1}\} \cup \{G^{(i)} : 1 \leq i \leq c_{j+1} + 1\}$.

(Σ4) If $\gamma(j) \in \{G^{(i)} : i \in \mathbb{N}\}$ then $\gamma(j+1) = B$.

The set of all infinite spectral- α -codes will be denoted as Σ_α . Similarly, the set of all spectral- α -codes in \mathcal{A}^{k+1} is denoted by $\Sigma_{\mathbf{c}_k}$. Moreover, the set $\Sigma_{\mathbf{c}_k}^{\text{spec}} \subseteq \Sigma_{\mathbf{c}_k}$ is defined as those $\gamma = (\gamma(0), \dots, \gamma(k)) \in \Sigma_{\mathbf{c}_k}$, who additionally satisfy

(Σ5) $\gamma(k) \in \{A^{(i)} : i \in \mathbb{N}\} \cup \{B\}$.

A depiction of conditions (Σ2) – (Σ4) in Definition 5.6 appears in Fig. 4.

Remark 5.7 There is a merit in embedding all the codes defined above in a tree graph. Our depiction of the codes in Figs. 4 and 5 uses this point of view. The tree representation explicitly appears in [3] using a directed rooted tree with a strict (i.e., irreflexive) partial order relation defined on its vertex set. It is called the *spectral- α -tree* in [3]. Here, we confine ourselves to the original presentation of [39] using the symbolic representation of codes (and appeal to the tree only via the figures). Finally, we note that in [3] the vertices of the tree graph are labeled only by A and B , as opposed to using also the label $G^{(i)}$ in the current paper.

The previous definition is in close relation with the forward property of a spectral band, see Definition 4.13. This is made precise in Proposition 5.8. Before, we define a partial order \leq on $\mathcal{A} := \{A^{(i)} : i \in \mathbb{N}\} \cup \{G^{(i)} : i \in \mathbb{N}\} \cup \{B\}$ by setting

$$G^{(1)} \leq A^{(1)} \leq G^{(2)} \leq A^{(2)} \leq \dots$$

Let $\alpha \in [0, 1] \setminus \mathbb{Q}$ with infinite continued fraction expansion $(c_k)_{k=0}^\infty$, convergents $\varphi(\mathbf{c}_k)$ and $\mathbf{c}_k = [0, c_0, c_1, \dots, c_k] \in \mathcal{C}$ for $k \in \mathbb{N}_0$. If $\gamma, \eta \in \bigsqcup_{k \in \mathbb{N}_0} \Sigma_{\mathbf{c}_k} \cup \Sigma_\alpha$, define

$$\gamma \leq \eta : \iff \begin{cases} \gamma(0) \leq \eta(0), \text{ or} \\ \gamma(j) = \eta(j) \text{ and } \gamma(j+1) \leq \eta(j+1) \text{ for some } j \in \mathbb{N}_0. \end{cases}$$

This defines a partial order on $\bigsqcup_{k \in \mathbb{N}_0} \Sigma_{\mathbf{c}_k}$, respectively, Σ_α . We continue defining an encoding of $\bigcup_{k \in \mathbb{N}_0} L_{\mathbf{c}_k, V}$ via the spectral- α -codes $\bigsqcup_{k \in \mathbb{N}_0} \Sigma_{\mathbf{c}_k}$ preserving the partial order relations, the types, and inclusions. This statement deviates slightly from [39] and follows the lines of [3, Proposition 7.1]. The reader is referred to Fig. 3, where an example of some spectra is plotted together with the associated code as described in the following proposition.

Proposition 5.8 *Let $\alpha \in [0, 1] \setminus \mathbb{Q}$ with infinite continued fraction expansion $(c_k)_{k=0}^\infty$ and $\mathbf{c}_k = [0, c_0, c_1, \dots, c_k] \in \mathcal{C}$ for $k \in \mathbb{N}_0$. Then there exists for each $V > 4$, a unique map*

$$b_V : \bigsqcup_{k \in \mathbb{N}_0} \Sigma_{\mathbf{c}_k} \rightarrow \bigcup_{k \in \mathbb{N}_0} L_{\mathbf{c}_k, V}$$

with the following properties:

- (a) For each $k \in \mathbb{N}_0$, b_V bijectively maps $\Sigma_{\mathbf{c}_k}$ onto $L_{\mathbf{c}_k, V}$.
- (b) For each $k \in \mathbb{N}$, we have for all $\gamma \in \Sigma_{\mathbf{c}_{k-1}}$ and $\eta = (\eta(0), \dots, \eta(k)) \in \Sigma_{\mathbf{c}_k}$,

$$\gamma = (\eta(0), \dots, \eta(k-1)) \Leftrightarrow b_V(\eta) \subseteq b_V(\gamma) \Leftrightarrow b_V(\gamma) \cap b_V(\eta) \neq \emptyset.$$

- (c) Let $\gamma, \eta \in \bigsqcup_{k \in \mathbb{N}_0} \Sigma_{\mathbf{c}_k}$. Then $\gamma < \eta$ if and only if $b_V(\gamma) <_{\text{str}} b_V(\eta)$.

- (d) If $\gamma \in \Sigma_{\mathbf{c}_k}$ for some $k \in \mathbb{N}_0$, then

- (1) $\gamma(k) \in A^{(i)}$ if and only if $b_V(\gamma) \subseteq \sigma_{\mathbf{c}_k}(V)$ is of type A .
- (2) $\gamma(k) \in B$ if and only if $b_V(\gamma) \subseteq \sigma_{\mathbf{c}_k}(V)$ is of type B .
- (3) $\gamma(k) \in G^{(i)}$ if and only if $b_V(\gamma) \subseteq \sigma_{[\mathbf{c}_k, 1]}(V)$ is of type B and $b_V(\gamma) \cap \sigma_{\mathbf{c}_k}(V) = \emptyset$.

Remark 5.9 Note that Proposition 5.8(d) asserts that the spectral band $b_V(\gamma)$ for $\gamma \in \Sigma_{\mathbf{c}_k}$ is contained in a spectral gap of $\sigma_{\mathbf{c}_k}(V)$ if and only if $\gamma(k) = G^{(i)}$ for some $i \in \mathbb{N}$. This, in particular, explains the notation $G^{(i)}$ standing for a gap.

Proof We first note that every such map satisfying (a) and (c) must be unique since $\Sigma_{\mathbf{c}_k}$ is totally ordered and $L_{\mathbf{c}_k, V}$ is totally ordered by Lemma 5.4.

First, suppose that such a map exists and justify that the equivalence $b_V(\eta) \subseteq b_V(\gamma) \Leftrightarrow b_V(\gamma) \cap b_V(\eta) \neq \emptyset$ in (b) holds. Suppose $b_V(\gamma) \cap b_V(\eta) \neq \emptyset$ holds. Since $L_{\mathbf{c}_{k-1}, V}$ is a cover of $L_{\mathbf{c}_k, V}$ by Lemma 5.5, we conclude $b_V(\eta) \subseteq \bigcup_{I \in L_{\mathbf{c}_{k-1}, V}} I$. Since the spectral bands in $L_{\mathbf{c}_{k-1}, V}$ do not touch (Lemma 5.4) and $b_V(\gamma) \cap b_V(\eta) \neq \emptyset$, we conclude $b_V(\eta) \subseteq b_V(\gamma)$. The reverse implication is trivial.

We continue inductively defining the map b_V .

Induction base: If $k = 0$, we have $\mathbf{c}_0 = [0, 0]$, $\Sigma_{[0, 0]} = \{(A^{(1)}), (G^{(2)})\}$ and $L_{\mathbf{c}_0, V} = \{[-2, 2], [-2 + V, 2 + V]\}$, see also Example 4.20. Define $b_V(A^{(1)}) = [-2, 2]$ and $b_V(G^{(2)}) = [-2 + V, 2 + V]$ satisfying (a)–(d) for $V > 4$ by construction.

If $k = 1$, we have $\mathbf{c}_1 = [0, 0, c_1]$ where $c_1 \in \mathbb{N}$. By Example 4.20, we have

$$\sigma_{[0,0,c_1]}(V) = \bigcup_{j=1}^{c_1-1} I_{[0,0,c_1]}^j(V) \cup K_{[0,0,c_1]}(V)$$

where

$$I_{[0,0,c_1]}^1(V) \prec_{\text{str}} I_{[0,0,c_1]}^2(V) \prec_{\text{str}} \dots \prec_{\text{str}} I_{[0,0,c_1]}^{c_1-1}(V) \prec_{\text{str}} K_{[0,0,c_1]}(V)$$

and $I_{[0,0,c_1]}^j(V) \subseteq [-2, 2]$ are of type A and $K_{[0,0,c_1]}(V) \subseteq [-2 + V, 2 + V]$ is of type B . Since $\sigma_{[0,0,c_1,1,-1]}(V) = \sigma_{[0,0]}(V)$, every spectral band in $\sigma_{[0,0,c_1,1]}(V)$ of type B is contained in $\sigma_{[0,0]}(V) = [-2, 2]$. Applying Proposition 4.18 to the spectral band $[-2, 2]$ of type A with $m = c_1$ implies that the spectral bands of type B in $\sigma_{[0,0,c_1,1]}(V)$ are $\{J^i(V)\}_{i=1}^{c_1}$ with

$$J^1(V) \prec_{\text{str}} I_{[0,0,c_1]}^1(V) \prec_{\text{str}} J^2(V) \prec_{\text{str}} \dots \prec_{\text{str}} I_{[0,0,c_1]}^{c_1-1}(V) \prec_{\text{str}} J^{c_1}(V)$$

and $J^i(V) \subseteq [-2, 2]$. Thus,

$$L_{\mathbf{c}_1, V} = \{I_{[0,0,c_1]}^i(V) : 1 \leq i \leq c_1 - 1\} \cup \{J^i(V) : 1 \leq i \leq c_1\} \cup \{K_{[0,0,c_1]}(V)\}.$$

Since $J^{c_1}(V) \subseteq [-2, 2]$ and $K_{[0,0,c_1]}(V) \subseteq [-2 + V, 2 + V]$, we conclude $J^{c_1}(V) \prec_{\text{str}} K_{[0,0,c_1]}(V)$ using $V > 4$. In addition, we have

$$\Sigma_{\mathbf{c}_1} = \{(A^{(1)}, A^{(i)}) : 1 \leq i \leq c_1 - 1\} \cup \{(A^{(1)}, G^{(i)}) : 1 \leq i \leq c_1\} \cup \{(G^{(2)}, B)\}.$$

With this at hand, define $b_V((A^{(1)}, A^{(i)})) := I_{[0,0,c_1]}^i(V)$, $b_V((A^{(1)}, G^{(i)})) := J^i(V)$, and $b_V((G^{(2)}, B)) := K_{[0,0,c_1]}(V)$ satisfying (a)–(d) by construction.

Induction step: Let $k \geq 2$ be such that $b_V : \bigsqcup_{l=0}^k \Sigma_{\mathbf{c}_k} \rightarrow \bigcup_{l=0}^k L_{\mathbf{c}_k, V}$ satisfies (a)–(d). We show how to extend $b_V : \Sigma_{\mathbf{c}_{k+1}} \rightarrow L_{\mathbf{c}_{k+1}, V}$. Let $\gamma' = (\gamma(0), \dots, \gamma(k)) \in \Sigma_{\mathbf{c}_k}$.

If $\gamma(k) = A^{(l)}$, then set $M = c_{k+1} - 1$ and if $\gamma(k) = B$, then set $M = c_{k+1}$. By the induction hypothesis and property (d), $b_V(\gamma') \subseteq \sigma_{\mathbf{c}_k}(V)$ is of type A if $\gamma(k) = A^{(l)}$ and of type B if $\gamma(k) = B$. Thus, Proposition 4.18 implies that there are exactly $\{I_{\mathbf{c}_{k+1}}^i\}_{i=1}^M \subseteq \sigma_{\mathbf{c}_{k+1}}(V)$ of type A and $\{I_{[\mathbf{c}_{k+1}, 1]}^j\}_{j=1}^{M+1} \subseteq \sigma_{[\mathbf{c}_{k+1}, 1]}(V)$ of type B such that $I_{\mathbf{c}_{k+1}}^i, I_{[\mathbf{c}_{k+1}, 1]}^j \subseteq_{\text{str}} b_V(\gamma')$ and

$$I_{[\mathbf{c}_{k+1}, 1]}^1 \prec_{\text{str}} I_{\mathbf{c}_{k+1}}^1 \prec_{\text{str}} \dots \prec_{\text{str}} I_{\mathbf{c}_{k+1}}^M \prec_{\text{str}} I_{[\mathbf{c}_{k+1}, 1]}^{M+1}.$$

Furthermore, $(\Sigma 2)$ implies that all choices for $\gamma(k+1)$ are $\{A^{(i)} : 1 \leq i \leq M\} \cup \{G^{(j)} : 1 \leq j \leq M+1\}$. Then define for $\gamma = (\gamma(0), \dots, \gamma(k+1)) \in \Sigma_{\mathbf{c}_{k+1}}$,

$$b_V(\gamma) = \begin{cases} I_{\mathbf{c}_{k+1}}^i & \text{if } \gamma(k+1) = A^{(i)}, \\ I_{[\mathbf{c}_{k+1}, 1]}^j & \text{if } \gamma(k+1) = G^{(j)}. \end{cases}$$

Thus, $b_V(\gamma) \subseteq b_V(\gamma')$ holds, namely, this definition satisfies (b) as well as (d). Furthermore, let $\gamma_1 := (\gamma(0), \dots, \gamma(k), \gamma(k+1))$ and $\gamma_2 := (\gamma(0), \dots, \gamma(k), \eta(k+1))$ for $\gamma(k) \in \{A^{(i)}, B\}$ and $\gamma(k+1), \eta(k+1) \in \{A^{(i)} : 1 \leq i \leq M\} \cup \{G^{(j)} : 1 \leq j \leq M+1\}$. By construction, we conclude

$$\gamma_1 \leq \gamma_2 \Leftrightarrow b_V(\gamma_1) \prec_{\text{str}} b_V(\gamma_2). \quad (5.3)$$

If $\gamma(k) = G^{(l)}$, then the induction hypothesis and property (d) imply that $b_V(\gamma') \subseteq \sigma_{[\mathbf{c}_k, 1]}(V)$ is of type B and $b_V(\gamma') \cap \sigma_{\mathbf{c}_k}(V) = \emptyset$. Thus, Corollary 4.17 asserts that there is a unique spectral band $J \in \sigma_{\mathbf{c}_{k+1}}(V)$ of type B with $J \subseteq b_V(\gamma')$. Note that if $c_{k+1} = 1$, then $J = b_V(\gamma')$. Define $b_V(\gamma(0), \dots, \gamma(k+1)) := J$. This definition satisfies (b) as well as (d).

By the previous considerations, we have defined the map $b_V : \Sigma_{\mathbf{c}_{k+1}} \rightarrow L_{\mathbf{c}_{k+1}, V}$ and by construction it is injective and it satisfies (b) and (d). Next, we prove that $b_V : \Sigma_{\mathbf{c}_{k+1}} \rightarrow L_{\mathbf{c}_{k+1}, V}$ is also surjective. Therefore, let $J \in L_{\mathbf{c}_{k+1}, V}$.

If $J \subseteq \sigma_{\mathbf{c}_{k+1}}(V)$ is of type A , then Corollary 4.21(a) and $k \geq 2$ imply that there is a unique spectral band $I_{\mathbf{c}_k} \subseteq \sigma_{\mathbf{c}_k}(V)$ such that $J = I_{[\mathbf{c}_k, c_{k+1}]}^i$ for some $1 \leq i \leq M$ (where $M = c_{k+1} - 1$ if $I_{\mathbf{c}_k}$ is of type A and $M = c_{k+1}$ if $I_{\mathbf{c}_k}$ is of type B). Since $b_V : \Sigma_{\mathbf{c}_k} \rightarrow L_{\mathbf{c}_k, V}$ is bijective by induction hypothesis, there is a $\gamma = (\gamma(0), \dots, \gamma(k)) \in \Sigma_{\mathbf{c}_k}$ with $b_V(\gamma) = I_{\mathbf{c}_k}$. Moreover, property (d) asserts $\gamma(k) = A^{(i)}$ if $I_{\mathbf{c}_k}$ is of type A and $\gamma(k) = B$ if $I_{\mathbf{c}_k}$ is of type B . Hence, $\gamma' := (\gamma(0), \dots, \gamma(k), A^{(i)}) \in \Sigma_{\mathbf{c}_{k+1}}$ by $(\Sigma 2)$ or $(\Sigma 3)$ and $b_V(\gamma') = J = I_{[\mathbf{c}_k, c_{k+1}]}^i$.

If $J \subseteq \sigma_{[\mathbf{c}_{k+1}, 1]}(V)$ is of type B , then Corollary 4.21(b) and $k \geq 2$ imply that there is a unique spectral band $I_{\mathbf{c}_k} \subseteq \sigma_{\mathbf{c}_k}(V)$ such that $J = I_{[\mathbf{c}_k, c_{k+1}, 1]}^i$ for some $1 \leq i \leq M+1$ (where $M = c_{k+1} - 1$ if $I_{\mathbf{c}_k}$ is of type A and $M = c_{k+1}$ if $I_{\mathbf{c}_k}$ is of type B). Since $b_V : \Sigma_{\mathbf{c}_k} \rightarrow L_{\mathbf{c}_k, V}$ is bijective by induction hypothesis, there is a $\gamma = (\gamma(0), \dots, \gamma(k)) \in \Sigma_{\mathbf{c}_k}$ with $b_V(\gamma) = I_{\mathbf{c}_k}$. Moreover, property (d) asserts $\gamma(k) = A^{(i)}$ if $I_{\mathbf{c}_k}$ is of type A and $\gamma(k) = B$ if $I_{\mathbf{c}_k}$ is of type B . Hence, $\gamma' := (\gamma(0), \dots, \gamma(k), G^{(i)}) \in \Sigma_{\mathbf{c}_{k+1}}$ by $(\Sigma 2)$ or $(\Sigma 3)$ and $b_V(\gamma') = J = I_{[\mathbf{c}_k, c_{k+1}, 1]}^i$.

If $J \subseteq \sigma_{\mathbf{c}_{k+1}}(V)$ is of type B , then Corollary 4.21(b) implies that there is a unique spectral band $I_{[\mathbf{c}_k, 1]} \subseteq \sigma_{[\mathbf{c}_k, 1]}(V)$ of type B such that $J \subseteq I_{[\mathbf{c}_k, 1]}$. Since $b_V : \Sigma_{\mathbf{c}_k} \rightarrow L_{\mathbf{c}_k, V}$ is bijective by induction hypothesis, there is a $\gamma = (\gamma(0), \dots, \gamma(k)) \in \Sigma_{\mathbf{c}_k}$ with $b_V(\gamma) = I_{[\mathbf{c}_k, 1]}$. Moreover, property (d) asserts $\gamma(k) = G^{(l)}$. Thus, $\gamma' = (\gamma(0), \dots, \gamma(k), B) \in \Sigma_{\mathbf{c}_{k+1}}$ by $(\Sigma 4)$ and $b_V(\gamma') = J$.

It is left to prove that $b_V : \Sigma_{\mathbf{c}_{k+1}} \rightarrow L_{\mathbf{c}_{k+1}, V}$ satisfies (c). Let $\gamma, \eta \in \Sigma_{\mathbf{c}_{k+1}}$. We need to treat two cases. If $\gamma(k) = \eta(k)$, then the equivalence $\gamma \leq \eta \Leftrightarrow b_V(\gamma) \prec_{\text{str}} b_V(\eta)$ follows from (5.3). If $\gamma(k) \neq \eta(k)$, then there is a $0 \leq l \leq k-1$ such that $\gamma(j) = \eta(j)$ for all $j \leq l$ and $\gamma(l+1) \neq \eta(l+1)$. Since $l+1 \leq k$, the induction hypothesis and (c) yield the equivalence $\gamma' \leq \eta' \Leftrightarrow b_V(\gamma') \prec_{\text{str}} b_V(\eta')$ where $\gamma' = (\gamma(0), \dots, \gamma(l+1))$ and $\eta' = (\eta(0), \dots, \eta(l+1))$. Thus, $b_V(\gamma') \cap b_V(\eta') =$

\emptyset holds. By property (b), we have $b_V(\gamma) \subseteq b_V(\gamma')$ and $b_V(\eta) \subseteq b_V(\eta')$. Hence, the previous considerations imply that $\gamma < \eta$ if and only if $b_V(\gamma) <_{\text{str}} b_V(\eta)$ proving (c) for $b_V : \Sigma_{\mathbf{c}_{k+1}} \rightarrow L_{\mathbf{c}_{k+1}, V}$. \square

Corollary 5.10 *Let $\alpha \in [0, 1] \setminus \mathbb{Q}$ with infinite continued fraction expansion $(c_k)_{k=0}^\infty$ and $\mathbf{c}_k = [0, c_0, c_1, \dots, c_k] \in \mathcal{C}$ for $k \in \mathbb{N}_0$. For all $V > 4$ and $k \in \mathbb{N}_0$, the image $b_V(\Sigma_{\mathbf{c}_k}^{\text{spec}})$ equals to $\{I : I \text{ spectral band of } \sigma_{\mathbf{c}_k}(V)\}$.*

Proof This follows immediately from Proposition 5.8 and Theorem 4.22 asserting that every spectral band in $\sigma_{\mathbf{c}_k}(V)$ is either of type A or B if $V > 4$. \square

Now we can use the previous considerations, to assign to each infinite code in Σ_α an element in $\sigma(H_{\alpha, V})$.

Lemma 5.11 *Let $V > 4$ and $\alpha \in [0, 1] \setminus \mathbb{Q}$. For all $\gamma \in \Sigma_\alpha$, the set $\bigcap_{k \in \mathbb{N}_0} b_V(\gamma|_{[0, k]})$ contains exactly one element and $\bigcap_{k \in \mathbb{N}_0} b_V(\gamma|_{[0, k]}) \subseteq \sigma(H_{\alpha, V})$.*

Proof Consider the sequence $\{b_V(\gamma|_{[0, k]})\}_{k \in \mathbb{N}_0}$ of intervals. This is a decreasing nested sequence of non-empty closed intervals, see Proposition 5.8(b). Applying Cantor intersection theorem yields that $\bigcap_{k \in \mathbb{N}_0} b_V(\gamma|_{[0, k]})$ is non-empty. Furthermore, it must be closed and convex (as intersection of closed and convex sets). Hence, it may be either an interval or a single point. Lemma 5.5 asserts $b_V(\gamma|_{[0, k]}) \subseteq \bigcup_{I \in L_{\mathbf{c}_k, V}} I = \Sigma_k(V)$ and

$$\bigcap_{k \in \mathbb{N}_0} b_V(\gamma|_{[0, k]}) \subseteq \bigcap_{k \in \mathbb{N}_0} \Sigma_k(V) = \sigma(H_{\alpha, V}).$$

According to [8], $\sigma(H_{\alpha, V})$ is of Lebesgue measure zero if $V \neq 0$. Thus, $\sigma(H_{\alpha, V})$ cannot contain an interval, and therefore $\bigcap_{k \in \mathbb{N}_0} b_V(\gamma|_{[0, k]})$ is a single point (which is contained in $\sigma(H_{\alpha, V})$). \square

A consequence of this lemma is, that we now get a well-defined map $E_{\alpha, V} : \Sigma_\alpha \rightarrow \sigma(H_{\alpha, V})$ by setting $E_{\alpha, V}(\gamma)$ to be the unique element in $\bigcap_{k \in \mathbb{N}_0} b_V(\gamma|_{[0, k]})$, which exists by Lemma 5.11.

Lemma 5.12 *Let $V > 4$ and $\alpha \in [0, 1] \setminus \mathbb{Q}$. Then the map $E_{\alpha, V} : \Sigma_\alpha \rightarrow \sigma(H_{\alpha, V})$ is a bijection.*

Proof Let $\varphi(\mathbf{c}_k)$, $k \in \mathbb{N}_0$ be the convergents of α . For each $k \in \mathbb{N}$, we have $\sigma(H_{\alpha, V}) \subseteq \bigcup_{I \in L_{\mathbf{c}_k, V}} I$ by Lemma 5.5. Furthermore, if $E \in \sigma(H_{\alpha, V})$ is fixed, then for each $k \in \mathbb{N}$, there exists a unique $I \in L_{\mathbf{c}_k, V}$ such that $E \in I$, since the spectral bands in $L_{\mathbf{c}_k, V}$ are disjoint. By Proposition 5.8, $b_V : \Sigma_{\mathbf{c}_k} \rightarrow L_{\mathbf{c}_k, V}$ is a bijection for each $k \in \mathbb{N}$. Thus, there exists a unique $\gamma_k \in \Sigma_{\mathbf{c}_k}$ for each $k \in \mathbb{N}$ such that $E \in b_V(\gamma_k)$. Then $E \in b_V(\gamma_k) \cap b_V(\gamma_{k+1}) \neq \emptyset$ follows. Thus, Proposition 5.8(b) asserts $b_V(\gamma_{k+1}) \subseteq b_V(\gamma_k)$ and the codes γ_{k+1} and γ_k coincide on the first $k+1$ digits. Hence, we inductively conclude for all $j \geq k$, $b_V(\gamma_j) \subseteq b_V(\gamma_k)$ and the codes $\gamma_j \in \Sigma_j$ and $\gamma_k \in \Sigma_k$ coincide on the first $k+1$ digits. Since k and j were arbitrary, there is a unique $\gamma \in \Sigma_\alpha$ such that γ and γ_k have the same first $k+1$ digits for all $k \in \mathbb{N}$. We claim

$E_{\alpha,V}(\gamma) = E$. By definition of $E_{\alpha,V}$, we get $E_{\alpha,V}(\gamma) \in \bigcap_{k \in \mathbb{N}_0} b_V(\gamma_k)$. On the other hand, also $E \in \bigcap_{k \in \mathbb{N}_0} b_V(\gamma_k)$ follows from our choice of γ_k . The uniqueness from Lemma 5.11 then yields $E_{\alpha,V}(\gamma) = E$. \square

Lemma 5.13 *Let $V > 4$ and $\alpha \in [0, 1] \setminus \mathbb{Q}$, then the map $E_{\alpha,V} : \Sigma_\alpha \rightarrow \sigma(H_{\alpha,V})$ is order preserving, i.e., if $\gamma, \eta \in \Sigma_\alpha$, then*

$$\gamma \leq \eta \iff E_{\alpha,V}(\gamma) < E_{\alpha,V}(\eta).$$

Proof Let $\varphi(c_k), k \in \mathbb{N}_0$ be the convergents of α . Also let $\gamma, \eta \in \Sigma_\alpha$ with $\gamma \leq \eta$. Then there is some $k \in \mathbb{N}_0$ such that $\gamma|_{[0,k]} \leq \eta|_{[0,k]}$. Thus, Proposition 5.8(c) leads to

$$E_{\alpha,V}(\gamma) \in b_V(\gamma|_{[0,k]}) \prec_{\text{str}} b_V(\eta|_{[0,k]}) \ni E_{\alpha,V}(\eta),$$

implying $E_{\alpha,V}(\gamma) < E_{\alpha,V}(\eta)$.

Conversely, suppose $E_{\alpha,V}(\gamma) < E_{\alpha,V}(\eta)$, then $\gamma \neq \eta$ follows by Lemma 5.12. Thus, there exists a $k_0 \in \mathbb{N}_0$ such that for all $k < k_0$, $\gamma|_{[0,k]} = \eta|_{[0,k]}$ and $\gamma(k_0) \neq \eta(k_0)$. Note that $\gamma(k_0) \neq B \neq \eta(k_0)$. Hence, either $\gamma(k_0) \leq \eta(k_0)$ or $\eta(k_0) \leq \gamma(k_0)$. Since

$$b_V(\gamma|_{[0,k_0]}) \ni E_{\alpha,V}(\gamma) < E_{\alpha,V}(\eta) \in b_V(\eta|_{[0,k_0]}),$$

we conclude $\gamma|_{[0,k_0]} \leq \eta|_{[0,k_0]}$ from Lemma 5.4 Proposition 5.8. Hence, $\gamma \leq \eta$ follows. \square

Lemma 5.14 *Let $V > 4$ and $\alpha \in [0, 1] \setminus \mathbb{Q}$ with convergents $\varphi(c_k), k \in \mathbb{N}_0$. Furthermore, let $\gamma \in \Sigma_\alpha$ with $E_{\alpha,V}(\gamma) = E$. Then for all $k \in \mathbb{N}$, the image of $\{\eta \in \Sigma_{c_k}^{\text{spec}} : \eta \leq \gamma|_{[0,k]}\}$ under b_V equals $\{I : I \text{ is a spectral band of } \sigma_{c_k}(V) \text{ with } I \prec_{\text{str}} \{E\}\}$.*

Proof Assume $\eta \in \Sigma_{c_k}^{\text{spec}}$ with $\eta \leq \gamma|_{[0,k]}$. Then $b_V(\eta)$ is a spectral band of σ_{c_k} with $b_V(\eta) \prec_{\text{str}} b_V(\gamma|_{[0,k]})$. In particular, $b_V(\eta) \cap b_V(\gamma|_{[0,k]}) = \emptyset$ follows from Proposition 5.8(b) and (c). By construction of the map $E_{\alpha,V}$, we have $E \in b_V(\gamma|_{[0,k]})$, which shows

$$b_V\left(\left\{\eta \in \Sigma_{c_k}^{\text{spec}} : \eta \leq \gamma|_{[0,k]}\right\}\right) \subseteq \{I : I \text{ is a spectral band of } \sigma_{c_k} \text{ with } I \prec_{\text{str}} \{E\}\}.$$

To show the other inclusion, consider a spectral band I of σ_{c_k} with $I \prec_{\text{str}} \{E\}$. We apply Proposition 5.8 to get $\eta \in \Sigma_{c_k}^{\text{spec}}$ such that $b_V(\eta) = I$ and $b_V(\eta) \cap b_V(\gamma|_{[0,k]}) = \emptyset$. Combining $E \in b_V(\gamma|_{[0,k]})$ and $I \prec_{\text{str}} \{E\}$, we get that $b_V(\eta) \prec_{\text{str}} b_V(\gamma|_{[0,k]})$. Hence, by Proposition 5.8 $\eta \leq \gamma|_{[0,k]}$ which finishes the proof. \square

As a consequence of the considerations of this subsection, we conclude with the following statement.

Proposition 5.15 *Let $V > 4$ and $\alpha \in [0, 1] \setminus \mathbb{Q}$ with convergents $\frac{p_k}{q_k} = \varphi(\mathbf{c}_k)$, $k \in \mathbb{N}_0$, where p_k, q_k are coprime. For each $E \in \sigma(H_{\alpha, V})$, there is a unique $\gamma \in \Sigma_\alpha$ such that $E = E_{\alpha, V}(\gamma)$ and*

$$N_{\alpha, V}(E) = N_{\alpha, V}(E_{\alpha, V}(\gamma)) = \lim_{k \rightarrow \infty} \frac{\#\{\eta \in \Sigma_{\mathbf{c}_k}^{\text{spec}} : \eta \prec_{[0, k]} \gamma\}}{q_k}. \quad (5.4)$$

Remark Note that the latter statement asserts that the value $N_{\alpha, V}(E_{\alpha, V}(\gamma))$ is independent of $V > 4$ as the limit on the right-hand side is so. In fact, the value is independent for all $V > 0$ as proven in [3, Theorem 1.9 (d)].

Proof Let $E \in \sigma(H_{\alpha, V})$. The existence of a unique $\gamma \in \Sigma_\alpha$ such that $E = E_{\alpha, V}(\gamma)$ is proven in Lemma 5.12. Thus, $N_{\alpha, V}(E) = N_{\alpha, V}(E_{\alpha, V}(\gamma))$ holds. Proposition 5.2 leads to

$$N_{\alpha, V}(E) = \lim_{k \rightarrow \infty} \frac{\#\left\{I : I \text{ is a spectral band of } \sigma(H_{\frac{p_k}{q_k}, V}) \text{ with } I \prec_{\text{str}} \{E\}\right\}}{q_k}.$$

First note that $\sigma(H_{\frac{p_k}{q_k}, V}) = \sigma_{\mathbf{c}_k}(V)$ by Proposition 3.5. Let $b_V : \bigsqcup_{k \in \mathbb{N}_0} \Sigma_{\mathbf{c}_k} \rightarrow \bigsqcup_{k \in \mathbb{N}_0} L_{\mathbf{c}_k, V}$ be the map defined in Proposition 5.8 satisfying $E = E_{\alpha, V}(\gamma) \in b_V(\gamma|_{[0, k]})$ for all $k \in \mathbb{N}_0$. Thus, Lemma 5.14 leads to

$$b_V\left(\left\{\eta \in \Sigma_{\mathbf{c}_k}^{\text{spec}} : \eta \prec_{[0, k]} \gamma\right\}\right) = \left\{I : I \subseteq \sigma_{\mathbf{c}_k}(V) \text{ spectral band with } I \prec_{\text{str}} \{E\}\right\}.$$

Hence, Proposition 5.8(a) (asserting that b_V is injective if restricted to $\Sigma_{\mathbf{c}_k}^{\text{spec}}$) implies

$$\#\{\eta \in \Sigma_{\mathbf{c}_k}^{\text{spec}} : \eta \prec_{[0, k]} \gamma\} = \#\{I : I \subseteq \sigma_{\mathbf{c}_k}(V) \text{ spectral band with } I \prec_{\text{str}} \{E\}\}$$

finishing the proof. \square

5.3 A Formula for the IDS Via the Spectral Coding

In this subsection, we use the hierarchical structure of the periodic spectra and its coding in order to provide an explicit formula for the IDS, $N_{\alpha, V}$. Proposition 5.15 is the starting point for the current subsection. Next, we provide some counting arguments in order to express the numerator in (5.4) and to obtain a convenient formula for the IDS, which is eventually proven in Proposition 5.21.

Example 5.16 We provide a guiding example to demonstrate some of the counting arguments which are developed in this subsection. Let $\alpha \notin \mathbb{Q}$ whose continued fraction expansion that starts with $(2, 1, 1, 2, \dots)$ and consider, for example, $\gamma = (G^{(2)}, B, G^{(2)}, B, G^{(2)}, \dots) \in \Sigma_\alpha$. We would like to compute the IDS at $E := E_{\alpha, V}(\gamma)$ using the sequence in Proposition 5.2. Here we show how to compute

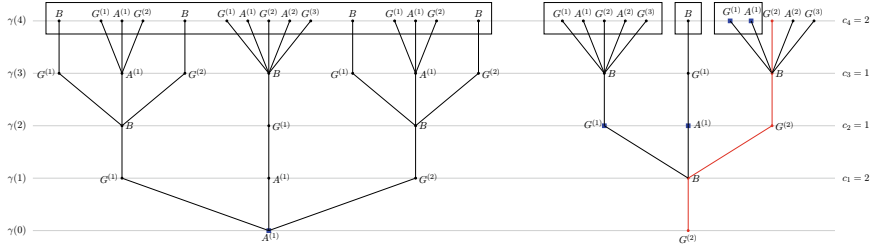


Fig. 5 Visualization of the codes in Example 5.16 as an ordered graph. The rectangles mark all the vertices in level 4 descending from a blue marked vertex in level $j \in \{0, 1, 2, 3, 4\}$

the $k = 4$ element of this sequence. First observe that $\frac{5}{13} = \frac{p_k}{q_k} = \varphi([0, 0, 2, 1, 1, 2])$. Since bands and codes are in a one-to-one relation by Proposition 5.8, we can rather think of codes and count the number of codes $\eta \in \Sigma_{c_4}^{\text{spec}}$ of length 5 with $\eta \leq \gamma|_{[0,4]}$. We demonstrate this situation in Figure 5—to better illustrate the example, we adapt here the tree formalism from [3], even though it did not originally appear in [39].

The beginning of the code γ is marked red and we need to count the codes $\eta = (\eta(0), \dots, \eta(4)) \in \Sigma_{c_4}^{\text{spec}}$ which correspond to spectral bands and which are to the left of this path γ . Specifically, one needs to count the vertices in the fourth level which are inside the rectangles, but only those vertices that are labeled $A^{(i)}$ or B should be counted since $\eta \in \Sigma_{c_4}^{\text{spec}}$. To do so, we follow the red path and at each level $j \in \{0, 1, 2, 3, 4\}$ we mark the vertices that branch off to the left. In Figure 5, we marked them with blue squares. The set of paths ending at a blue square in level j with label $\star = A$ if $\eta(j) = A^{(i)}$ and $\star = G$ if $\eta(j) = G$ are denoted by $\Gamma_j(\gamma, \star)$. For instance, $\Gamma_0(\gamma, A) = \{(A^{(1)})\}$ and $\Gamma_0(\gamma, G) = \emptyset$. Then we use the evolution laws $(\Sigma 2)$, $(\Sigma 3)$ and $(\Sigma 4)$ to calculate how many codes of length 5 are descendants of these blue squares and end with an $A^{(i)}$ or an B . This number is denoted by $d_j^4(\star)$, see Definition 5.19. For instance, $d_0^4(A) = 8$ and $d_1^4(G) = 3$. Then $d_j^4(\star) \cdot \sharp \Gamma_j(\gamma, \star)$ is the total number of codes $\eta \in \Sigma_{c_4}^{\text{spec}}$ where $\eta(j)$ has the label \star and $\eta \leq \gamma|_{[0,4]}$ since $\eta(j) \leq \gamma(j)$. Let $\sharp D_j^4(\gamma) = d_j^4(A) \cdot \sharp \Gamma_j(\gamma, A) + d_j^4(G) \cdot \sharp \Gamma_j(\gamma, G)$ be the sum of these numbers for the different labels $\star \in \{A, G\}$, see Lemma 5.17 and Eq. (5.5). For this specific example, we now can check directly in Fig. 5 that

$$\begin{aligned}
 \sharp D_0^4(\gamma) &= 8 \cdot 1 + 5 \cdot 0 &= 8, \\
 \sharp D_1^4(\gamma) &= 2 \cdot 0 + 3 \cdot 0 &= 0, \\
 \sharp D_2^4(\gamma) &= 1 \cdot 1 + 2 \cdot 1 &= 3, \\
 \sharp D_3^4(\gamma) &= 1 \cdot 0 + 1 \cdot 0 &= 0, \\
 \sharp D_4^4(\gamma) &= 1 \cdot 1 + 0 \cdot 1 &= 1,
 \end{aligned}$$

and $\sharp \{ \eta \in \Sigma_{\mathbf{c}_4}^{\text{spec}} : \eta \leq \gamma|_{[0,4]} \} = 12$ coinciding with the sum of $\sharp D_j^4(\gamma)$. Thus,

$$\frac{\sharp \{ \eta \in \Sigma_{\mathbf{c}_4}^{\text{spec}} : \eta \leq \gamma|_{[0,4]} \}}{q_4} = \frac{12}{13}$$

follows.

In this subsection, we perform this counting in a general manner and the final result is given in Proposition 5.21. Let $\alpha \in [0, 1] \setminus \mathbb{Q}$ and $\gamma \in \Sigma_\alpha$ an infinite spectral- α -code. Define

$$D_j^k(\gamma) := \{ \gamma' \in \Sigma_{\mathbf{c}_k}^{\text{spec}} : \gamma'(j) \leq \gamma(j) \text{ and } \forall i < j, \gamma'(i) = \gamma(i) \},$$

for all $0 \leq j \leq k$. Notice that, in particular,

$$D_0^k(\gamma) = \{ \gamma' \in \Sigma_{\mathbf{c}_k}^{\text{spec}} : \gamma'(0) \leq \gamma(0) \},$$

and, for example, $D_0^k(\gamma) = \emptyset$ if $\gamma(0) = A^{(1)}$.

We intend to employ the sets $D_j^k(\gamma)$ in order to compute the numerator in (5.4), see, e.g., (a) in the following lemma.

Lemma 5.17 *Let $V > 4$, $\alpha \in [0, 1] \setminus \mathbb{Q}$ with convergents $\varphi(\mathbf{c}_k)$, $k \in \mathbb{N}_0$, and $\gamma \in \Sigma_\alpha$. Then the following assertions hold.*

(a) We have

$$\{ \eta \in \Sigma_{\mathbf{c}_k}^{\text{spec}} : \eta \leq \gamma|_{[0,k]} \} = \bigsqcup_{j=0}^k D_j^k(\gamma).$$

(b) Let $R_j^k : \Sigma_{\mathbf{c}_k} \rightarrow \Sigma_{\mathbf{c}_j}$, $\gamma \mapsto R_j^k(\gamma) = \gamma|_{[0,j]}$ be the restriction map. Then

$$\sharp D_j^k(\gamma) = \sum_{\eta \in R_j^k(D_j^k(\gamma))} \sharp ((R_j^k)^{-1}(\eta) \cap \Sigma_{\mathbf{c}_k}^{\text{spec}}).$$

(c) If $\eta \in D_j^k(\gamma)$, then $\eta(j) \neq B \neq \gamma(j)$. In particular $D_j^k = \emptyset$ if $\gamma(j) = B$.

(d) For any $0 \leq j \leq k$, we have $R_j^k(D_j^k(\gamma)) = \Gamma_j(\gamma, A) \sqcup \Gamma_j(\gamma, G)$, where

$$\begin{aligned} \Gamma_j(\gamma, A) &:= \left\{ \eta \in \Sigma_{\mathbf{c}_j} : \eta \leq \gamma|_{[0,j]}, \eta|_{[0,j-1]} = \gamma|_{[0,j-1]}, \eta(j) \in \{A^{(i)} : i \in \mathbb{N}\} \right\}, \\ \Gamma_j(\gamma, G) &:= \left\{ \eta \in \Sigma_{\mathbf{c}_j} : \eta \leq \gamma|_{[0,j]}, \eta|_{[0,j-1]} = \gamma|_{[0,j-1]}, \eta(j) \in \{G^{(i)} : i \in \mathbb{N}\} \right\}. \end{aligned}$$

Proof (a) Let $\eta \in D_j^k(\gamma)$ for $0 \leq j \leq k$. By construction of \prec on $\Sigma_{\mathbf{c}_k}^{\text{spec}}$, $\eta(j) \prec \gamma(j)$ implies $\eta \prec \gamma|_{[0,k]}$. Thus

$$D_j^k(\gamma) \subseteq \{\gamma' \in \Sigma_{\mathbf{c}_k}^s : \eta \prec \gamma|_{[0,k]}\},$$

follows for all $0 \leq j \leq k$. For the converse inclusion observe that if $\eta \in \Sigma_{\mathbf{c}_k}^{\text{spec}}$ satisfies $\eta \prec \gamma|_{[0,k]}$, then either $\eta(0) \prec \gamma(0)$, or there is some $0 \leq j \leq k$ such that

$$\eta(j) \prec \gamma(j) \quad \text{and} \quad \eta(i) = \gamma(i) \text{ for all } 0 \leq i < j.$$

(b) Let $\eta \in R_j^k(D_j^k(\gamma))$, so we have $\eta(j) \prec \gamma(j)$. Thus, if $\tilde{\gamma} \in (R_j^k)^{-1}(\{\eta\})$, then $\tilde{\gamma}|_{[0,j]} = \eta$ holds and so $\tilde{\gamma} \prec \gamma|_{[0,k]}$. If, additionally, $\tilde{\gamma} \in \Sigma_{\mathbf{c}_k}^{\text{spec}}$, then we $\tilde{\gamma} \in D_j^k(\gamma)$. With this the claim follows.

(c) This follows ($\Sigma 4$) in Definition 5.6 asserting that if $\gamma(j) = B$, then $\gamma(j-1) = G^{(i)}$ for some $i \in \mathbb{N}$. Therefore, there is no code $\eta \in \Sigma_{\mathbf{c}_j}$ with $\eta(j-1) = \gamma(j-1)$, $\eta(j) \prec \gamma(j)$ and $\eta(j) = B$ or $\gamma(j) = B$.

(d) This follows directly from (c). \square

To continue the counting arguments, we find it useful to partition finite codes according to their finite letter. Toward this we introduce another notation. Let $\alpha \in [0, 1] \setminus \mathbb{Q}$ with continued fraction expansion $(c_k)_{k=0}^\infty$ and $\mathbf{c}_k = [0, c_0, \dots, c_k] \in \mathcal{C}$. Consider a subset $\mathcal{E} \subseteq \Sigma_{\mathbf{c}_k}$. Define

$$\begin{aligned} \varrho(\mathcal{E}, A) &:= \# \{ \eta \in \mathcal{E} : \eta(k) = A^{(i)} \text{ for some } i \in \mathbb{N} \}, \\ \varrho(\mathcal{E}, G) &:= \# \{ \eta \in \mathcal{E} : \eta(k) = G^{(i)} \text{ for some } i \in \mathbb{N} \}, \\ \varrho(\mathcal{E}, B) &:= \# \{ \eta \in \mathcal{E} : \eta(k) = B \}. \end{aligned}$$

For instance, $\varrho(\mathcal{E}, A)$ is the number of those spectral- α -codes in \mathcal{E} which end on an $A^{(i)}$. Let $l \in \mathbb{N}$. Then $\varrho((R_k^{k+l})^{-1}(\mathcal{E}), A)$ is the number of those codes in $\Sigma_{\mathbf{c}_{k+l}}$ that are extensions of codes in \mathcal{E} and end with a letter $A^{(i)}$. The next lemma provides identities for counting the number of such code extensions. Therefore, recall that the convergents $\frac{p_k}{q_k} = \varphi(\mathbf{c}_k)$, $k \in \mathbb{N}_0$, of $\alpha \in [0, 1] \setminus \mathbb{Q}$ with p_k, q_k coprime satisfy the recursive relation (2.3).

Lemma 5.18 ([39, Proposition 4.1]) *Let $\alpha \in [0, 1] \setminus \mathbb{Q}$ with continued fraction expansion $(c_k)_{k=0}^\infty$ and convergents $\frac{p_k}{q_k} = \varphi(\mathbf{c}_k)$, $k \in \mathbb{N}_0$, where p_k, q_k are coprime.*

(a) *Let $\mathcal{E} \subseteq \Sigma_{\mathbf{c}_k}$, $k \in \mathbb{N}_0$. Then*

$$\begin{pmatrix} \varrho((R_k^{k+1})^{-1}(\mathcal{E}), G) \\ \varrho((R_k^{k+1})^{-1}(\mathcal{E}), B) \\ \varrho((R_k^{k+1})^{-1}(\mathcal{E}), A) \end{pmatrix} = T_{k+1} \begin{pmatrix} \varrho(\mathcal{E}, G) \\ \varrho(\mathcal{E}, B) \\ \varrho(\mathcal{E}, A) \end{pmatrix},$$

where

$$T_{k+1} := T_{k+1}(\mathbf{c}_{k+1}) := \begin{pmatrix} 1 & c_{k+1} + 1 & c_{k+1} \\ 1 & 0 & 0 \\ 0 & c_{k+1} & c_{k+1} - 1 \end{pmatrix}.$$

(b) If $\ell \in \mathbb{N}$, then

$$\begin{pmatrix} \varrho \left((R_k^{k+\ell})^{-1}(\mathcal{E}), G \right) \\ \varrho \left((R_k^{k+\ell})^{-1}(\mathcal{E}), B \right) \\ \varrho \left((R_k^{k+\ell})^{-1}(\mathcal{E}), A \right) \end{pmatrix} = S_{k+\ell} S_k^{-1} \begin{pmatrix} \varrho(\mathcal{E}, G) \\ \varrho(\mathcal{E}, B) \\ \varrho(\mathcal{E}, A) \end{pmatrix}$$

with $S_k := S_k(\mathbf{c}_k) := T_k T_{k-1} \dots T_1$ and $S_0 = \mathbb{I}$ the identity matrix.

(c) The matrix S_k is given by

$$S_k = \begin{pmatrix} p_k + (-1)^k & q_k - (-1)^k & q_k - p_k - (-1)^k \\ p_{k-1} - (-1)^k & q_{k-1} + (-1)^k & q_{k-1} - p_{k-1} + (-1)^k \\ p_k - p_{k-1} + (-1)^k & q_k - q_{k-1} - (-1)^k & q_k - q_{k-1} - p_k + p_{k-1} - (-1)^k \end{pmatrix}$$

and its inverse S_k^{-1} equals to

$$S_k^{-1} = (-1)^k \begin{pmatrix} 1 - p_k & p_{k-1} - 1 & p_{k-1} + p_k - 1 \\ q_k - 1 & 1 - q_{k-1} & 1 - q_k - q_{k-1} \\ 1 - p_k - q_k & q_{k-1} + p_{k-1} - 1 & p_k + p_{k-1} + q_k + q_{k-1} - 1 \end{pmatrix}.$$

Proof (a) This is a direct consequence of the defining properties $(\Sigma 2)$ to $(\Sigma 4)$.

(b) This is proven via induction over $\ell \in \mathbb{N}$. For $\ell = 1$ this statement is just part (a) of this Lemma. Now assume the statement holds for an arbitrary $\ell \in \mathbb{N}$. By observing $R_k^{k+\ell+1} = R_k^{k+\ell} \circ R_{k+\ell}^{k+\ell+1}$ we get

$$(R_k^{k+\ell+1})^{-1}(\mathcal{E}) = (R_{k+\ell}^{k+\ell+1})^{-1} \left((R_k^{k+\ell})^{-1}(\mathcal{E}) \right).$$

Using (a) and our induction hypothesis then yields

$$\begin{aligned} \left(\varrho \left((R_k^{k+\ell+1})^{-1}(\mathcal{E}), G \right) \right) &= \left(\varrho \left((R_{k+\ell}^{k+\ell+1})^{-1} \left((R_k^{k+\ell})^{-1}(\mathcal{E}) \right), G \right) \right) \\ &= T_{k+\ell+1} \left(\varrho \left((R_k^{k+\ell})^{-1}(\mathcal{E}), G \right) \right) \\ &= T_{k+\ell+1} S_{k+\ell} S_k^{-1} \left(\varrho(\mathcal{E}, G) \right) \\ &= S_{k+\ell+1} S_k^{-1} \left(\varrho(\mathcal{E}, G) \right). \end{aligned}$$

(c) The stated form for S_k can be computed inductively. Then one checks by direct computations that S_k^{-1} is given by the stated matrix. Occasionally, the formula

$q_k p_{k-1} - p_k q_{k-1} = (-1)^k$ (see [27, Theorem 2]) is used. We leave the computational details to the reader. \square

Let $\gamma \in \Sigma_{\mathbf{c}_j}$ such that $\gamma(j) = A^{(i)}$ for some i . Then, for $k > j$, we wish to count how many $\eta \in \Sigma_{\mathbf{c}_k}^{\text{spec}}$ there are such that $\eta|_{[0,j]} = \gamma$. By the previous lemma, this number depends only on j and k , but it does not depend on the particular $\gamma \in \Sigma_{\mathbf{c}_j}$ satisfying $\gamma(j) = A^{(i)}$. Indeed, using Lemma 5.18 we define

Definition 5.19 For $\alpha \in [0, 1] \setminus \mathbb{Q}$, define

$$d_j^k(A) := (0 \ 1 \ 1) S_k S_j^{-1} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix},$$

and

$$d_j^k(G) := (0 \ 1 \ 1) S_k S_j^{-1} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}.$$

With this definition we may express the number of elements in the sets $D_j^k(\gamma)$ (which are used in Lemma 5.17(a))

$$\#D_j^k(\gamma) = d_j^k(A) \cdot \#\Gamma_j(\gamma, A) + d_j^k(G) \cdot \#\Gamma_j(\gamma, G), \quad (5.5)$$

where the sets $\Gamma_j(\gamma, A)$, $\Gamma_j(\gamma, G)$ were defined in Lemma 5.17. To verify identity (5.5) one first observes that the set $D_j^k(\gamma)$ may be decomposed into codes $\eta \in D_j^k(\gamma)$ for which $\eta(j) = A^{(i)}$ (for some i) and codes $\eta \in D_j^k(\gamma)$ for which $\eta(j) = G^{(i)}$ (for some i). This decomposition is thorough, since there are no codes $\eta \in D_j^k(\gamma)$ for which $\eta(j) = B$, see Lemma 5.17(c). To count the codes $\eta \in D_j^k(\gamma)$ for which $\eta(j) = A^{(i)}$, we notice that the prefix of each such code, $(\eta(0), \dots, \eta(j-1), A^{(i)})$ belongs to $\Gamma_j(\gamma, A)$ and there are exactly $d_j^k(A)$ ways to extend such a prefix to get an element in $D_j^k(\gamma)$.

Next, we provide an explicit formula for $d_j^k(A)$ and $d_j^k(G)$ using the convergents $\frac{p_k}{q_k} = \varphi(\mathbf{c}_k)$, $k \in \mathbb{N}_0$, of α with p_k, q_k coprime. Therefore, we like to remind the reader on the recursive definition of $\{p_k\}_{k=-1}^\infty$ and $\{q_k\}_{k=-1}^\infty$ in (2.3) with initial condition:

$$p_{-1} = 1, \quad p_0 = 0, \quad q_{-1} = 0, \quad q_0 = 1.$$

Lemma 5.20 Let $\alpha \in [0, 1] \setminus \mathbb{Q}$ with convergents $\frac{p_k}{q_k} = \varphi(\mathbf{c}_k)$, $k \in \mathbb{N}_0$, with p_k, q_k coprime. Consider the numbers

$$\mathcal{P}_j^k := (-1)^j [q_j p_k - p_j q_k] \quad \text{for } -1 \leq j \leq k.$$

Then

$$d_j^k(A) = \mathcal{P}_{j-1}^k - \mathcal{P}_j^k \quad \text{and} \quad d_j^k(G) = \mathcal{P}_j^k$$

hold for $0 \leq j \leq k$.

Proof We sketch the computation of $d_j^k(G)$. We have

$$S_k S_j^{-1} \cdot \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = (-1)^j S_k \cdot \begin{pmatrix} 1 - p_j \\ q_j - 1 \\ 1 - p_j - q_j \end{pmatrix}.$$

Performing this matrix multiplication and simplifying then yields

$$\begin{aligned} (0 \ 1 \ 0) \cdot S_k S_j^{-1} \cdot \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} &= (-1)^j [q_j p_{k-1} - p_j q_{k-1} - (-1)^k], \\ (0 \ 0 \ 1) \cdot S_k S_j^{-1} \cdot \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} &= (-1)^j [p_j q_{k-1} + q_j p_k - q_j p_{k-1} - p_j q_k + (-1)^k], \end{aligned}$$

and hence

$$d_j^k(G) = (-1)^j [q_j p_k - p_j q_k] = \mathcal{P}_j^k.$$

To compute $d_j^k(A)$, one proceeds analogously. □

Now, we have collected all the pieces in order to provide the promised formula for the IDS $N_{\alpha, V}$.

Proposition 5.21 *Let $V > 4$, $\alpha \in [0, 1] \setminus \mathbb{Q}$ with convergents $\frac{p_k}{q_k} = \varphi(c_k)$, $k \in \mathbb{N}_0$, with p_k, q_k coprime. Then, for each $\gamma \in \Sigma_\alpha$,*

$$N_{\alpha, V}(E_{\alpha, V}(\gamma)) = \sum_{k=-1}^{\infty} (-1)^k \mu_k(\gamma) (q_k \alpha - p_k)$$

where

$$\mu_{-1}(\gamma) := \#\Gamma_0(\gamma, A) \quad \text{and} \quad \mu_k(\gamma) := \#\Gamma_k(\gamma, G) - \#\Gamma_k(\gamma, A) + \#\Gamma_{k+1}(\gamma, A), \quad k \in \mathbb{N}_0.$$

Proof Let $\gamma \in \Sigma_\alpha$. Our starting point is Proposition 5.15, to which we consequently apply Lemma 5.17(a), (5.5) and Lemma 5.20,

$$\begin{aligned}
N_{\alpha,V}(E_{\alpha,V}(\gamma)) &= \lim_{k \rightarrow \infty} \frac{\#\{\eta \in \Sigma_{\mathbf{c}_k}^{\text{spec}} : \eta \leq \gamma\}}{q_k} \\
&= \lim_{k \rightarrow \infty} \frac{\sum_{j=0}^k \#D_j^k(\gamma)}{q_k} \\
&= \lim_{k \rightarrow \infty} \frac{1}{q_k} \sum_{j=0}^k \# \Gamma_j(\gamma, A) \cdot d_j^k(A) + \# \Gamma_j(\gamma, G) \cdot d_j^k(G) \\
&= \lim_{k \rightarrow \infty} \frac{1}{q_k} \sum_{j=0}^k \# \Gamma_j(\gamma, A) \cdot (\mathcal{P}_{j-1}^k - \mathcal{P}_j^k) + \# \Gamma_j(\gamma, G) \cdot \mathcal{P}_j^k \\
&= \lim_{k \rightarrow \infty} \frac{1}{q_k} \sum_{j=0}^k \mathcal{P}_j^k \cdot (\# \Gamma_j(\gamma, G) - \# \Gamma_j(\gamma, A) + \# \Gamma_{j+1}(\gamma, A)) \\
&\quad + \frac{1}{q_k} \mathcal{P}_{-1}^k \cdot \# \Gamma_0(\gamma, A) - \frac{1}{q_k} \underbrace{\mathcal{P}_k^k}_{=0} \cdot \# \Gamma_{k+1}(\gamma, A) \\
&= \lim_{k \rightarrow \infty} \frac{1}{q_k} \sum_{j=-1}^k \mathcal{P}_j^k \cdot \mu_j(\gamma) \\
&= \lim_{k \rightarrow \infty} \sum_{j=-1}^k \underbrace{(-1)^j \mu_j(\gamma) \cdot \left(q_j \frac{p_k}{q_k} - p_j \right)}_{=: f_k(j)},
\end{aligned}$$

where in the last two equalities we substitute $\mu_j(\gamma)$ from this proposition statement and the \mathcal{P}_j^k from Lemma 5.20.

According to [27, Theorem 4], the sequence $\left\{ \frac{p_{2l}}{q_{2l}} \right\}_{l=1}^{\infty}$ is monotonically increasing, $\left\{ \frac{p_{2l-1}}{q_{2l-1}} \right\}_{l=1}^{\infty}$ is monotonically decreasing and both sequences converge to α . Hence, we conclude for all $k \in \mathbb{N}$,

$$(-1)^j \left(q_j \frac{p_k}{q_k} - p_j \right) \geq 0 \quad \text{for all } j \leq k \quad \text{and} \quad (-1)^k (q_k \alpha - p_k) \geq 0.$$

Since $\mu_j(\gamma) \geq 0$ if $j \geq 1$, we conclude $f_k(j) \geq 0$ for all $j \in \mathbb{N}$. Thus, $\lim_{k \rightarrow \infty} \sum_{j=-1}^k f_k(j)$ converges absolutely using that the limit exists. For each $k \in \mathbb{N}$, we also have $f_{2k}(2l)$ is monotone increasing in $l \in \mathbb{N}$ and $f_{2k}(2l-1)$ is monotone decreasing in $l \in \mathbb{N}$. Note also that $\lim_{k \rightarrow \infty} f_k(j) = (-1)^j \mu_j(\gamma) \cdot (q_j \alpha - p_j)$ for each $j \geq -1$. Hence, the monotone convergence theorem applied to the following two summands separately leads to

$$N_{\alpha,V}(E_{\alpha,V}(\gamma)) = \lim_{k \rightarrow \infty} \left(\sum_{j=0}^{2k} f_{2k}(2j-1) + \sum_{l=0}^{2k} f_{2k}(2l) \right) = \sum_{j=-1}^{\infty} (-1)^j \mu_j(\gamma) \cdot (q_j \alpha - p_j)$$

where we used in the first step that the limit exists and so we can pass to the subsequence of even numbers $2k$. \square

Remark 5.22 Recognizing the importance of the functions $\mu_k(\gamma)$, $k \geq -1$ for the representation of the IDS in Proposition 5.21, we wish to elaborate on their possible values and their connection to the spectral code.

We have

$$\mu_{-1}(\gamma) = \begin{cases} 0, & \gamma(0) = A^{(1)}, \\ 1, & \gamma(0) = G^{(2)}. \end{cases}$$

For $k \in \mathbb{N}_0$ one can read the value of $\mu_k(\gamma)$ from the following table.

	$k = 0$			$k \geq 1$				
$\gamma(k)$	$A^{(1)}$		$G^{(2)}$	$A^{(i)}$		B		$G^{(i)}$
$\gamma(k+1)$	$A^{(j)}$		$G^{(j)}$	$A^{(j)}$		$G^{(j)}$		B
$\#\Gamma_k(\gamma, A)$	0	0	1	$i-1$	$i-1$	0	0	$i-1$
$\#\Gamma_k(\gamma, G)$	0	0	0	i	i	0	0	$i-1$
$\#\Gamma_{k+1}(\gamma, A)$	$j-1$	$j-1$	0	$j-1$	$j-1$	$j-1$	$j-1$	0
$\mu_k(\gamma)$	$j-1$	$j-1$	-1	j	j	$j-1$	$j-1$	0

Therefore we can conclude for all $k \in \mathbb{N}_{-1}$

$$\mu_k(\gamma) = \delta_{A,\gamma}(k) + \#\Gamma_{k+1}(\gamma, A) - \delta_{k,0}$$

where

$$\delta_{A,\gamma}(k) := \begin{cases} 1 & \gamma_k \in \{A^{(i)} : i \in \mathbb{N}\} \text{ and } k \geq 0, \\ 0 & \text{else.} \end{cases}$$

Remark 5.23 Comparing the IDS formula in Proposition 5.21 to the formula in [39, Theorem 4.7] shows that they are similar up to an additional term of $-\alpha$ which appears in [39, Theorem 4.7], but not in Proposition 5.21. The source for this difference is the connection between the coefficients $\mu_k(\gamma)$, we used above, and similar coefficients $\pi_k(\gamma)$ in [39]. It can be checked that the connection between both type of coefficients is given by

$$\pi_k(\gamma) = \mu_k(\gamma) + \delta_{k,0}.$$

We conclude this subsection by making a connection between the set of all possible infinite codes, $\gamma \in \Sigma_\alpha$ and the set of all possible infinite sequences, $(\mu_k)_{k \in \mathbb{N}_{-1}}$. The latter set is given by

$$\mathcal{M}_\alpha := \left\{ (\mu_k)_{k \in \mathbb{N}_{-1}} \in \mathbb{N}_{-1}^{\mathbb{N}_{-1}} \left| \begin{array}{ll} \mu_{-1} \in \{0, 1\} & \text{and } \mu_{-1} = 1 \iff \mu_0 = -1, \\ \mu_0 \in \{-1, \dots, c_1 - 1\} & \text{and } \mu_0 = c_1 - 1 \implies \mu_1 = 0, \\ \mu_j \in \{0, \dots, c_{j+1}\} & \text{and } \mu_j = c_{j+1} \implies \mu_{j+1} = 0 \text{ for } j \geq 1 \end{array} \right. \right\},$$

where $(c_k)_{k \in \mathbb{N}}$ is the continued fraction expansion of α .

Lemma 5.24 ([39, Proposition 4.4]) *Let $\alpha \in [0, 1] \setminus \mathbb{Q}$. Then there is a bijection between Σ_α and \mathcal{M}_α . The bijection is explicitly given by $\gamma \mapsto (\mu_k(\gamma))_{k \in \mathbb{N}_{-1}}$ where*

$$\mu_{-1}(\gamma) := \#\Gamma_0(\gamma, A) \quad \text{and} \quad \mu_k(\gamma) := \#\Gamma_k(\gamma, G) - \#\Gamma_k(\gamma, A) + \#\Gamma_{k+1}(\gamma, A), \quad k \in \mathbb{N}_0.$$

Proof It is straightforward to verify that the map in the statement is well defined: given $\gamma \in \Sigma_\alpha$, one can check that $(\mu_k(\gamma))_{k \in \mathbb{N}_{-1}} \in \mathcal{M}_\alpha$. To see this compare the definition of \mathcal{M}_α with Remark 5.22 which shows a table which characterizes $(\mu_k)_{k \in \mathbb{N}_{-1}}$. To show that this map is a bijection, we take $(\mu_k)_{k \in \mathbb{N}_{-1}} \in \mathcal{M}_\alpha$ and inductively compute the corresponding $\gamma(k)$. On the way, we prove that $\gamma(k)$ is uniquely determined by $(\mu_{-1}, \mu_0, \dots, \mu_{k+1})$.

To aid this computation confer the table in Remark 5.22 and recall that for all $k \in \mathbb{N}_{-1}$

$$\mu_k(\gamma) = \delta_{A,\gamma}(k) + \#\Gamma_{k+1}(\gamma, A) - \delta_{k,0}.$$

First, if $\mu_{-1} = 1$, then we set $\gamma(0) = G^{(2)}$ and otherwise if $\mu_{-1} = 0$, then we set $\gamma(0) = A^{(1)}$.

If $\mu_0 = -1$, then $\mu_{-1} = 1$ and therefore $\gamma(0) = G^{(2)}$. Now property $(\Sigma 4)$ from Definition 5.6 implies $\gamma(1) = B$. Else, if $\mu_0 = i \in \{0, \dots, c_1 - 1\}$, then $\gamma(0) = A^{(1)}$ follows. If in addition $\mu_1 = 0$, then we conclude $\gamma(1) = G^{(i)}$, and if $\mu_1 \neq 0$, then $\gamma(1) = A^{(i)}$ holds. Notice that the code $(\gamma(0), \gamma(1))$ generated this way fulfills Definition 5.6. This describes the induction base of the construction.

Now assume γ was uniquely determined by μ up to $\gamma(k)$ for some $k \geq 1$. If $\gamma(k)$ was $G^{(i)}$, then property $(\Sigma 4)$ yields again $\gamma(k+1) = B$. If $\gamma(k) \in \{A^{(i)} : i \in \mathbb{N}\} \cup \{B\}$, then $(\Sigma 2)$ and $(\Sigma 4)$ imply $\gamma(k+1) \in \{A^{(i)} : i \in \mathbb{N}\} \cup \{G^{(i)} : i \in \mathbb{N}\}$. Assume $\mu_k = j$. Then we get even $\gamma(k+1) \in \{A^{(j)}, G^{(j)}\}$. If $\mu_{k+1} = 0$, then $\gamma(k+1) = G^{(j)}$ and otherwise $\gamma(k+1) = A^{(j)}$. Thus $\gamma(k)$, μ_k and μ_{k+1} uniquely determine $\gamma(k+1)$. Observe again, that the code $(\gamma(0), \dots, \gamma(k+1))$ fulfills Definition 5.6. \square

5.4 Finding all the Gap Labels

Our aim in this subsection is to prove the following.

Theorem 5.25 *Let $V > 4$. For $\alpha \in [0, 1] \setminus \mathbb{Q}$ we have*

$$\{N_{\alpha,V}(E) : E \in \mathbb{R} \setminus \sigma(H_{\alpha,V})\} = \{\ell\alpha \mod 1 : \ell \in \mathbb{Z}\} \cup \{1\} = (\mathbb{Z} + \mathbb{Z}\alpha) \cap [0, 1].$$

A main tool in the proof of the theorem is Proposition 5.21. Therefore, we need the following auxiliary lemma.

Lemma 5.26 ([39, Proposition 5.2]) *Let $\alpha \in [0, 1] \setminus \mathbb{Q}$ with convergents $\frac{p_k}{q_k} = \varphi(\mathbf{c}_k)$. For each $\ell \in \mathbb{Z}$, there is some $k_0 \in \mathbb{N}$ and $\mu = (\mu_j)_{j \in \mathbb{N}_{-1}} \in \mathcal{M}_\alpha$ such that $\mu_j = 0$ for $j > k_0$ and*

$$\ell = \sum_{j=-1}^{\infty} (-1)^j \mu_j q_j = \sum_{j=-1}^{k_0} (-1)^j \mu_j q_j. \quad (5.6)$$

Moreover, if $\ell \notin \{-1, 0, 1\}$, then $\mu_{k_0} \geq 1$.

Proof We prove the statement inductively over $m \in \mathbb{N}$ that

- (a) For all $\ell \in [-q_{2m}, q_{2m-1})$ there is a $k_0 \leq 2m$ and a $\mu = (\mu_j) \in \mathcal{M}_\alpha$ satisfying (5.6) $\mu_j = 0$ if $j > k_0$.
- (b) If $\mu_{k_0-1} = c_{k_0}$, then $\ell \in [-q_{k_0}, -q_{k_0} + q_{k_0-1})$ if k_0 is even and $\ell \in [-q_{k_0-1} + q_{k_0}, q_{k_0})$ if k_0 is odd.

To do this, we check the claim in an alternating manner on the positive and negative part of these intervals. Also recall the recursive behavior of the sequence $(q_k)_{k \in \mathbb{N}_0}$, that is:

$$q_{-1} = 0, \quad q_0 = 1 \quad \text{and} \quad q_k = c_k q_{k-1} + q_{k-2} \quad \text{for } k \in \mathbb{N}.$$

First, let $m = 1$ and consider $\ell \in [-q_2, q_1) = [-q_2, -q_0) \cup \{-q_0\} \cup (-q_0, q_1)$ and we separately consider each of the cases

$$\ell \in \{-q_0\}, \quad \ell \in (-q_0, q_1) \quad \text{and} \quad \ell \in [-q_2, -q_0).$$

If $\ell = -q_0 = -1$, then we choose $k_0 = 0 \leq 2m - 1$ and $\mu := (\mu_j)_{j \in \mathbb{N}_{-1}} := (1, -1, 0, 0, \dots)$. In this case we get $\mu \in \mathcal{M}_\alpha$ and

$$\sum_{j=-1}^{\infty} (-1)^j \mu_j q_j = \mu_0 = -1 = \ell.$$

For the second case, if $\ell \in (-q_0, q_1) \cap \mathbb{Z} = [0, c_1) \cap \mathbb{Z}$, choose $k_0 = 0 \leq 2m - 1$ and $\mu := (0, \ell, 0, 0, \dots)$. Again, observe that $\mu \in \mathcal{M}_\alpha$ satisfies (5.6). For the third case we assume $\ell \in [-q_2, -q_0)$. Notice that we can decompose this interval into the c_2 intervals

$$[-q_2, -q_0) = \bigsqcup_{j=1}^{c_2} [-q_0 - (c_2 + 1 - j)q_1, q_0 - (c_2 - j)q_1).$$

That is, there is a unique $\mu_1 \in \{1, \dots, c_2\}$ with

$$-q_0 - \mu_1 q_1 \leq \ell < -q_0 - (\mu_1 - 1)q_1.$$

Equivalently, we can write this as

$$-q_0 \leq \ell + \mu_1 q_1 < -q_0 + q_1 = c_1 - 1.$$

If $\ell + \mu_1 q_1$ happen to be $-q_0 = -1$, then we can apply the first case to it and get

$$\ell + \mu_1 q_1 = \sum_{j=-1}^0 (-1)^j \mu_j q_j,$$

with $\mu_{-1} = 1$ and $\mu_0 = -1$. Then $\mu := (1, -1, \mu_1, 0, 0, \dots) \in \mathcal{M}_\alpha$ and $k_0 = 1 \leq 2m - 1$ satisfy (5.6) for the given ℓ . We proceed similarly when

$$-q_0 < \ell + \mu_1 q_1 < -q_0 + q_1 = c_1 - 1.$$

More precisely, if this holds, the second case yields

$$\ell + \mu_1 q_1 = \sum_{j=-1}^0 (-1)^j \mu_j q_j,$$

with $\mu_{-1} = 0$ and $\mu_0 = \ell + \mu_1 q_1$. Thus for $\mu := (0, \mu_0, \mu_1, 0, 0, \dots)$ we have $\mu \in \mathcal{M}_\alpha$ as $\mu_0 \neq c_1 - 1$ (we need this since $\mu_1 \neq 0$) and, by construction, μ satisfies (5.6) for the given ℓ and $k_0 = 1 \leq 2m - 1$. This ends the induction base.

For the induction step suppose (a) and (b) hold for some $m \in \mathbb{N}$. Let $\ell \in [-q_{2m+2}, q_{2m+1})$. Again, we separately discuss the three cases

$$\ell \in [-q_{2m+2}, -q_{2m}), \quad \ell \in [-q_{2m}, q_{2m-1}) \quad \text{and} \quad \ell \in [q_{2m-1}, q_{2m+1}).$$

For $\ell \in [-q_{2m}, q_{2m-1})$ there is nothing to do, as (5.6) holds by the induction hypothesis.

If $\ell \in [q_{2m-1}, q_{2m+1}) = [q_{2m-1}, q_{2m-1} + c_{2m+1} q_{2m})$, then there exists some $\mu_{2m} \in \{1, \dots, c_{2m+1}\}$ such that

$$q_{2m-1} + (\mu_{2m} - 1)q_{2m} \leq \ell < q_{2m-1} + \mu_{2m} q_{2m}, \quad (5.7)$$

or equivalently

$$-q_{2m} + q_{2m-1} \leq \ell - \mu_{2m} q_{2m} < q_{2m-1}.$$

In particular we observe $\ell - \mu_{2m} q_{2m} \notin [-q_{2m}, -q_{2m} + q_{2m-1})$. Thus the induction hypothesis implies that there exists $(\mu_{-1}, \dots, \mu_{2m-1}, 0, 0, \dots) \in \mathcal{M}_\alpha$ with $\mu_{2m-1} \neq c_{2m}$ such that

$$\ell - \mu_{2m} q_{2m} = \sum_{j=-1}^{2m-1} (-1)^j \mu_j q_j.$$

Note that if $\mu_{2m-1} = c_{2m}$, then the induction hypothesis for (b) and $k_0 = 2m$ yields $\ell - \mu_{2m}q_{2m} \in [-q_{2m}, -q_{2m} + q_{2m-1})$, a contradiction.

Therefore we set $\mu := (\mu_{-1}, \dots, \mu_{2m-1}, \mu_{2m}, 0, 0, \dots)$ and observe $\mu \in \mathcal{M}_\alpha$, as $\mu_{2m-1} \neq c_{2m}$. Then (5.6) hold for the given ℓ and $k_0 = 2m \leq 2(m+1) - 1$. Note that if $\mu_{2m} = c_{2m+1}$, i.e., $k_0 = 2m + 1$ odd then (5.7) implies

$$\ell \in [q_{2m+1} - q_{2m}, q_{2m+1}) = [-q_{k_0-1} + q_{k_0}, q_{k_0}).$$

This proves (b) if k_0 is odd for $m + 1$.

Finally, we suppose $\ell \in [-q_{2m+2}, -q_{2m}) = [-c_{2m+2}q_{2m+1} - q_{2m}, -q_{2m})$. Then there exists some $\mu_{2m+1} \in \{1, \dots, c_{2m+2}\}$ such that

$$-\mu_{2m+1}q_{2m+1} - q_{2m} \leq \ell < -(\mu_{2m+1} - 1)q_{2m+1} - q_{2m}, \quad (5.8)$$

or equivalently

$$-q_{2m} \leq \ell + \mu_{2m+1}q_{2m+1} < -q_{2m} + q_{2m+1} = -q_{2m} + c_{2m+1}q_{2m} + q_{2m-1}.$$

In particular, we observe $\ell + \mu_{2m+1}q_{2m+1} \notin [-q_{2m} + q_{2m+1}, q_{2m+1})$. Thus, the induction hypothesis implies that there are some $(\mu_{-1}, \dots, \mu_{2m}, 0, 0, \dots) \in \mathcal{M}_\alpha$ with $\mu_{2m} \neq c_{2m+1}$ such that

$$\ell + \mu_{2m+1}q_{2m+1} = \sum_{j=-1}^{2m} (-1)^j \mu_j q_j.$$

Note that if $\mu_{2m} = c_{2m+1}$, then the induction hypothesis for (b) and $k_0 = 2m + 1$ yields $\ell + \mu_{2m+1}q_{2m+1} \in [-q_{2m} + q_{2m+1}, q_{2m+1})$, a contradiction.

Therefore we set $\mu := (\mu_{-1}, \dots, \mu_{2m}, \mu_{2m+1}, 0, 0, \dots)$ and observe $\mu \in \mathcal{M}_\alpha$, as $\mu_{2m} \neq c_{2m+1}$. Then (5.6) hold for the given ℓ and $k_0 = 2m + 1 \leq 2(m+1) - 1$. Note that if $\mu_{2m+1} = c_{2m+2}$, i.e., $k_0 = 2m + 2$ even then (5.8) implies

$$\ell \in [-q_{2m+2}, -q_{2m+2} - q_{2m+1}).$$

Thus, (b) holds if k_0 is even for $m + 1$.

Note that $\mu_{k_0} \geq 0$ holds for all $k_0 \geq 1$. The cases where $k_0 \in \{-1, 0\}$ and $\mu_{k_0} = 0$ are exactly when $\ell \in \{-1, 0, 1\}$. Therefore $\ell \in \mathbb{Z} \setminus \{-1, 0, 1\}$ and $\mu_{k_0} \neq 0$ imply $\mu_{k_0} \geq 1$. \square

Proof (Proof of Theorem 5.25) We start by recalling that the gap labeling theorem [4, Proposition 5.2.4] already provides the inclusion,

$$\mathcal{G} := \{N_{\alpha,V}(E) : E \in \mathbb{R} \setminus \sigma(H_{\alpha,V})\} \subseteq \{\ell\alpha \pmod{1} : \ell \in \mathbb{Z}\} \cup \{1\}.$$

First note that the spectrum $\sigma(H_{\alpha,V})$ is a compact subset of \mathbb{R} . Then if $E < \inf \sigma(H_{\alpha,V})$, we obtain $N_{\alpha,V}(E) = 0$. Similarly if $E > \sup \sigma(H_{\alpha,V})$, then $N_{\alpha,V}(E) = 1$ and so $\{0, 1\} \subseteq \mathcal{G}$ holds. We continue proving $\ell\alpha \bmod 1 \in \mathcal{G}$ for $\ell \in \mathbb{Z} \setminus \{-1, 0\}$. The case $\ell = -1$ will be treated separately at the end.

Let $\ell \in \mathbb{Z} \setminus \{-1, 0\}$ and let $\mu = (\mu_{-1}, \mu_0, \dots) \in \mathcal{M}_\alpha$ be such that there is some $k_0 \in \mathbb{N}_0$ with $\ell = \sum_{j=-1}^{k_0} (-1)^j \mu_j q_j$ and $\mu_j = 0$ for all $j \geq k_0 + 1$, which exists by Lemma 5.26. In addition, Lemma 5.26 asserts that $\mu_{k_0} \geq 1$. Then define

$$\mu' = (\mu_{-1}, \mu_0, \dots, \mu_{k_0-1}, (\mu_{k_0} - 1), c_{k_0+2}, 0, c_{k_0+4}, 0, c_{k_0+6}, \dots). \quad (5.9)$$

Observe that $\mu' \in \mathcal{M}_\alpha$ using $\mu_{k_0} \geq 1$. Then Lemma 5.24 implies that there are unique $\gamma, \gamma' \in \Sigma_\alpha$ such that $E := E_{\alpha,V}(\gamma)$ and $E' := E_{\alpha,V}(\gamma')$ satisfy

$$N_{\alpha,V}(E) = \sum_{j=-1}^{\infty} (-1)^j \mu_j (q_j \alpha - p_j) \quad \text{and} \quad N_{\alpha,V}(E') = \sum_{j=-1}^{\infty} (-1)^j \mu'_j (q_j \alpha - p_j).$$

With this choice we get

$$\begin{aligned} [0, 1] \ni N_{\alpha,V}(E) &= \sum_{j=-1}^{\infty} (-1)^j \mu_j (q_j \alpha - p_j) \\ &= \sum_{j=-1}^{k_0} (-1)^j \mu_j (q_j \alpha - p_j) \\ &= \underbrace{\sum_{j=-1}^{k_0} (-1)^j \mu_j q_j \alpha}_{=\ell\alpha} - \underbrace{\sum_{j=-1}^{k_0} (-1)^j \mu_j p_j}_{\in \mathbb{Z}} \end{aligned}$$

and therefore $N_{\alpha,V}(E) = \ell\alpha \bmod 1$.

We also claim $E \neq E'$. Assume differently, i.e., $E = E'$, then $\gamma = \gamma'$ due to Lemma 5.12. Hence, $\mu_j(\gamma) = \mu_j(\gamma')$ follows for all $j \in \mathbb{N}_{-1}$ by the definition of $(\mu_j)_{j \in \mathbb{N}_{-1}}$ in Proposition 5.21. This yields a contradiction for $j \geq k_0$.

Next we observe

$$\begin{aligned} |N_{\alpha,V}(E') - N_{\alpha,V}(E)| &= |(-1)^{k_0+1} (q_{k_0} \alpha - p_{k_0}) + (-1)^{k_0+1} c_{k_0+2} (q_{k_0+1} \alpha - p_{k_0+1}) \\ &\quad + \sum_{j=k_0+3}^{\infty} (-1)^j \mu'_j (q_j \alpha - p_j)| \\ &= \left| (-1)^{k_0+1} (q_{k_0+2} \alpha - p_{k_0+2}) + \sum_{j=k_0+3}^{\infty} (-1)^j \mu'_j (q_j \alpha - p_j) \right|. \end{aligned}$$

Using the recursion formulas for $\{p_k\}_{k \in \mathbb{N}_{-1}}$ and $\{q_k\}_{k \in \mathbb{N}_{-1}}$ from Eq. (2.3), we inductively conclude

$$\begin{aligned} & \left| (-1)^{k_0+1} (q_{k_0+2n}\alpha - p_{k_0+2n}) + \sum_{j=k_0+2n+1}^{\infty} (-1)^j \mu'_j (q_j\alpha - p_j) \right| \\ &= \left| (-1)^{k_0+1} q_{k_0+2(n+1)}\alpha - p_{k_0+2(n+1)} + \sum_{j=k_0+2(n+1)+1}^{\infty} (-1)^j \mu'_j (q_j\alpha - p_j) \right|, \end{aligned}$$

for all $n \in \mathbb{N}$. Hence, we obtain

$$|N_{\alpha,V}(E') - N_{\alpha,V}(E)| \leq |q_{k+2n}\alpha - p_{k+2n}| + \left| \sum_{j=k+2n+1}^{\infty} (-1)^j \mu'_j (q_j\alpha - p_j) \right|,$$

for all $n \in \mathbb{N}$. Sending $n \rightarrow \infty$ and using that the sum exists, we conclude

$$|N_{\alpha,V}(E') - N_{\alpha,V}(E)| \leq \lim_{n \rightarrow \infty} |q_{k+2n}\alpha - p_{k+2n}| \leq 0,$$

by properties of the Diophantine approximation [27, Theorem 9]. Therefore $\ell\alpha \bmod 1 = N_{\alpha,V}(E) = N_{\alpha,V}(E')$ while $E \neq E'$. Since the IDS is monotonously increasing (IDS1) and constant on the gaps (IDS2), we conclude that (E, E') is completely contained in $\mathbb{R} \setminus \sigma(H_{\alpha,V})$. That is for all $E'' \in (E, E')$ we still get

$$N_{\alpha,V}(E'') = N_{\alpha,V}(E) = \ell\alpha \bmod 1$$

and so we conclude $\ell\alpha \bmod 1 \in \mathcal{G}$.

We now treat the last case $\ell = -1$ and the gap label $\ell\alpha \bmod 1 = 1 - \alpha$ for $\ell = -1$. Let $\mu = (1, -1, 0, 0, \dots)$ and $\mu' = (0, c_1 - 1, 0, c_3, 0, c_5, \dots)$. By Lemma 5.24 there are again unique $\gamma, \gamma' \in \Sigma_\alpha$ such that $\mu(\gamma) = \mu$ and $\mu(\gamma') = \mu'$. Following similar computations as above, we get $N_{\alpha,V}(E_{\alpha,V}(\gamma)) = 1 - \alpha = N_{\alpha,V}(E_{\alpha,V}(\gamma'))$. Since $\gamma \neq \gamma'$, Lemma 5.12 implies $E_{\alpha,V}(\gamma) \neq E_{\alpha,V}(\gamma')$. Hence we also get in this case $1 - \alpha \in \mathcal{G}$. \square

6 A Recursive Relation for Periods of Mechanical Words

This section is devoted to the proof of Lemma 2.4 and deriving a consequence of its proof (given as Corollary 6.5). Let $\alpha \in [0, 1] \setminus \mathbb{Q}$ with infinite continued fraction expansion $(c_k)_{k=0}^\infty$ and convergents $\alpha_k = \varphi([0, c_0, c_1, \dots, c_k])$ for $k \in \mathbb{N}_0$. Recall from (2.6) the definition

$$W_k(i) := \omega_{\alpha_k}(i), \quad 0 \leq i \leq q_k - 1,$$

for the period of those mechanical words ω_{α_k} . Further recall the statement of Lemma 2.4:

$$W_0 = 0, \quad W_1 = \underbrace{0 \dots 0}_{c_1-1} 1,$$

and if $k \geq 2$, then

$$W_k = \begin{cases} W_{k-2} W_{k-1}^{c_k}, & k \equiv 0 \pmod{2}, \\ W_{k-1}^{c_k} W_{k-2}, & k \equiv 1 \pmod{2}, \end{cases}$$

where the power means a concatenation of words. We now bring four auxiliary lemmas (Lemmas 6.1, 6.2, 6.3, and 6.4) which are needed to prove Lemma 2.4.

Lemma 6.1 (Period prefixes) *Let $\alpha \in [0, 1] \setminus \mathbb{Q}$ and $k \geq 2$.*

(a) *If $k \equiv 0 \pmod{2}$ then*

$$W_k(i) = W_{k-1}(i) \quad \text{for all } 0 \leq i \leq q_{k-1} - 2 \quad (6.1)$$

and

$$W_k(i) = W_{k-2}(i \pmod{q_{k-2}}) \quad \text{for all } 0 \leq i \leq q_{k-1} - 2. \quad (6.2)$$

(b) *If $k \equiv 1 \pmod{2}$ then*

$$W_k(i) = W_{k-1}(i \pmod{q_{k-1}}) \quad \text{for all } 0 \leq i \leq q_k - 2 \quad (6.3)$$

and

$$W_k(i) = W_{k-2}(i) \quad \text{for all } 0 \leq i \leq q_{k-2} - 2. \quad (6.4)$$

Proof (a) Start by treating the case $k \equiv 0 \pmod{2}$. Since k is even, standard theory of rational convergents ([27, Theorem 4]) implies $\frac{p_{k-2}}{q_{k-2}} < \frac{p_k}{q_k} < \frac{p_{k-1}}{q_{k-1}}$.

We start by showing that for all $0 \leq i \leq q_{k-1} - 1$, $\left\lfloor \frac{p_k}{q_k} i \right\rfloor = \left\lfloor \frac{p_{k-1}}{q_{k-1}} i \right\rfloor$ from which (6.1) of the Lemma follows when using Lemmas 2.3 and (2.6).

Assume toward contradiction that there exists $0 \leq i \leq q_{k-1} - 1$ such that $\left\lfloor \frac{p_k}{q_k} i \right\rfloor \neq \left\lfloor \frac{p_{k-1}}{q_{k-1}} i \right\rfloor$. Clearly, $i > 0$ must hold. Using $\frac{p_k}{q_k} < \frac{p_{k-1}}{q_{k-1}}$, we infer that there exists an $m \in \mathbb{N}$ such that

$$\frac{p_k}{q_k} i < m \leq \frac{p_{k-1}}{q_{k-1}} i,$$

or, equivalently,

$$\frac{p_k}{q_k} < \frac{m}{i} \leq \frac{p_{k-1}}{q_{k-1}}. \quad (6.5)$$

Since k is even, [27, Theorem 2] implies

$$\frac{p_{k-1}}{q_{k-1}} - \frac{p_k}{q_k} = \frac{1}{q_{k-1}q_k}. \quad (6.6)$$

By (6.5), $mq_k - ip_k > 0$ holds and so $mq_k - ip_k \geq 1$. Thus, (6.6) and $i \leq q_{k-1} - 1$ lead to

$$\frac{1}{q_{k-1}q_k} = \frac{p_{k-1}}{q_{k-1}} - \frac{p_k}{q_k} \geq \frac{m}{i} - \frac{p_k}{q_k} = \frac{mq_k - ip_k}{iq_k} > \frac{mq_k - ip_k}{q_{k-1}q_k} \geq \frac{1}{q_{k-1}q_k},$$

a contradiction.

Next, we show that for all $0 \leq i \leq q_{k-1} - 1$, $\left\lfloor \frac{p_{k-2}}{q_{k-2}} i \right\rfloor = \left\lfloor \frac{p_k}{q_k} i \right\rfloor$ from which (6.2) of the Lemma follows when using Lemmas 2.3 and (2.6).

Assume toward contradiction that there exists $0 \leq i \leq q_{k-1} - 1$ such that $\left\lfloor \frac{p_{k-2}}{q_{k-2}} i \right\rfloor \neq \left\lfloor \frac{p_k}{q_k} i \right\rfloor$. Clearly, $i > 0$ must hold. Using $\frac{p_{k-2}}{q_{k-2}} < \frac{p_k}{q_k}$, we infer that there exists an $m \in \mathbb{N}$ such that

$$\frac{p_{k-2}}{q_{k-2}} i < m \leq \frac{p_k}{q_k} i,$$

or, equivalently,

$$\frac{p_{k-2}}{q_{k-2}} < \frac{m}{i} \leq \frac{p_k}{q_k}. \quad (6.7)$$

Let $(c_i)_{i \in \mathbb{N}_0}$ be the infinite continued fraction expansion of α . Since k is even, [27, Theorem 3] implies

$$\frac{p_k}{q_k} - \frac{p_{k-2}}{q_{k-2}} = \frac{c_k}{q_k q_{k-2}}. \quad (6.8)$$

By (6.7), $mq_{k-2} - ip_{k-2} > 0$ holds and so $mq_{k-2} - ip_{k-2} \geq 1$. Thus, (6.7) and (6.8) lead to

$$\frac{c_k}{q_k q_{k-2}} = \frac{p_k}{q_k} - \frac{p_{k-2}}{q_{k-2}} \geq \frac{m}{i} - \frac{p_{k-2}}{q_{k-2}} = \frac{mq_{k-2} - ip_{k-2}}{iq_{k-2}} > \frac{mq_{k-2} - ip_{k-2}}{q_{k-1}q_{k-2}}.$$

Since $k \geq 2$, we have $q_{k-2} > 0$ and so (2.3) and the previous estimate leads to

$$1 \leq mq_{k-2} - ip_{k-2} < \frac{c_k q_{k-1}}{q_k} = \frac{c_k q_{k-1}}{c_k q_{k-1} + q_{k-2}} < 1,$$

a contradiction.

(b) For the case $k \equiv 1 \pmod{2}$, we get by standard theory of rational convergents ([27, Theorem 4]) that $\frac{p_{k-1}}{q_{k-1}} < \frac{p_k}{q_k} < \frac{p_{k-2}}{q_{k-2}}$.

To prove (6.3) we need to show that for all $0 \leq i \leq q_k - 1$, $\left\lfloor \frac{p_{k-1}}{q_{k-1}} i \right\rfloor = \left\lfloor \frac{p_k}{q_k} i \right\rfloor$, which can be done similar to the way that (6.1) was proven above (but exchanging

the roles of $\frac{p_k}{q_k}$ and $\frac{p_{k-1}}{q_{k-1}}$. Note that statement (6.3) is stronger than (6.1) in the sense that we show equality for a longer subset (up to $q_k - 2$ rather than up to $q_{k-1} - 2$).

Assume toward contradiction that there exists $0 \leq i \leq q_k - 1$ such that $\left\lfloor \frac{p_{k-1}}{q_{k-1}} i \right\rfloor \neq \left\lfloor \frac{p_k}{q_k} i \right\rfloor$. Clearly, $i > 0$ must hold. Using $\frac{p_{k-1}}{q_{k-1}} < \frac{p_k}{q_k}$, we infer that there exists an $m \in \mathbb{N}$ such that

$$\frac{p_{k-1}}{q_{k-1}} < \frac{m}{i} \leq \frac{p_k}{q_k}.$$

Thus, $q_{k-1}m - p_{k-1}i \geq 1$ follows. Since k is odd, [27, Theorem 2] implies

$$\frac{p_k}{q_k} - \frac{p_{k-1}}{q_{k-1}} = \frac{1}{q_{k-1}q_k}.$$

Hence, $i \leq q_k - 1$ lead to

$$\frac{1}{q_{k-1}q_k} = \frac{p_k}{q_k} - \frac{p_{k-1}}{q_{k-1}} \geq \frac{m}{i} - \frac{p_{k-1}}{q_{k-1}} = \frac{q_{k-1}m - p_{k-1}i}{iq_{k-1}} > \frac{q_{k-1}m - p_{k-1}i}{q_{k-1}q_k} \geq \frac{1}{q_{k-1}q_k},$$

a contradiction.

To prove (6.4) we need to show that for all $0 \leq i \leq q_{k-2} - 1$, $\left\lfloor \frac{p_k}{q_k} i \right\rfloor = \left\lfloor \frac{p_{k-2}}{q_{k-2}} i \right\rfloor$. Next, we show that for all $0 \leq i \leq q_{k-2} - 1$, $\left\lfloor \frac{p_{k-2}}{q_{k-2}} i \right\rfloor = \left\lfloor \frac{p_k}{q_k} i \right\rfloor$ from which (6.2) of the Lemma follows when using Lemmas 2.3 and (2.6).

Assume toward contradiction that there exists $0 \leq i \leq q_{k-2} - 1$ such that $\left\lfloor \frac{p_{k-2}}{q_{k-2}} i \right\rfloor \neq \left\lfloor \frac{p_k}{q_k} i \right\rfloor$. Clearly, $i > 0$ must hold. Using $\frac{p_k}{q_k} < \frac{p_{k-2}}{q_{k-2}}$, we infer that there exists an $m \in \mathbb{N}$ such that

$$\frac{p_k}{q_k} < \frac{m}{i} \leq \frac{p_{k-2}}{q_{k-2}}.$$

Let $(c_i)_{i \in \mathbb{N}_0}$ be the infinite continued fraction expansion of α . Since k is odd, [27, Theorem 3] implies

$$\frac{c_k}{q_k q_{k-2}} = \frac{p_{k-2}}{q_{k-2}} - \frac{p_k}{q_k} > \frac{p_{k-2}}{q_{k-2}} - \frac{m}{i} = \frac{p_{k-2}i - mq_{k-2}}{iq_{k-2}}.$$

Hence, $i \leq q_{k-1} - 1$ and the recursive relation (2.3)

$$1 \geq \frac{c_k q_{k-1}}{q_k} > \frac{c_k i}{q_k} > p_{k-2}i - mq_{k-2} \geq 0.$$

Thus, $p_{k-2}i - mq_{k-2} = 0$ follows or equivalently $\frac{m}{i} = \frac{p_{k-2}}{q_{k-2}}$. This contradicts $i \leq q_{k-2} - 1$ and p_{k-1}, q_{k-1} are coprime. \square

The proof of the previous lemma allows to conclude the following, which will be used to prove the second part of Lemma 2.4.

Lemma 6.2 (The period as a prefix of a Sturmian sequence) *Let $\alpha \in [0, 1] \setminus \mathbb{Q}$ and $k \geq 2$.*

(a) *If $k \equiv 0 \pmod{2}$ then*

$$\omega_\alpha(i) = W_{k-1}(i) \quad \text{for all } 0 \leq i \leq q_{k-1} - 2.$$

(b) *If $k \equiv 1 \pmod{2}$ then*

$$\omega_\alpha(i) = W_{k-1}(i \pmod{q_{k-1}}) \quad \text{for all } 0 \leq i \leq q_k - 2.$$

Proof For the first part of the lemma, we use that when $k \equiv 0 \pmod{2}$ then $\frac{p_k}{q_k} < \alpha < \frac{p_{k-1}}{q_{k-1}}$ ([27, Theorem 8]). We have shown in the first part of the proof of Lemma 6.1 that for all $0 \leq i \leq q_{k-1} - 1$, $\left\lfloor \frac{p_k}{q_k} i \right\rfloor = \left\lfloor \frac{p_{k-1}}{q_{k-1}} i \right\rfloor$. Combining this with $\frac{p_k}{q_k} < \alpha < \frac{p_{k-1}}{q_{k-1}}$ we get that $\lfloor \alpha i \rfloor = \left\lfloor \frac{p_{k-1}}{q_{k-1}} i \right\rfloor$, for all $0 \leq i \leq q_{k-1} - 1$. Now, the first part of the current lemma follows when using the mechanical word representation as in Lemma 2.3.

For the second part of the lemma, we use that when $k \equiv 1 \pmod{2}$ then $\frac{p_{k-1}}{q_{k-1}} < \alpha < \frac{p_k}{q_k}$ ([27, Theorem 8]). We have shown in the second part of the proof of Lemma 6.1 that for all $0 \leq i \leq q_k - 1$, $\left\lfloor \frac{p_{k-1}}{q_{k-1}} i \right\rfloor = \left\lfloor \frac{p_k}{q_k} i \right\rfloor$. Combining this with $\frac{p_{k-1}}{q_{k-1}} < \alpha < \frac{p_k}{q_k}$ we get that $\left\lfloor \frac{p_{k-1}}{q_{k-1}} i \right\rfloor = \lfloor \alpha i \rfloor$, for all $0 \leq i \leq q_k - 1$. Now, the second part of the current lemma follows when using the mechanical word representation as in Lemma 2.3. \square

Lemma 6.3 (Period suffixes) *Let $\alpha \in [0, 1] \setminus \mathbb{Q}$ and $k \geq 2$.*

(a) *If $k \equiv 0 \pmod{2}$, then*

$$W_k(q_k - i) = W_{k-1}(q_{k-1} - i) \quad \text{for all } 1 \leq i \leq q_{k-1}. \quad (6.9)$$

(b) *If $k \equiv 1 \pmod{2}$, then*

$$W_k(q_k - i) = W_{k-2}(q_{k-2} - i) \quad \text{for all } 1 \leq i \leq q_{k-2}. \quad (6.10)$$

Proof Using (2.5) in Lemma 2.3 gives for all $k \geq 1$,

$$W_k(q_k - 1) = \lfloor (q_k - 1 + 1) \frac{p_k}{q_k} \rfloor - \lfloor (q_k - 1) \frac{p_k}{q_k} \rfloor = 1, \quad (6.11)$$

which proves the case $i = 1$ in (6.9) and (6.10). If $c_1 = 1$ and $k \in \{2, 3\}$, we conclude $q_1 = 1$ from (2.3), and hence the statement holds in this case (as we have shown that it holds for $i = 1$). Thus, in the sequel of the proof, when treating $k \in \{2, 3\}$, we will assume $c_1 > 1$.

We show another auxiliary statement which aids in the proof—that the sub-word $W_k|_{\{1, \dots, q_k-2\}}$ is a palindrome, i.e.:

$$W_k(i) = W_k(q_k - (i + 1)) \quad \text{for all } 1 \leq i \leq q_k - 2. \quad (6.12)$$

To prove this identity, observe for $1 \leq i \leq q - 2$ and p, q coprime,

$$\begin{aligned} \left\lfloor (q - i) \frac{p}{q} \right\rfloor - \left\lfloor (q - 1 - i) \frac{p}{q} \right\rfloor &= \left\lfloor -i \frac{p}{q} \right\rfloor - \left\lfloor -(i + 1) \frac{p}{q} \right\rfloor \\ &= -\left(\left\lfloor i \frac{p}{q} \right\rfloor + 1\right) + \left(\left\lfloor (i + 1) \frac{p}{q} \right\rfloor + 1\right) \\ &= \left\lfloor (i + 1) \frac{p}{q} \right\rfloor - \left\lfloor i \frac{p}{q} \right\rfloor. \end{aligned}$$

Thus, (6.12) follows from (2.5) in Lemma 2.3. We now proceed to prove the lemma using the above.

(a) Assume that $k \equiv 0 \pmod{2}$. For $2 \leq i \leq q_{k-1} - 1$, we have

$$W_k(q_k - i) = W_k(i - 1) = W_{k-1}(i - 1) = W_{k-1}(q_{k-1} - i),$$

where the first and third equalities follow from (6.12), and the second equality follows from (6.1) in Lemma 6.1. To finish this part of the proof we only need to show that (6.9) holds for $i = q_{k-1}$, i.e., that $W_k(q_k - q_{k-1}) = W_{k-1}(0) = 0$. Using [27, Theorem 2] we calculate

$$q_{k-1} \frac{p_k}{q_k} = \frac{1}{q_k} (q_{k-1} p_k - q_k p_{k-1}) + p_{k-1} = -\frac{1}{q_k} + p_{k-1}.$$

Hence,

$$\begin{aligned} W_k(q_k - q_{k-1}) &= \left\lfloor (q_k - q_{k-1} + 1) \frac{p_k}{q_k} \right\rfloor - \left\lfloor (q_k - q_{k-1}) \frac{p_k}{q_k} \right\rfloor \\ &= \left\lfloor p_k - p_{k-1} + \frac{1}{q_k} + \frac{p_k}{q_k} \right\rfloor - \left\lfloor p_k - p_{k-1} + \frac{1}{q_k} \right\rfloor \\ &= \left\lfloor \frac{p_k + 1}{q_k} \right\rfloor - \left\lfloor \frac{1}{q_k} \right\rfloor = 0, \end{aligned}$$

follows where in the last equality we used that $q_k > p_k + 1$, which holds if $k > 2$ or if $k = 2$ and $c_1 > 1$ (which we can assume since we have already dealt the case $k = 2$, $c_1 = 1$ in the beginning of the proof).

(b) Assume that $k \equiv 1 \pmod{2}$. For $2 \leq i \leq q_{k-2} - 1$ we have

$$W_k(q_k - i) = W_k(i - 1) = W_{k-2}(i - 1) = W_{k-2}(q_{k-2} - i),$$

where the first and third equalities follow from (6.12), and the second equality follows from (6.4) in Lemma 6.1. To finish this part of the proof we only need to show that (6.10) holds for $i = q_{k-2}$, i.e., that $W_k(q_k - q_{k-2}) = W_{k-2}(0) = 0$. Using [27, Theorem 3] we calculate

$$q_{k-2} \frac{p_k}{q_k} = \frac{1}{q_k} (q_{k-2} p_k - q_k p_{k-2}) + p_{k-2} = -\frac{c_k}{q_k} + p_{k-2}.$$

Hence, we conclude

$$\begin{aligned} W_k(q_k - q_{k-2}) &= \left\lfloor (q_k - q_{k-2} + 1) \frac{p_k}{q_k} \right\rfloor - \left\lfloor (q_k - q_{k-2}) \frac{p_k}{q_k} \right\rfloor \\ &= \left\lfloor p_k - p_{k-2} + \frac{c_k}{q_k} + \frac{p_k}{q_k} \right\rfloor - \left\lfloor p_k - p_{k-2} + \frac{c_k}{q_k} \right\rfloor \\ &= \left\lfloor \frac{p_k + c_k}{q_k} \right\rfloor - \left\lfloor \frac{c_k}{q_k} \right\rfloor. \end{aligned}$$

To conclude $W_k(q_k - q_{k-2}) = 0$, we now show $\frac{c_k}{q_k} < 1$ and $\frac{p_k + c_k}{q_k} < 1$. The recursions (2.3) lead to

$$\frac{c_k}{q_k} = \frac{1}{q_k} \frac{q_k - q_{k-2}}{q_{k-1}} < 1$$

and

$$\frac{p_k + c_k}{q_k} = \frac{c_k (p_{k-1} + 1) + p_{k-2}}{c_k q_{k-1} + q_{k-2}} < 1,$$

where to get the last inequality we observe that for $k \geq 3$ (recalling that $k \geq 2$ and we consider now odd k values) $p_{k-2} \leq q_{k-2}$ and $p_{k-1} + 1 \leq q_{k-1}$, and equality in both of these may be achieved only if $k = 3$ and $c_1 = 1$ (which yields $p_1 = q_1 = 1$ and $p_2 + 1 = c_2 = q_2$), but we have already dealt with this case in the beginning of the proof. □

Lemma 6.4 (Sub-periods of the period) *Let $\alpha \in [0, 1] \setminus \mathbb{Q}$ and $k \geq 2$.*

(a) *If $k \equiv 0 \pmod{2}$, then*

$$W_k(i) = W_k(i + q_{k-1} \pmod{q_k}) \quad \text{for all } 1 \leq i \leq q_k - 2. \quad (6.13)$$

(b) *If $k \equiv 1 \pmod{2}$, then*

$$W_k(i \pmod{q_k}) = W_k(i + q_{k-1} \pmod{q_k}) \quad \text{for all } -q_{k-1} + 1 \leq i \leq q_k - q_{k-1} - 2. \quad (6.14)$$

Proof As before we use frequently (2.5) in Lemma 2.3.

(a) Let $k \equiv 0 \pmod{2}$. Let $1 \leq i \leq q_k - 2$. Since p_k, q_k are coprime, we conclude

$j \frac{p_k}{q_k} \notin \mathbb{Z}$ and $\left\lfloor j \frac{p_k}{q_k} - \frac{1}{q_k} \right\rfloor = \left\lfloor j \frac{p_k}{q_k} \right\rfloor$ for all $1 \leq j \leq q_k - 1$. Then

$$\begin{aligned} W_k(i + q_{k-1} \pmod{q_k}) &= \left\lfloor (i + 1 + q_{k-1}) \frac{p_k}{q_k} \right\rfloor - \left\lfloor (i + q_{k-1}) \frac{p_k}{q_k} \right\rfloor \\ &= \left\lfloor (i + 1) \frac{p_k}{q_k} + \left(q_{k-1} \frac{p_k}{q_k} - p_{k-1} \right) \right\rfloor - \left\lfloor i \frac{p_k}{q_k} + \left(q_{k-1} \frac{p_k}{q_k} - p_{k-1} \right) \right\rfloor \\ &= \left\lfloor (i + 1) \frac{p_k}{q_k} - \frac{1}{q_k} \right\rfloor - \left\lfloor i \frac{p_k}{q_k} - \frac{1}{q_k} \right\rfloor \\ &= \left\lfloor (i + 1) \frac{p_k}{q_k} \right\rfloor - \left\lfloor i \frac{p_k}{q_k} \right\rfloor = W_k(i) \end{aligned}$$

follows where we used [27, Theorem 2] in the third equality.

(b) Let $k \equiv 1 \pmod{2}$. Let $-q_{k-1} + 1 \leq i \leq q_k - q_{k-1} - 2$.

$$\begin{aligned} W_k(i + q_{k-1}) &= \left\lfloor (i + 1 + q_{k-1}) \frac{p_k}{q_k} \right\rfloor - \left\lfloor (i + q_{k-1}) \frac{p_k}{q_k} \right\rfloor \\ &= \left\lfloor (i + 1) \frac{p_k}{q_k} + \left(q_{k-1} \frac{p_k}{q_k} - p_{k-1} \right) \right\rfloor - \left\lfloor i \frac{p_k}{q_k} + \left(q_{k-1} \frac{p_k}{q_k} - p_{k-1} \right) \right\rfloor \\ &= \left\lfloor (i + 1) \frac{p_k}{q_k} + \frac{1}{q_k} \right\rfloor - \left\lfloor i \frac{p_k}{q_k} + \frac{1}{q_k} \right\rfloor. \end{aligned} \tag{6.15}$$

Thus, it suffices to prove (quite similar to the proof of the first part) that for all $-q_{k-1} + 1 \leq j \leq q_k - q_{k-1} - 1$,

$$\left\lfloor j \frac{p_k}{q_k} + \frac{1}{q_k} \right\rfloor = \left\lfloor j \frac{p_k}{q_k} \right\rfloor.$$

Assume toward contradiction that $\left\lfloor j \frac{p_k}{q_k} + \frac{1}{q_k} \right\rfloor \neq \left\lfloor j \frac{p_k}{q_k} \right\rfloor$ for some $-q_{k-1} + 1 \leq j \leq q_k - q_{k-1} - 1$. This means that there exists $m \in \mathbb{Z}$ such that $j \frac{p_k}{q_k} + \frac{1}{q_k} = m$. Therefore,

$$j p_k \equiv -1 \pmod{q_k}. \tag{6.16}$$

By [27, Theorem 2] $-q_{k-1} p_k + p_{k-1} q_k = -1$. Thus, $j = -q_{k-1}$ is a solution to (6.16). In fact, since p_k, q_k are coprime any solution to (6.16) satisfies $j \equiv -q_{k-1} \pmod{q_k}$. We now obtain a contradiction since there is no such value in the range $j \in \{-q_{k-1} + 1, \dots, q_k - q_{k-1} - 1\}$.

□

We now combine the last three lemmas to prove Lemma 2.4.

Proof (Proof of Lemma 2.4) A short computation leads to $W_0 = 0$ with $\alpha_0 = \frac{0}{1}$ and $W_1 = \underbrace{0 \dots 0}_{c_1-1} 1$ with $\alpha_1 = \frac{1}{c_1}$.

We start by observing that the second part of the lemma follows quite straightforwardly from Lemma 6.2. To see this note that Lemma 6.2 connects ω_α to W_{k-1} (rather than to W_k as in the statement of Lemma 2.4), so an appropriate conversion (and a switch of the parity of k) should be done. Further note that when treating the case $k \equiv 0 \pmod 2$ we have by (2.3) that $q_{k+1} \geq q_k + 1$, which allows to conclude that the equality for this case holds for all $0 \leq i \leq q_k - 1$ (by Lemma 6.2, (b) it holds for $0 \leq i \leq q_{k+1} - 2$).

We proceed to prove the first part of the lemma and, as before, distinguish between two cases according to the parity of k :

- (a) Let $k \equiv 0 \pmod 2$. We first treat the case $k = 2$ and $c_1 = 1$. In this case, we have $W_0 = 0$ and $W_1 = 1$. Then the recursion relation (2.3) asserts $\alpha_1 = \frac{p_1}{q_1} = \frac{1}{1}$ and $\alpha_2 = \frac{p_2}{q_2} = \frac{c_2}{c_2+1}$. Thus, $W_2 = 0 \underbrace{1 \dots 1}_{c_2} = W_0 W_1^{c_2}$ follows as claimed by (2.4) and

(2.6). Therefore, we can from now on assume that if $k = 2$, then $c_1 > 1$.

Next, observe that $q_{k-1} = q_{k-2}$ can happen only for $k = 2$ and $c_1 = 1$ (as can be verified from (2.3)). Therefore, we may continue the proof assuming that $q_{k-1} > q_{k-2}$.

Applying (6.2) in Lemma 6.1 establishes the required statement for the prefix of W_k , i.e.:

$$W_{k-2} = W_k|_{\{0, \dots, q_{k-2}-1\}} = W_k|_{\{0, \dots, q_k - c_k q_{k-1} - 1\}},$$

where we used $q_{k-1} > q_{k-2}$ and the recursive relation (2.3) of $\{q_k\}$.

Applying (6.9) in Lemma 6.3 gives

$$W_k|_{\{q_k - q_{k-1}, \dots, q_k - 1\}} = W_{k-1}.$$

The last equality together with (6.13) in Lemma 6.4 yields

$$W_k|_{\{q_k - c_k q_{k-1}, \dots, q_k - 1\}} = W_{k-1}^{c_k},$$

and completes the proof of this part.

- (b) Let $k \equiv 1 \pmod 2$.

Applying (6.10) in Lemma 6.3 establishes the required statement for the suffix of W_k , i.e.:

$$W_{k-2} = W_k|_{\{q_k - q_{k-2}, \dots, q_k - 1\}} = W_k|_{\{c_k q_{k-1}, \dots, q_k - 1\}},$$

where we used the recursive relation (2.3) of $\{q_k\}$. Applying (6.3) in Lemma 6.1 gives

$$W_k|_{\{0, \dots, q_{k-1}-1\}} = W_{k-1}.$$

We observe that in this case we have $k \geq 3$ and $q_{k-2} \geq 1$. Hence, the last equality together with (6.14) in Lemma 6.4 yields

$$W_k|_{\{0, \dots, c_k q_{k-1} - 1\}} = W_{k-1}^{c_k},$$

and completes the proof. \square

Having proven Lemma 2.4, we use the arguments from the proof in order to draw useful insights on the corresponding dynamical system. We refer the reader to [6, 7, 12, 13] for more background on the dynamical perspective.

Let \mathcal{A} be a finite set (frequently called an alphabet). The set $\mathcal{A}^{\mathbb{Z}} = \{\omega : \mathbb{Z} \rightarrow \mathcal{A}\}$ is a compact metrizable space if equipped with the product topology. The shift $T : \mathcal{A}^{\mathbb{Z}} \rightarrow \mathcal{A}^{\mathbb{Z}}$ is defined by $(T\omega)(n) := \omega(n-1)$ for all $n \in \mathbb{Z}$, and it is a homeomorphism. Then we can define the action of the group \mathbb{Z} on $\mathcal{A}^{\mathbb{Z}}$, where the shift T is the generator of \mathbb{Z} and hence $(\mathcal{A}^{\mathbb{Z}}, T)$ defines a topological dynamical system. Denote by $\text{Orb}(\omega) := \{T^n \omega : n \in \mathbb{Z}\}$ the orbit of $\omega \in \mathcal{A}^{\mathbb{Z}}$ under this action. For a given $\alpha \in [0, 1]$, the orbit closure $\overline{\text{Orb}(\omega_\alpha)}$ is denoted by Ω_α where $\omega_\alpha \in \mathcal{A}^{\mathbb{Z}}$ is the sequence defined in Eq. (2.4). Since Ω_α is shift invariant (i.e., $T(\Omega_\alpha) = \Omega_\alpha$) and closed, (Ω_α, T) is also a dynamical system. If $\alpha \in [0, 1] \setminus \mathbb{Q}$, then (Ω_α, T) is called a *Sturmian dynamical system*. Using the previous results, we provide in the following a representation of Ω_β for $\beta \in [0, 1] \cap \mathbb{Q}$.

Consider the alphabet $\mathcal{A} = \{0, 1\}$. A finite word is a concatenation $v_1 v_2 \dots v_k$ of letters $v_n \in \mathcal{A}$ for $1 \leq n \leq k$. For a finite continued fraction expansion $\mathbf{c} = [0, 0, c_1, \dots, c_k] \in \mathcal{C}$, with $c_k \notin \{-1, 0\}$, recursively define the finite words $s_n := s_n(\mathbf{c})$ for $-1 \leq n \leq k$ by

$$s_{-1} = 1, \quad s_0 = 0, \quad s_1 = 0^{c_1-1} 1, \quad s_n = s_{n-1}^{c_n} s_{n-2} \text{ for } 2 \leq n \leq k,$$

where s^m denotes the m -times concatenation of the word s . The two-sided infinite concatenation of the word s is denoted by $s^\infty \in \mathcal{A}^{\mathbb{Z}}$. We further denote $s(\mathbf{c}) := s_k(\mathbf{c})$ for a finite continued fraction $\mathbf{c} = [0, 0, c_1, \dots, c_k]$.

Given a rational number $\beta \in (0, 1) \cap \mathbb{Q}$, a finite continued fraction expansions \mathbf{c} satisfying $\varphi(\mathbf{c}) = \beta$ is not unique, see Remark 2.1. However, the corresponding dynamical system Ω_β can be represented via $s(\mathbf{c})^\infty$ for any \mathbf{c} satisfying $\varphi(\mathbf{c}) = \beta$:

Corollary 6.5 *Let $\beta = \frac{p}{q} \in (0, 1) \cap \mathbb{Q}$ be such that p, q are coprime. Fix a finite continued fraction expansion $\mathbf{c} = [0, 0, c_1, \dots, c_k] \in \mathcal{C}$, with $c_k \notin \{-1, 0\}$, such that $\varphi(\mathbf{c}) = \beta$. Then $\text{Orb}(s(\mathbf{c})^\infty) = \Omega_\beta$. Furthermore, $\text{Orb}(s([0, 0])^\infty) = \Omega_0$ and $\text{Orb}(s([0, 0, 1])^\infty) = \Omega_1$.*

Proof If $\beta = 0$, then only $\mathbf{c} = [0, 0]$ satisfies $\varphi(\mathbf{c}) = \beta$. Thus, $s(\mathbf{c}) = s_0 = 0$ and $\omega_\beta = 0^\infty$ proving the claim. If $\beta = 1$, then only $\mathbf{c} = [0, 0, 1]$ satisfies $\varphi(\mathbf{c}) = \beta$. Thus, $s(\mathbf{c}) = s_1 = 1$ and $\omega_\beta = 1^\infty$ proving the claim.

Now, let $\beta \in (0, 1) \cap \mathbb{Q}$. We first note that there exist exactly two (using $\beta \in (0, 1)$ and $c_k \notin \{-1, 0\}$) finite continued fraction expansions for β (a short and a long one) denoted by

$$\mathbf{c}_s = [0, 0, c_1, \dots, c_m + 1] \quad \text{and} \quad \mathbf{c}_l = [0, 0, c_1, \dots, c_m, 1].$$

We first show that $\text{Orb}(s(\mathbf{c}_s)^\infty) = \text{Orb}(s(\mathbf{c}_l)^\infty)$. Since the continued fractions \mathbf{c}_s and \mathbf{c}_l share the same digits up to $m - 1$, we have $s_k := s_k(\mathbf{c}_s) = s_k(\mathbf{c}_l)$ for all $k \leq m - 1$. Hence, $s(\mathbf{c}_s) = s_{m-1}^{c_m+1} s_{m-2}$ and $s(\mathbf{c}_l) = s_{m-1}^{c_m} s_{m-2} s_{m-1}$ follows by the recursive definition. Thus, $\text{Orb}(s(\mathbf{c}_s)^\infty) = \text{Orb}(s(\mathbf{c}_l)^\infty)$ follows since $s(\mathbf{c}_s)^\infty$ is the same word as $s(\mathbf{c}_l)^\infty$ up to a shift (by the length of the word s_{m-1}).

Define

$$\mathbf{c} := \begin{cases} \mathbf{c}_s & m \equiv 0 \pmod{2}, \\ \mathbf{c}_l & m \equiv 1 \pmod{2}. \end{cases}$$

Note that the words $s(\mathbf{c}_s)$ and $s(\mathbf{c}_l)$ generate the same orbit by the previous considerations. By construction, $\mathbf{c} = [0, 0, c_1, \dots, c_j]$ is a tuple of an even length, i.e., $j \in \mathbb{N}$ is even. Choose $\alpha \in [0, 1] \setminus \mathbb{Q}$ with continued fraction expansion $(d_k)_{k \in \mathbb{N}_0}$ such that $\mathbf{c} = [0, 0, d_1, \dots, d_j]$, namely $c_k = d_k$ for all $k \leq j$. Applying [31, prop. 2.2.24] to α yields $\omega_\alpha|_{[1, q_j]} = s([0, 0, d_1, \dots, d_j]) = s(\mathbf{c})$. Note that $s(\mathbf{c})$ is a finite word of length q_j and let $v_i \in \{0, 1\}$ be the letters of this word, namely $s(\mathbf{c}) = v_1 \dots v_{q_j}$. Set $u = v_1 \dots v_{q_j-1}$, which is the prefix of $s(\mathbf{c})$ where we deleted the last letter. Since $\beta = \varphi(\mathbf{c}) = \alpha_j$ and $j \in \mathbb{N}$ is even, Lemma 6.2 implies $\omega_\alpha|_{[0, q_j-1]} = W_j = \omega_{\alpha_j}|_{[0, q_j-1]}$. Since $\alpha < 1$, we have $\omega_\alpha(0) = 0$. Combined with the previous considerations, we have $\omega_{\alpha_j}|_{[0, q_j-1]} = 0u$, a word of length q_j . Thus,

$$\Omega_\beta = \Omega_{\alpha_j} = \text{Orb}((0u)^\infty).$$

Since we wish to prove $\text{Orb}(s(\mathbf{c})^\infty) = \Omega_\beta$, it suffices to show that $v_{q_j} = 0$, since then $s(\mathbf{c}) = u0$ and $\text{Orb}((0u)^\infty) = \text{Orb}((u0)^\infty)$ holds trivially. The claim that the last digit of $s(\mathbf{c})$ is zero (i.e., $v_{q_j} = 0$) follows inductively from the definition of the words using $s_0 = 0$ and $s_k = s_{k-1}^{c_k} s_{k-2}$ and since j is even (such a statement also appears in [31, problem 2.2.10]). \square

7 Floquet-Bloch Theory Via Finite-Dimensional Hamiltonian Matrices

This section complements Sect. 3 by providing an alternative approach for the spectral analysis of the periodic operators, $H_{\frac{p}{q}, V}$. In Sect. 3.1 the Floquet-Bloch theory is described in terms of transfer matrices and the discriminant, whereas here we make use of finite Hamiltonian matrices $H_{\mathbf{c}, V}(\theta)$. These matrices $H_{\mathbf{c}, V}(\theta)$ play a crucial

role in [3] and henceforth it is advantageous to introduce them already here and make the appropriate connection to the transfer matrices.

We use here the continued fraction notation, $\mathbf{c} \in \mathcal{C}$ and denote the corresponding rational number by $\frac{p}{q} := \varphi(\mathbf{c})$. The corresponding operator is

$$(H_{\frac{p}{q},V}\psi)(n) := \psi(n+1) + \psi(n-1) + V\omega_{\frac{p}{q}}(n)\psi(n),$$

where the potential is given by the mechanical word,

$$\omega_{\frac{p}{q}}(n) := \chi_{[1-\frac{p}{q},1)}\left(n\frac{p}{q} \bmod 1\right),$$

which is q periodic (see Sect. 2.2). To describe the relevant Floquet-Bloch theory, we define the following finite-dimensional auxiliary matrix

$$H_{\mathbf{c},V}(\theta) := \begin{cases} 2 \cos(\theta) + V\omega_{\frac{p}{q}}(0), & q = 1, \\ \begin{pmatrix} V\omega_{\frac{p}{q}}(0) & 1 + e^{-i\theta} \\ 1 + e^{i\theta} & V\omega_{\frac{p}{q}}(1) \end{pmatrix}, & q = 2, \\ \begin{pmatrix} V\omega_{\frac{p}{q}}(0) & 1 & 0 & \dots & e^{-i\theta} \\ 1 & V\omega_{\frac{p}{q}}(1) & 1 & \dots & 0 \\ 0 & 1 & \ddots & & \vdots \\ \vdots & \ddots & & \ddots & 0 \\ 0 & & & & 1 \\ e^{i\theta} & 0 & \dots & 0 & 1 \end{pmatrix} V\omega_{\frac{p}{q}}(q-1) \end{pmatrix}, & q > 2. \end{cases} \quad (7.1)$$

The characteristic polynomial of the matrix above is denoted by

$$P_{\mathbf{c},V}(\theta; E) := \det(E - H_{\mathbf{c},V}(\theta)).$$

Using the auxiliary matrices defined above, we get the following by standard Floquet-Bloch theory (see e.g., [46, Sect. 7.2], [43, Sect. 5.3]).

Proposition 7.1 *Let $V \in \mathbb{R}$ and $\mathbf{c} \in \mathcal{C}$ with $\frac{p}{q} = \varphi(\mathbf{c}) \neq \infty$.*

(a) *The spectrum of $H_{\frac{p}{q},V}$ is given by*

$$\sigma(H_{\frac{p}{q},V}) = \bigcup_{\theta \in [0, \pi]} \sigma(H_{\mathbf{c},V}(\theta)).$$

(b) Suppose p and q are coprime. Denoting the roots of $P_{\mathbf{c},V}(\theta; \cdot)$ by $\left\{ \lambda_i^{(\theta)} \right\}_{i=1}^q$ we have

$$\lambda_{q-1}^{(0)} > \lambda_{q-1}^{(\pi)} > \lambda_{q-2}^{(\pi)} > \lambda_{q-2}^{(0)} > \lambda_{q-3}^{(0)} > \lambda_{q-3}^{(\pi)} > \dots \quad (7.2)$$

and get that $\sigma(H_{\frac{p}{q},V})$ is the following union of q disjoint closed intervals

$$\sigma(H_{\frac{p}{q},V}) = \dots \sqcup \left[\lambda_{q-3}^{(\pi)}, \lambda_{q-3}^{(0)} \right] \sqcup \left[\lambda_{q-2}^{(0)}, \lambda_{q-2}^{(\pi)} \right] \sqcup \left[\lambda_{q-1}^{(\pi)}, \lambda_{q-1}^{(0)} \right], \quad (7.3)$$

which are commonly called spectral bands.

The general statement of Proposition 7.1 within Floquet-Bloch theory is with weak inequalities in (7.2) and possible intersections of the spectral bands in (7.3) at their edges. Specifically, in our case where the potential is given by $\omega_{\frac{p}{q}}(n)$, this slightly stronger version holds since p, q are coprime—a proof is found in Proposition 4.1 using transfer matrices.

Since Floquet-Bloch theory may be described either in terms of transfer matrices (as in Sect. 3.1) and in terms of finite-dimensional Hamiltonian matrices (as in this section), it makes sense to draw a direct connection between both. Hence, we explicitly state the connection between the trace $t_{\mathbf{c}}$ of the transfer matrix (i.e., the discriminant) and the characteristic polynomial $P_{\mathbf{c},V}$:

Lemma 7.2 For all $\theta \in [0, 2\pi]$,

$$P_{\mathbf{c},V}(\theta; E) = t_{\mathbf{c}}(E, V) - 2 \cos(\theta).$$

A standard way to prove the identity in the lemma is to develop the Floquet-Bloch theory using both the discriminant $t_{\mathbf{c}}$ and the characteristic polynomial $P_{\mathbf{c},V}$ and note that these two polynomials have common roots. See for example [43, Theorem 5.4.1.(iii)]. Nevertheless, we bring here a direct computational proof⁴ which exploits the structure of the matrix $H_{\mathbf{c},V}(\theta)$.

Proof As usual, denote $\frac{p}{q} := \varphi(\mathbf{c})$, with coprime p, q . We first prove the statement assuming $q \geq 3$ and at the end check that it holds also for the cases $q = 1$ and $q = 2$. Start by examining $P_{\mathbf{c},V}(\theta; E) + 2 \cos(\theta) = \det(E\mathbf{1} - H_{\mathbf{c},V}(\theta)) + 2 \cos(\theta)$ and decomposing it into summands. We use the Leibniz formula for determinants to get

$$P_{\mathbf{c},V}(\theta; E) = \sum_{\sigma \in S_q} \text{sign}(\sigma) \prod_{n=1}^q [E\mathbf{1} - H_{\mathbf{c},V}(\theta)]_{n,\sigma(n)}, \quad (7.4)$$

where S_q is the set of all permutations on $[q] := \{1, 2, \dots, q\}$. We examine only permutations with a non-vanishing contribution to the sum above. Let $\sigma \in S_q$ be such permutation and $n \in [q]$. We have that $[E\mathbf{1} - H_{\mathbf{c},V}(\theta)]_{n,\sigma(n)} \neq 0$ only if $\sigma(n) \in \{n-1, n, n+1\}$ (noting that we consider a cyclic ordering of the indices in the set

⁴ An idea toward such a proof is also found in remark 3 after [43, Theorem 5.4.1].

$[q]$, such that if $n = 1$ then $n - 1 := q$ and if $n = q$ then $n + 1 = 1$). If $\sigma(n) = n + 1$, then we can have either $\sigma(n + 1) = n$ or $\sigma(n + 1) = n + 2$ (so that the corresponding product in (7.4) differs than zero). In the first case, we see that the permutation σ contains an involution, $(n \ n + 1)$. The second case imposes that σ is the cyclic permutation, $\sigma_{\text{cyc}}^+ = (1 \ 2 \ \dots \ q - 1 \ q)$, as all other permutations which satisfy both $\sigma(n) = n + 1$ and $\sigma(n + 1) = \sigma(n + 2)$ have a vanishing contribution to (7.4). Explicitly the contribution of σ_{cyc}^+ to this sum is

$$\text{sign}(\sigma_{\text{cyc}}^+) \left(\prod_{n=1}^{q-1} [E\mathbf{1} - H_{\mathbf{c}, V}(\theta)]_{n, n+1} \right) [-H_{\mathbf{c}, V}(\theta)]_{q, 1} = (-1)^{q+1} (-1)^{q-1} (-e^{i\theta}) = -e^{i\theta}.$$

If we repeat the arguments above for the case $\sigma(n) = n - 1$ we get that either σ contains the involution $(n - 1 \ n)$ or that it is the cyclic permutation $\sigma_{\text{cyc}}^- = (q \ q - 1 \ \dots \ 2 \ 1)$ whose contribution to (7.4) is $-e^{-i\theta}$. Hence, the contribution of both σ_{cyc}^+ and σ_{cyc}^- sums to $-2 \cos(\theta)$. All other permutations with non-vanishing contribution to (7.4) contain only involutions of the form $(n - 1 \ n)$ or fixed points (n) . We denote the set of such permutations by \tilde{S}_q and summarize the discussion so far by writing

$$P_{\mathbf{c}, V}(\theta; E) + 2 \cos(\theta) = \sum_{\sigma \in \tilde{S}_q} (-1)^{|I(\sigma)|} \prod_{n \in F(\sigma)} \left(E - V \omega_{\frac{p}{q}}(n - 1) \right), \quad (7.5)$$

where $I(\sigma)$ is the set of involutions $(n \ n + 1)$ of σ and $F(\sigma)$ is the set of fixed points of σ .

Now, we consider $t_{\mathbf{c}}(E, V)$ and decompose it into summands. To do so, we recall (see Sect. 3.1) the definition of $M_{\mathbf{c}}(E, V)$ as the product of one-step transfer matrices,

$$A_{\alpha}(n)(E, V) := \begin{pmatrix} E - V \omega_{\alpha}(n - 1) & -1 \\ 1 & 0 \end{pmatrix},$$

and write

$$t_{\mathbf{c}}(E, V) = \text{tr}(M_{\mathbf{c}}(E, V)) \quad (7.6)$$

$$= \text{tr} \left(\prod_{n=1}^q A_{\varphi(\mathbf{c})}(n)(E, V) \right) \quad (7.7)$$

$$= \sum_{\nu \in \{1, 2\}^q} \prod_{n=1}^q [A_{\varphi(\mathbf{c})}(n)(E, V)]_{\nu_n, \nu_{n+1}}, \quad (7.8)$$

where we have the interpretation $\nu_{q+1} := \nu_1$ due to the cyclic property of the trace. In the sum above, a summand which corresponds to $\nu \in \{1, 2\}^q$ is non-zero if and only

if there is no n such that $\nu_n = \nu_{n+1} = 2$. We denote the set of all such $\nu \in \{1, 2\}^q$ with non-vanishing contribution by $\tilde{\mathcal{N}}_q$, so that

$$t_{\mathbf{c}}(E, V) = \sum_{\nu \in \tilde{\mathcal{N}}_q} \prod_{n=1}^q [A_{\varphi(\mathbf{c})}(n)(E, V)]_{\nu_n, \nu_{n+1}}. \quad (7.9)$$

For the last part of this proof, we show a bijection $h : \tilde{\mathcal{S}}_q \rightarrow \tilde{\mathcal{N}}_q$ such that the contribution of $\sigma \in \tilde{\mathcal{S}}_q$ to (7.5) equals the contribution of $h(\sigma)$ to (7.9). We explicitly construct this bijection as follows: for any fixed point $n \in F(\sigma)$ we set

$$h(\sigma)_n = h(\sigma)_{n+1} = 1,$$

and for any involution $(n \ n+1) \in I(\sigma)$ we set

$$h(\sigma)_n = 1, \quad h(\sigma)_{n+1} = 2, \quad h(\sigma)_{n+2} = 1.$$

First, the map $h : \tilde{\mathcal{S}}_q \rightarrow \tilde{\mathcal{N}}_q$ is well defined, as no two subsequent entries of $h(\sigma)$ may be equal to 2. Furthermore, one can see that it is a bijection and for each $\nu \in \tilde{\mathcal{N}}_q$ one can uniquely construct the corresponding $\sigma \in \tilde{\mathcal{S}}_q$ such that $h(\sigma) = \nu$. Finally, it is also not hard to check that the contribution to the corresponding sum ((7.5) or (7.9)) is preserved under the map h .

We end the proof by checking that the statement holds for the particular cases of $q = 1$ and $q = 2$.

For $q = 1$ we have

$$P_{\mathbf{c}, V}(\theta; E) = E - \left(2 \cos + V \omega_{\frac{p}{q}}(0)\right),$$

and

$$t_{\mathbf{c}}(E, V) = \text{tr} \left(A_{\frac{p}{q}}(1)(E, V) \right) = \text{tr} \begin{pmatrix} E - V \omega_{\frac{p}{q}}(0) & -1 \\ 1 & 0 \end{pmatrix} = E - V \omega_{\frac{p}{q}}(0).$$

For $q = 2$ we have

$$\begin{aligned} P_{\mathbf{c}, V}(\theta; E) &= \det \begin{pmatrix} E - V \omega_{\frac{p}{q}}(0) & -(1 + e^{-i\theta}) \\ -(1 + e^{i\theta}) & E - V \omega_{\frac{p}{q}}(1) \end{pmatrix} \\ &= \left(E - V \omega_{\frac{p}{q}}(1) \right) \left(E - V \omega_{\frac{p}{q}}(0) \right) - 2 - 2 \cos(\theta), \end{aligned}$$

and

$$\begin{aligned}
t_c(E, V) &= \text{tr} \left(A_{\frac{p}{q}}(2)(E, V) \cdot A_{\frac{p}{q}}(1)(E, V) \right) \\
&= \text{tr} \left[\begin{pmatrix} E - V\omega_{\frac{p}{q}}(1) & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} E - V\omega_{\frac{p}{q}}(0) & -1 \\ 1 & 0 \end{pmatrix} \right] \\
&= \text{tr} \left[\begin{pmatrix} (E - V\omega_{\frac{p}{q}}(1))(E - V\omega_{\frac{p}{q}}(0)) - 1 & -E + V\omega_{\frac{p}{q}}(1) \\ E - V\omega_{\frac{p}{q}}(1) & -1 \end{pmatrix} \right] \\
&= (E - V\omega_{\frac{p}{q}}(1))(E - V\omega_{\frac{p}{q}}(0)) - 2.
\end{aligned}$$

□

8 Dilated Chebychev Polynomials of the Second Kind

In this section we collect proofs to the statements and identities around the dilated Chebychev polynomials of second kind. Recall that we defined these polynomials recursively by setting

$$S_{-1}(x) := 0, \quad S_0(x) := 1 \quad \text{and} \quad S_n(x) := xS_{n-1}(x) - S_{n-2}(x) \text{ for all } n \in \mathbb{N}.$$

We also remind the reader that the classical Chebychev polynomials of second kind can be defined using the recursion formula

$$U_{-1}(x) := 0, \quad U_0(x) := 1 \quad \text{and} \quad U_n(x) := 2xU_{n-1}(x) - U_{n-2}(x) \text{ for all } n \in \mathbb{N}.$$

Lemma 8.1 *For all $n \in \mathbb{N}_{-1}$ and all $x \in \mathbb{R}$ we have $S_n(2x) = U_n(x)$.*

Proof We perform a proof by induction over $n \in \mathbb{N}_{-1}$. For $n = -1$ and $n = 0$ the statement follows directly from the definition. Therefore let $n \in \mathbb{N}$ and assume $S_{n-1}(2x) = U_{n-1}(x)$ and $S_{n-2}(2x) = U_{n-2}(x)$ for all $x \in \mathbb{R}$. Then we get

$$S_n(2x) = 2xS_{n-1}(2x) - S_{n-2}(2x) = 2xU_{n-1}(x) - U_{n-2}(x) = U_n(x).$$

□

Lemma 8.2 *Let $x \in \mathbb{R}$ and $n \in \mathbb{N}_0$. Then the following holds.*

- (a) *We have $S_{n+1}(x)S_{n-1}(x) - S_n(x)^2 = -1$.*
- (b) *If $|x| = 2$, then $\text{sign}(x)^{n-1}S_{n-1}(x) = n$.*
- (c) *If $|x| \geq 2$, then $2|S_n(x)| - |S_{n-1}| \geq 0$.*
- (d) *If $|x| \geq 2$, then $\text{sign}(x)^n S_n(x) = |S_n(x)|$ and*

$$\text{sign}(x)^n x S_{n-1}(x) \geq 2|S_{n-1}(x)|.$$

(e) If $|x| \geq 2$, then

$$\text{sign}(x)^n \left(S_n(x) - \frac{x}{2} S_{n-1}(x) \right) \geq 1.$$

(f) If $|x| \geq 2$, then $|S_n(x)| \geq 1$.

(g) If $|x| > 2$ and $n \geq 1$, then

$$\text{sign}(x)^n \left(S_n(x) - \frac{x}{2} S_{n-1}(x) \right) > 1.$$

Proof We prove each statement by an induction over n .

(a) For $n = 0$ and $n = 1$, observe

$$S_1(x)S_{-1}(x) - S_0(x)^2 = -1^2 = -1,$$

and

$$S_2(x)S_0(x) - S_1(x)^2 = (x^2 - 1) - x^2 = -1.$$

Suppose the statement is true for $n \in \mathbb{N}$ and $n - 1$, then

$$\begin{aligned} S_{n+1}S_{n-1} - S_n^2 &= (xS_n - S_{n-1})S_{n-1} - S_n^2 \\ &= S_n \underbrace{(xS_{n-1} - S_n)}_{=S_{n-2}} - S_{n-1}^2 \\ &= S_nS_{n-2} - S_n = -1 \end{aligned}$$

follows.

(b) Let $|x| = 2$. For $n = 0$ and $n = 1$, observe in these cases

$$\text{sign}(x)^{-1}S_{-1}(x) = 0 \quad \text{and} \quad \text{sign}(x)^0S_0(x) = 1.$$

Suppose the statement is true for $n \in \mathbb{N}$ and $n - 1$, then

$$\begin{aligned} \text{sign}(x)^{n+1}S_{n+1} &= \text{sign}(x)^{n+1}(xS_n - S_{n-1}) \\ &= |x|(n+1) - n = 2(n+1) - n = (n+1) + 1. \end{aligned}$$

(c) Let $|x| \geq 2$. If $n = 0$, then $2|S_n| - |S_{n-1}| = 2 - 0 \geq 0$. Suppose the statement is true for $n \in \mathbb{N}_0$. Then

$$\begin{aligned} 2|S_{n+1}| - |S_n| &= 2|xS_n - S_{n-1}| - |S_n| \geq 2|x| \cdot |S_n| - |S_{n-1}| - |S_n| \\ &\geq 4|S_n| - |S_{n-1}| - |S_n| \\ &\geq 2|S_n| - |S_{n-1}| \geq 0 \end{aligned}$$

by induction hypothesis.

(d) Again, let $|x| \geq 2$ and consider $n = 0$ and $n = 1$ for the induction base. Then

$$\text{sign}(x)^0 S_0(x) = 1 = |S_0(x)| \quad \text{and} \quad \text{sign}(x)^1 S_1(x) = \text{sign}(x) \cdot x = |x| = |S_1(x)|.$$

Suppose it holds for $n \in \mathbb{N}$. Then

$$\begin{aligned} \text{sign}(x)^{n+1} S_{n+1}(x) &= \text{sign}(x)^{n+1} (x S_n - S_{n-1}) \\ &= |x| \cdot |S_n| - |S_{n-1}| \geq 2|S_n| - |S_{n-1}| \geq 0, \end{aligned}$$

where the last follows by the previous induction. Hence, $\text{sign}(x)^{n+1} S_{n+1}(x) = |S_{n+1}(x)|$ follows proving the first part of (8.2). Moreover, this and $|x| \geq 2$ lead to

$$\text{sign}(x)^n x S_{n-1}(x) = |x| |S_{n-1}(x)| \geq 2 |S_{n-1}(x)|$$

proving the second part of (8.2).

(e) Let $|x| \geq 2$ and suppose $n = 0$ for the induction base. Then

$$\text{sign}(x)^0 \left(S_0(x) - \frac{x}{2} S_{-1}(x) \right) = 1.$$

Suppose the statement is true for $n \in \mathbb{N}_0$. Then

$$\begin{aligned} &\text{sign}(x)^{n+1} \left(S_{n+1}(x) - \frac{x}{2} S_n(x) \right) \\ &= \underbrace{\text{sign}(x) \frac{x}{2}}_{\geq 1 \text{ if } |x| \geq 2} \text{sign}(x)^n \left(S_n(x) - \frac{x}{2} S_{n-1}(x) \right) + \underbrace{\left(\frac{x^2}{4} - 1 \right)}_{\geq 0} \underbrace{\text{sign}(x)^{n-1} S_{n-1}(x)}_{\geq 0 \text{ by (b)}} \\ &\geq \text{sign}(x)^n \left(S_n(x) - \frac{x}{2} S_{n-1}(x) \right) \end{aligned}$$

follows. Thus, the induction hypothesis implies the desired claim.

(f) Let $|x| \geq 2$ and $n \in \mathbb{N}_0$. Then (d) and (e) imply

$$|S_n(x)| = \text{sign}(x)^n S_n(x) \geq 1 + \text{sign}(x)^n \frac{x}{2} S_{n-1}(x) \geq 1.$$

(g) Let $|x| > 2$. If $n = 1$, then

$$\text{sign}(x)^1 \left(S_1(x) - \frac{x}{2} S_0(x) \right) = \text{sign}(x) \left(x - \frac{x}{2} \right) = \frac{|x|}{2} > 1$$

follows. A similar computation as in (e) leads to

$$\operatorname{sign}(x)^{n+1} \left(S_{n+1}(x) - \frac{x}{2} S_n(x) \right) \geq \operatorname{sign}(x)^n \left(S_n(x) - \frac{x}{2} S_{n-1}(x) \right) > 1,$$

where the last estimate follows by the induction hypothesis.

□

Lemma 8.3 ([36, (18.5.2)]) *For all $n \in \mathbb{N}$ and all $\theta \in \mathbb{R}$ we have*

$$S_n(2 \cos \theta) = U_n(\cos \theta) = \frac{\sin(n+1)\theta}{\sin \theta}.$$

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