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Extremal values of semi-regular continuants and codings of interval exchange transformations

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Abstract

Given a set \mathbb{A} consisting of positive integers $a_1 < a_2 < \dots < a_k$ and a k -term partition $P : n_1 + n_2 + \dots + n_k = n$, find the extremal denominators of the regular and semi-regular continued fraction $[0; x_1, x_2, \dots, x_n]$ with partial quotients $x_i \in \mathbb{A}$ and where each a_i occurs precisely n_i times in the sequence x_1, x_2, \dots, x_n . In 1983, G. Ramharter gave an explicit description of the extremal arrangements of the regular continued fraction and the minimizing arrangement for the semi-regular continued fraction and showed that in each case the arrangement is unique up to reversal and independent of the actual values of the positive integers a_i . However, an explicit determination of a maximizing arrangement for the semi-regular continuant turned out to be substantially more difficult. Ramharter conjectured that as in the other three cases, the maximizing arrangement is unique (up to reversal) and depends only on the partition P and not on the actual values of the a_i . He further verified the conjecture in the special case of a binary alphabet. In this paper, we confirm Ramharter's conjecture for sets \mathbb{A} with $|\mathbb{A}| = 3$ and give an algorithmic procedure for constructing the unique maximizing arrangement. We also show that Ramharter's conjecture fails for sets with $|\mathbb{A}| \geq 4$ in that the maximizing arrangement is in general neither unique nor independent of the values of the digits in \mathbb{A} . The central idea, is that the extremal arrangements satisfy a strong combinatorial condition. This combinatorial condition may also be stated more or less verbatim in the context of infinite sequences on an ordered set. We show that in the context of bi-infinite binary words, this condition coincides with the Markoff property, discovered by A.A. Markoff in 1879 in his study of minima of binary quadratic forms. We further show that this same combinatorial condition is the fundamental property which describes the orbit structure of the natural codings of points under a symmetric k -interval exchange transformation.

Keywords: Continued fractions, extremal values of continuants, Markoff property, Sturmian words and interval exchange transformations.

MSC[2010]: Primary 11J70; 37B10, 68R15.

1 Introduction

Given a finite sequence of positive integers $y = y_1, y_2, \dots, y_n$, describe an arrangement or permutation $x = x_1, x_2, \dots, x_n$ of the sequence y which maximizes (resp. minimizes) the regular continuant $K(x) = K_n(x_1, x_2, \dots, x_n)$. The continuant $K_n(x_1, x_2, \dots, x_n)$ is defined recursively by $K_0() = 1$, $K_1(x_1) = x_1$ and

$$K_n(x_1, x_2, \dots, x_n) = x_n K_{n-1}(x_1, x_2, \dots, x_{n-1}) + K_{n-2}(x_1, x_2, \dots, x_{n-2}) \quad (1)$$

and is equal to the denominator of the finite regular continued fraction $[0; x_1, x_2, \dots, x_n]$. This problem appears to be first attributed to C.A. Nicol (see [27]). There is no reason a priori that such an extremal arrangement should be unique. In fact, since $K_n(x_1, x_2, \dots, x_n) = K_n(x_n, \dots, x_2, x_1)$, the reversal (or mirror image) of any extremal arrangement is again extremal. But more generally, the function $K(\cdot)$ is far from being injective and it happens that many different permutations of the sequence y have the same K value [33]. There are many open questions concerning the distribution of the continuants $K_n(x_1, x_2, \dots, x_n)$ ($n \in \mathbb{N}$) where the x_i are restricted to a bounded subset of positive integers, including the famous Zaremba conjecture [37]. The distribution of the continuants with the x_i belonging to a bounded subset \mathbb{A} is also extremely relevant in estimating the Hausdorff dimension of the set $E_{\mathbb{A}} \subset \mathbb{R}$ consisting of all finite and infinite (regular) continued fractions whose partial quotients all belong to \mathbb{A} (see for instance [10, 9, 19]).

T.S. Motzkin and E.G. Straus [27] provided a first partial answer to Nicol's question in the special case in which y_1, y_2, \dots, y_n , are pairwise distinct. In [9], T.W. Cusick found the maximizing arrangement for an arbitrary sequence y_1, y_2, \dots, y_n consisting of 1s and 2s. But the general problem was settled by G. Ramharter [29]. He gave an explicit description of both extremal arrangements and showed that they are unique (up to reversal) and independent of the actual values of the digits (see Theorem 1 in [29]). For example, if $y = y_1, y_2, \dots, y_n$ is given in the form $a_1^{n_1} \cdots a_k^{n_k}$ with $1 \leq a_1 < a_2 < \cdots < a_k$ and $n_1 + n_2 + \cdots + n_k = n$, then the maximizing arrangement for $K(\cdot)$ is unique up to reversal and given by:

$$a_k L_{k-1} a_{k-2} L_{k-3} \cdots a_1^{n_1} \cdots a_{k-3} L_{k-2} a_{k-1} L_k$$

where $L_i = a_i^{n_i - 1}$. The fact that the extremal arrangements are unique is quite surprising as is remarkable that they do not involve the ring structure of the integers but rather only the relative order of the digits involved. Ramharter's theorem was later reproved by C. Baxa in [4] and used to prove a criterion for the transcendence of continued fractions whose partial quotients are contained in a finite set (see also [13]).

Motivated by a question in diophantine approximation [32], Ramharter also considered the analogous problem in the context of the semi-regular continuant $\dot{K}_n(x_1, x_2, \dots, x_n)$ defined recursively by $\dot{K}_0() = 1$, $\dot{K}_1(x_1) = x_1$ and

$$\dot{K}_n(x_1, x_2, \dots, x_n) = x_n \dot{K}_{n-1}(x_1, x_2, \dots, x_{n-1}) - \dot{K}_{n-2}(x_1, x_2, \dots, x_{n-2}). \quad (2)$$

For semi-regular continuants, the digit 1 needs to be excluded and in this case, $\dot{K}(x)$ is the denominator of the terminating semi-regular continued fraction

$$[x]^\bullet = \frac{1}{x_1 - \frac{1}{x_2 - \frac{1}{\ddots - \frac{1}{x_n}}}}$$

Letting X be the tridiagonal matrix

$$X = \begin{pmatrix} x_1 & 1 & 0 & \cdots & 0 \\ 1 & x_2 & 1 & \ddots & \vdots \\ 0 & 1 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & x_{n-1} & 1 \\ 0 & \cdots & 0 & 1 & x_n \end{pmatrix}$$

we have that $K_n(x_1, x_2, \dots, x_n) = \text{perm}(X)$ while $\dot{K}_n(x_1, x_2, \dots, x_n) = \det(X)$ where $\text{perm}(X)$ (resp. $\det(X)$) denotes the permanent (resp. determinant) of the matrix X .

As in the case of the extremal arrangements for the regular continuant, Ramharter showed that the minimizing arrangement for $\dot{K}(\cdot)$ is unique (up to reversal) and independent of the choice of digits a_1, \dots, a_k . However, the determination of the maximizing arrangement for $\dot{K}(\cdot)$ turned out to be more difficult. In fact, Ramharter points out that in contrast with the other three cases, there is an infinity of essentially different patterns and the maximizing arrangements for $\dot{K}(\cdot)$ must be described in terms of an algorithmic procedure as “their combinatorial structure is exceptionally complicated.” Ramharter conjectured that, as in the case of the other three extremal arrangements, for general sequences $a_1^{n_1} \cdots a_k^{n_k}$ the maximizing arrangement for the semi-regular continuant $\dot{K}(\cdot)$ is always unique (up to reversal) and independent of the values of the digits $2 \leq a_1 < a_2 < \cdots < a_k$. The conjecture has been verified by Ramharter in two special cases : i) for sequence $y = y_1, y_2, \dots, y_n$ on a binary alphabet, i.e., $y_1, \dots, y_n \in \{a_1, a_2\}$ for some choice of positive integers $2 \leq a_1 < a_2$ (see theorems 1 and 2 in [29]); ii) for sequences y_1, y_2, \dots, y_n with pairwise different entries (see Theorem 1 in [31]).

The central idea, as was first observed by Ramharter in [29], is that the extremal arrangements for both the regular and semi-regular continuants satisfy a very special combinatorial condition. In the case of the maximising arrangement $x = x_1, x_2, \dots, x_n$ (with each $x_i \geq 2$) for the semi-regular continuant, this condition, denoted \dot{K}_{\max} , is as follows :

\dot{K}_{\max} : For each factorization $x = \bar{u}vw$ with $v \neq \bar{v}$ and $u \neq w$ one has that $v < \bar{v}$ if and only if $w < u$.

Here \bar{u} denotes the reversal of the sequence u , (i.e., if $u = u_1, u_2, \dots, u_j$ then $\bar{u} = u_j, \dots, u_2, u_1$), and $<$ denotes the lexicographic order induced by the natural order on

\mathbb{R} where however one takes the opposite convention of the true dictionary order with respect to proper prefixes, i.e., we declare $u < v$ whenever v is a proper prefix of u . We remark that condition \dot{K}_{\max} makes sense for any finite sequence x over any totally ordered set \mathbb{A} , i.e., the entries of x need not be positive whole numbers. As Ramharter points out, the central question is to understand whether for each sequence y over an ordered alphabet \mathbb{A} there exists a *unique* permutation x of y verifying condition \dot{K}_{\max} , which, if true, would imply a unique global maximum for the semi-regular continuant. He further conjectured that this should be the case in general [31].

The following theorem confirms Ramharter's conjecture for sequences y over any ternary ordered alphabet \mathbb{A} :

Theorem 1. *Let \mathbb{A} be any totally ordered ternary alphabet and $y = y_1, y_2, \dots, y_n$ be any sequence with each $y_i \in \mathbb{A}$. Then there is precisely one permutation x of y (up to reversal) which verifies condition \dot{K}_{\max} .*

We also give an algorithmic procedure for constructing the permutation x verifying condition \dot{K}_{\max} . It follows that for each sequence $y = a_1^{n_1} a_2^{n_2} a_3^{n_3}$ of positive integers with $2 \leq a_1 < a_2 < a_3$, there exists a unique (up to reversal) permutation x of y which maximizes the semi-regular continuant $\dot{K}(\cdot)$. Moreover the maximizing arrangement is independent of the actual values of the digits a_1, a_2 and a_3 and depends only on the vector (n_1, n_2, n_3) . Thus for sequences y involving at most three distinct positive integers, condition \dot{K}_{\max} gives a full characterization of the maximizing arrangement for the semi-regular continuant $\dot{K}(\cdot)$.

However, for sequences y over ordered alphabets \mathbb{A} of cardinality 4 or more, it may happen that y admits more than one permutation verifying condition \dot{K}_{\max} . This in itself does not disprove the existence of a unique global maximum for the semi-regular continuant $\dot{K}(\cdot)$ which is independent of the actual choice of positive integers assigned to the elements of \mathbb{A} , however, it provides a basis for constructing such examples. In fact, we show the existence of a sequence y over an ordered alphabet $\mathbb{A} = \{a < b < c < d\}$ having two permutations x and x' (with $x' \neq \bar{x}$) each verifying \dot{K}_{\max} and depending on the values assigned to each of a, b, c , and d in the sequence y , the maximum of $\dot{K}(\cdot)$ is assumed at x and not at x' , or inversely the maximum occurs at x' and not x or the maximum occurs simultaneously at both x and x' (see Example 3.23). It follows from this that for sequences y involving 4 or more distinct positive integers, \dot{K}_{\max} is not a strong enough condition to guarantee a maximizing arrangement.

A primary objective of this paper is to study condition \dot{K}_{\max} in its full generality. Given a totally ordered set \mathbb{A} , let \mathbb{A}^+ denote the free semigroup generated by \mathbb{A} consisting of all finite words $x = x_1 x_2 \cdots x_n$ with each $x_i \in \mathbb{A}$. We let $\mathbb{A}^* = \mathbb{A}^+ \cup \{\varepsilon\}$ be the free monoid generated by \mathbb{A} in which we adjoin the empty word ε regarded as the unique word of length 0. We also let $\mathbb{A}^{\mathbb{N}}$ (resp. $\mathbb{A}^{\mathbb{Z}}$) denote the set of all one sided (resp. two-sided) infinite words $x = x_1 x_2 x_3 \cdots$ (resp. $x = \cdots x_{-2} x_{-1} x_0 x_1 x_2 \cdots$) with each $x_i \in \mathbb{A}$.

We introduce the following definition which amounts to a reformulation of \dot{K}_{\max} to a more general setting which includes both finite and infinite words:

Definition 2. Let \mathbb{A} be any totally ordered alphabet, and $x \in \mathbb{A}^+ \cup \mathbb{A}^{\mathbb{N}} \cup \mathbb{A}^{\mathbb{Z}}$. We say that x is *singular* if for all factorizations $x = \bar{u}vw$ ($v \in \mathbb{A}^+$, $u, w \in \mathbb{A}^* \cup \mathbb{A}^{\mathbb{N}}$) with $v \neq \bar{v}$ and $u \neq w$ we have $v < \bar{v}$ if and only if $w < u$.

The order $<$ is taken to be the lexicographic order on $\mathbb{A}^* \cup \mathbb{A}^{\mathbb{N}}$ induced by the order on \mathbb{A} (where as in \dot{K}_{\max} , we take the opposite convention of the true dictionary order when it comes to proper prefixes).

In [31, 30], Ramharter showed that each finite singular word x over a binary alphabet $\mathbb{A} = \{a, b\}$ is a finite Sturmian word, and that the palindromic binary maximizing arrangements for $\dot{K}(\cdot)$ are in one-to-one correspondence with the extremal cases of the Fine and Wilf theorem [17] with two co-prime periods (see Theorem 3 in [31]). We give a more precise reformulation of this result in terms of more standard notions in the theory of finite Sturmian words and already existing algorithms:

Theorem 3. *A finite word x over a binary ordered alphabet $\{a < b\}$ is singular if and only if x or \bar{x} is of the form b^n , ab^n ($n \geq 0$) or aya where ayb is a power of a Christoffel word $C_{p,q}$ with co-prime periods p and q .*

If we now consider bi-infinite words x over a binary alphabet $\mathbb{A} = \{a, b\}$, then we show that the singular property in Definition 2 coincides with the so-called Markoff property, first identified by A.A. Markoff in [24] in his study of minima of binary quadratic forms, and again in [25] (see in particular page 28) in which he answers a question posed by J. Bernoulli in [5]. The Markoff property applies to bi-infinite words x over a binary alphabet $\mathbb{A} = \{a, b\}$ and may be formulated as follows:

- (M) For each factorization $x = \bar{u}a'b'w$ with $\{a', b'\} = \{a, b\}$ and $u, w \in \mathbb{A}^{\mathbb{N}}$, either $u = w$ or if $i \in \mathbb{N}$ is the least index j for which $u_j \neq w_j$, then $u_i = b'$ and $w_i = a'$.

Although both \dot{K}_{\max} and property (M) were discovered in the context of extremal problems involving continued fractions, the former relates to semi-regular continuants while the latter concerns inequalities relating real numbers and convergents of infinite continued fractions. So the connection between the two is not fully transparent. As was first observed by T.W. Cusick and M.E. Flahive in [11] and later proved by C. Reutenauer in [34], property (M) is equivalent to the balanced property of Morse-Hedlund [26].

We show that a bi-infinite binary word verifies the Markoff property (M) if and only if it is singular (see Corollary 4.2). One way to establish the equivalence is to show that a bi-infinite binary word is singular if and only if it is balanced (see Proposition 4.1) and then use Theorem 3.1 in [34]. Alternatively, a direct proof (which bypasses the balance property) may be given using Sturmian morphisms. As for one sided-infinite binary words, we show

Theorem 4. *Let $x \in \{a, b\}^{\mathbb{N}}$ be an aperiodic binary (one sided) infinite word. Then x is singular if and only if x is a Sturmian Lyndon word.*

Recall that a finite or infinite word x over an ordered alphabet is said to be *Lyndon* if and only if x is lexicographically smaller than each of its proper suffixes.

The next question is to understand bi-infinite singular words over higher alphabets. We show that the singular property is the fundamental property which distinguishes the orbit structure of codings of symmetric interval exchange transformations from other subshifts of the same factor complexity including Arnoux-Rauzy subshifts [2]. A *symmetric k -interval exchange transformation* \mathcal{I} is given by a probability vector of k lengths $(\alpha_1, \dots, \alpha_k)$. The unit interval is partitioned into k subintervals of lengths $\alpha_1, \dots, \alpha_k$ labeled $1, 2, \dots, k$ which are then re-arranged according to the permutation $\sigma(j) = k+1-j$. A natural coding of a point $x \in [0, 1]$ under \mathcal{I} is given by a bi-infinite word $(x_n)_{n \in \mathbb{Z}}$ over the alphabet $\{1, 2, \dots, k\}$ where $x_n = i$ whenever the n -th iterate of x lies in i th interval. By the language of \mathcal{I} we mean the language defined by all natural codings under \mathcal{I} . We obtain the following characterization of singular bi-infinite words x whose associated language is *symmetric* (i.e., closed under reversal) and which constitutes a generalization of Theorem 3.1 in [34]:

Theorem 5. *Let $\mathbb{A}_k = \{1, 2, \dots, k\}$ ($k \geq 2$) and let $x \in \mathbb{A}_k^{\mathbb{Z}}$ be uniformly recurrent and assume that each $i \in \mathbb{A}_k$ occurs in x . Then the following are equivalent:*

1. $L(x)$ is the language of a symmetric k -interval exchange transformation.
2. x is singular and $L(x)$ is symmetric.

As in Theorem 4, if we take x to be a one-sided infinite word, then in item 2. of Theorem 5 we need to add the condition that x is Lyndon. We also give a characterization of natural codings of symmetric k -interval exchange transformations satisfying Keane's infinite discrete orbit condition (or i.d.o.c.) in terms of infinite singular words.

2 Preliminaries

Let $\mathbb{A} = \{a_1, a_2, \dots, a_k\}$ be a totally ordered set with $a_1 < a_2 < \dots < a_k$. For each $x \in \mathbb{A}^+$ and $a \in \mathbb{A}$ we let $|x|_a$ denote the number of occurrences of the letter a in x and write $|x| = \sum_{a \in \mathbb{A}} |x|_a$ for the length of x . The *Parikh vector* of x is defined by $(|x|_{a_1}, |x|_{a_2}, \dots, |x|_{a_k})$. Two finite words $x, y \in \mathbb{A}^+$ are said to be *abelian equivalent* if they define the same Parikh vector, i.e., $|x|_a = |y|_a$ for each $a \in \mathbb{A}$. We define the abelian class of a word $x \in \mathbb{A}^+$ to be the set of all words $y \in \mathbb{A}^+$ which are abelian equivalent to x . If $x \in \mathbb{A}^{\mathbb{N}} \cup \mathbb{A}^{\mathbb{Z}}$, then a factor u of x is said to be recurrent in x if every suffix of x contains an occurrence of u . We say x is recurrent if every factor u of x is recurrent in x . For $x \in \mathbb{A}^+ \cup \mathbb{A}^{\mathbb{N}} \cup \mathbb{A}^{\mathbb{Z}}$, we let $L(x)$ denote its *language*, i.e., the set of all factors of x . We say x is *balanced* if for all factors u, v of x with $|u| = |v|$ we have $||u|_a - |v|_a| \leq 1$ for each $a \in \mathbb{A}$. For all other word combinatorial definitions which have not been explicitly defined herein, we refer the reader to [23].

The total order \leq on \mathbb{A} defines a lexicographic order on $\mathbb{A}^* \cup \mathbb{A}^{\mathbb{N}}$, also denoted \leq , where we write $x < y$ if either y is a proper prefix of x (so we are adopting the opposite convention of the true dictionary order) or if $x = ua_i x'$, $y = ua_j y'$ for some $u \in \mathbb{A}^*$, $x', y' \in \mathbb{A}^* \cup \mathbb{A}^{\mathbb{N}}$ and $i < j$. For $x, y \in \mathbb{A}^* \cup \mathbb{A}^{\mathbb{N}}$, we write $x \leq y$ if either $x = y$ or $x < y$.

Definition 2.1. Let $x \in \mathbb{A}^* \cup \mathbb{A}^{\mathbb{N}} \cup \mathbb{A}^{\mathbb{Z}}$. A factorization $x = \bar{u}vw$ (with $v \in \mathbb{A}^+$, $u, w \in \mathbb{A}^* \cup \mathbb{A}^{\mathbb{N}}$) and with $v \neq \bar{v}$ and $u \neq w$ is called *reversible* (resp. *singular*) if $v < \bar{v}$ and $u < w$ or $\bar{v} < v$ and $w < u$ (resp. if $v < \bar{v}$ and $w < u$ or $\bar{v} < v$ and $u < w$). We say x is *reversible* if x admits a reversible factorization.

It follows immediately that each word $x \in \mathbb{A}^* \cup \mathbb{A}^{\mathbb{N}} \cup \mathbb{A}^{\mathbb{Z}}$ is either reversible or singular, but not both. A reversible word may admit more than one reversible factorization. For example, if $\mathbb{A} = \{a, b\}$ with $a < b$, then the reversible word $x = aabb$ admits the reversible factorization $x = (a)(ab)(b)$ as well as $x = (a)(abb)\varepsilon$. We also note that the property of being reversible (resp. singular) is invariant under reversal, i.e., x is reversible (resp. singular) if and only if \bar{x} is reversible (resp. singular). To check that a word x is singular, it suffices to show that any factorization $x = \bar{u}vw$ with $u \neq w$ and where v begins and ends in distinct letters is singular. In fact, writing $v = \bar{z}cydz$ with $z, y \in \mathbb{A}^*$ and $c, d \in \mathbb{A}$ distinct, we see that if the factorization $x = \bar{u}vw$ is reversible, then so is the factorization $x = \bar{z}\bar{u}(cyd)zw$.

3 Finite singular words

We begin this section with a characterization of finite binary singular words. We then study finite ternary singular words and show that corresponding to each Parikh vector $\mathbf{v} = (n_a, n_b, n_c)$ there exists a unique (up to reversal) singular word x over the ordered alphabet $\{a < b < c\}$ whose Parikh vector is equal to \mathbf{v} . We also describe an algorithm for constructing the singular word x . Finally, we show that on ordered alphabets of size greater than three, there may exist many abelian equivalent singular words. In particular, we show that the abelian class defined by the ordered Parikh vector $(n_a, n_b, n_c, n_d) = (1, 2, 1, 2)$ over the ordered alphabet $\{a < b < c < d\}$ contains up to reversal two distinct singular words x and x' and that the maximizing arrangement for $\dot{K}(\cdot)$ depends on the actual values of the positive integers assigned to each of the letters a, b, c and d .

We begin with a simple lemma which applies to arbitrary ordered alphabets \mathbb{A} . For a word $x \in \mathbb{A}^+$, let $\min x$ denote the smallest letter occurring in x .

Lemma 3.1. *Let \mathbb{A} be a totally ordered alphabet, $x \in \mathbb{A}^+$ be a singular word, and $a = \min x$. Then x must either begin or end in a . If $x = ax'$ (resp. $x = x'a$) for some $x' \in \mathbb{A}^+$, then x' ends (resp. begins) with $\min x'$.*

Proof. For $b \in \mathbb{A}$ and $u, v \in \mathbb{A}^*$, the factorization $x = \bar{u} \cdot avb \cdot \varepsilon$ is reversible if $u \neq \varepsilon$ and $b \neq a$. Thus x has a as its first or last letter. Short of replacing x by \bar{x} , we may assume without loss of generality that $x = avb = ax'$. If $v = \bar{u}'cv'$ with $c \in \mathbb{A}$, then since the factorization $\overline{au'} \cdot cv'b \cdot \varepsilon$ is not reversible, we obtain $c \geq b$. Hence $b = \min x'$. \square

Remark 3.2. Note that Lemma 3.1 implies that for a singular word x , if $x = sat$ with $s, t \in \mathbb{A}^+$ and $a = \min \mathbb{A}$, then a is a prefix of s and a suffix of t ; whereas if x begins in c where $c = \max \mathbb{A}$, then $x = c^n b$ for some $n \geq 1$ and $b \in \mathbb{A}$.

We now study binary singular words.

Lemma 3.3. *Let \mathbb{A} be an ordered binary alphabet $\{a < b\}$ and let $x \in \mathbb{A}^* \cup \mathbb{A}^{\mathbb{N}} \cup \mathbb{A}^{\mathbb{Z}}$ be singular. Then x is balanced.*

Proof. Let x be singular and assume to the contrary that x is not balanced. By Proposition 2.1.3 in [23], there exists a palindrome $z \in \mathbb{A}^*$ such that both aza and bzb are factors of x . Since the factors aza and bzb cannot overlap one another, there exist distinct $a', b' \in \mathbb{A}$ and a factorization $x = \bar{u}vw$ where v begins in a' and ends in b' , za' is a prefix of u and zb' a prefix of w . It follows that $a' < b'$ if and only if $u < w$ and hence we obtain a reversible factorization of x , a contradiction. \square

Theorem 3.4. *A finite word x over a binary ordered alphabet $\mathbb{A} = \{a < b\}$ is singular if and only if x or \bar{x} is of the form b^n , ab^n , ($n \geq 0$) or aya where y is a bispecial Sturmian word.*

A word $y \in \{a, b\}^*$ is a *bispecial Sturmian word* if ay, by, ya and yb are each a factor of an infinite Sturmian word, or equivalently if they are each balanced (see Proposition 2.1.17 in [23]).

Remark 3.5. If $x \in \{a, b\}^{\mathbb{N}}$ is a Sturmian word, then the bispecial factors of x are called *central words* and are bispecial Sturmian words. The factors of x of the form aya , with y a central word, are already known in the literature and called *singular Sturmian words* [36]. The reason for the term *singular* is that if $n = |y| + 2$, then the $n + 1$ factors of x of length n are partitioned into two distinct abelian classes, one class contains n words (which are all cyclically conjugate to the Christoffel word ayb) while the other class consists only of the word aya . Thus relative to the order $a < b$, every singular Sturmian word of the form aya is singular in the sense of Definition 2, but not every singular binary word of the form aya is a singular Sturmian word since a bispecial Sturmian word need not be central (e.g. ab).

Proof of Theorem 3.4. Assume first that $x \in \mathbb{A}^+$ is singular. By Lemma 3.1, if $|x|_a = 1$, then $x = ab^n$ or $x = b^na$ with $n = |x|_b$, whereas if $|x|_a \geq 2$, then we may write $x = aya$ for some $y \in \mathbb{A}^*$. To see that y is a bispecial Sturmian word, it suffices to show that each of ay, by, ya and yb is balanced (see Proposition 2.1.17 in [23]). Since x itself is balanced by Lemma 3.3, it suffices to show that by and yb are balanced. Let us assume to the contrary that by is not balanced, and pick a palindrome z such that aza and bzb are factors of by . Since y is balanced, it follows that bzb is a prefix of by . Thus we can write $by = bz \cdot v \cdot zay'$ with $y' \in \mathbb{A}^*$ and where v begins in b and ends in a . This gives a factorization $x = \bar{u}vw$ where $u = za$ and $w = zay'a$. It follows that $\bar{v} < v$ and $w < u$ (since u is a proper prefix of w) whence x is reversible, a contradiction. Similarly, one shows that yb is also balanced.

For the converse, we first note that any word of the form b^n or ab^n is clearly singular. So let us assume that $x = aya$ with y a bispecial Sturmian word. To see that x is singular, fix a factorization $x = \bar{u}vw$ with $v = a'v'b'$, $u \neq w$ and $\{a', b'\} = \mathbb{A}$. Short of replacing x by \bar{x} we may assume without loss of generality that $v < \bar{v}$, whence $v = av'b$. We will show that $w < u$. If u is a proper prefix of w , then clearly $w < u$. So let us next suppose that w is a proper prefix of u . If w is empty, then $v = av'b$ is a suffix of x ,

which contradicts $x = aya$. If $w \neq \varepsilon$ then we may write $w = ra$ and $u = rau'$ for some $r \in \mathbb{A}^*$ and $u' \in \mathbb{A}^+$. It follows that $a\bar{r}vw = a\bar{r}av'bra$ is a proper suffix of x and hence $a\bar{r}av'brb$ is a suffix of yb , contradicting that yb is balanced.

Finally, if neither u nor w are proper prefixes of one another, then we may write $u = rcu'$ and $w = rdw'$ where $r, u', w' \in \mathbb{A}^*$ and $\{c, d\} = \mathbb{A}$. Thus

$$x = \bar{u}vw = \bar{u}'c\bar{r}av'brdw'.$$

If w' is empty, then $d = a$ and so $c = b$ and $w < u$. If $w' \neq \varepsilon$, then $c\bar{r}av'brd$ is a factor of ay and since ay is balanced, it follows that $d = a$ and $c = b$, whence $w < u$ as required. \square

As a consequence, we can now prove

Theorem 3. *A finite word x over a binary ordered alphabet $\{a < b\}$ is singular if and only if x or \bar{x} is of the form b^n, ab^n ($n \geq 0$) or aya where ayb is a power of a Christoffel word $C_{p,q}$ with co-prime periods p and q .*

Proof. This follows immediately from the fact that a word $y \in \{a, b\}^*$ is a bispecial Sturmian word if and only if ayb or $a\bar{y}b$ is a power of a Christoffel word $C_{p,q}$ with $\gcd(p, q) = 1$ (see Theorem 3.11 in [16]). \square

Example 3.6. Theorem 3 may be used to construct binary singular words having a specified Parikh vector (n_a, n_b) via standard algorithms for constructing Christoffel words. For example, suppose we want to find a singular word $x \in \{a, b\}^+$ whose corresponding Parikh vector is $(7, 14)$. Then we shall first build a word of the form $x' = ayb$ (with y a Sturmian bispecial) with Parikh vector $(6, 15)$ and then $x = aya = x'b^{-1}a$. To construct x' , we first note that $\gcd(6, 15) = 3$ and hence we must find the Christoffel word $C_{2,5}$. Using standard algorithms (see [6]) we find that $C_{2,5} = abbabbb$. It follows that $x' = C_{2,5}^3 = abbabbb \cdot abbabbb \cdot abbabbb$ and hence $x = abbabbb \cdot abbabbb \cdot abbabba$.

Before moving to the ternary case, let us give a few more results which apply to arbitrary ordered alphabets. We say that a letter a is *separating* for a word $x \in \mathbb{A}^+$ if a occurs in every factor of x of length 2. Notice that two distinct letters a, b are both separating for x if and only if x is one of the following, for a suitable $n \geq 0$: $(ab)^n, (ba)^n, (ab)^na,$ or $(ba)^nb$.

Lemma 3.7. *Let $d \in \{\min \mathbb{A}, \max \mathbb{A}\}$. If a singular word x has dd as a factor, then d is separating for x .*

Proof. Assume to the contrary that x contains both dd and ab as factors, with $a, b \in \mathbb{A} \setminus \{d\}$. We may assume without loss of generality that dd occurs in x before ab , and hence $x = \bar{u}d \cdot dva \cdot bw$ for suitable $u, v, w \in \mathbb{A}^*$. As d is either smaller or bigger than both a and b , this factorization is reversible, a contradiction. \square

Lemma 3.8. *Let $a = \min \mathbb{A}$, and $x \in \mathbb{A}^*$ be a singular word with $|x|_a > 1$. Then a is separating in x if and only if*

$$|x|_a \geq \sum_{a' \in \mathbb{A} \setminus \{a\}} |x|_{a'} + 1, \quad (3)$$

and $aa \in L(x)$ if and only if the inequality is strict.

Proof. By Lemma 3.1, x begins and ends with a . Thus if a is separating for x , then every occurrence in x of a letter $a' \neq a$ must be immediately preceded by a . In particular, if a is separating, then (3) holds.

Conversely, assume (3) holds, and suppose to the contrary that a is not separating for x . This means that x has at least one factor bc with $b, c \in \mathbb{A} \setminus \{a\}$. But then (3) implies $aa \in L(x)$, which is absurd in view of Lemma 3.7. It is now clear that aa occurs if and only if the inequality in (3) is strict. \square

The following analogue for $\max \mathbb{A}$ can be proved in a similar way.

Lemma 3.9. *Let $c = \max \mathbb{A}$, and $x \in \mathbb{A}^*$ a singular word. Then c is separating for x if and only if*

$$|x|_c \geq \sum_{c' \in \mathbb{A} \setminus \{c\}} |x|_{c'} - 1.$$

When $|x| - |x|_c > 1$, the above inequality is strict if and only if $cc \in L(x)$.

For a letter $d \in \mathbb{A}$, let λ_d and ρ_d denote the morphisms defined by $\lambda_d(d') = dd'$, $\rho_d(d') = d'd$ for letters $d' \neq d$, and $\lambda_d(d) = \rho_d(d) = d$. The following properties are easy to verify and will be useful in the sequel: for all $d \in \mathbb{A}$ and $x \in \mathbb{A}^*$,

$$d\overline{\lambda_d(x)} = \lambda_d(\overline{x})d \quad \text{and} \quad d\rho_d(x) = \lambda_d(x)d. \quad (4)$$

Lemma 3.10. *Let $a \in \mathbb{A}$ and $x, y \in \mathbb{A}^*$. Then $x < y \iff \lambda_a(x)a < \lambda_a(y)a$.*

Proof. If y is a proper prefix of x , then clearly $\lambda_a(y)a$ is a prefix of $\lambda_a(x)$, and hence a proper prefix of $\lambda_a(x)a$. Conversely, if $\lambda_a(x)a = \lambda_a(y)aWa$ for some $W \in \mathbb{A}^*$, then there exists $w \in \mathbb{A}^+$ such that $aW = \lambda_a(w)$ and $x = yw$.

If $x = ubv$ and $y = ucw$ for some $u, v, w \in \mathbb{A}^*$ and $b, c \in \mathbb{A}$ such that $b < c$, then in all cases $\lambda_a(x)a$ begins with $\lambda_a(u)ab$ and $\lambda_a(y)a$ begins with $\lambda_a(u)ac$. Conversely, assume $\lambda_a(x)a < \lambda_a(y)a$, the latter not being a prefix of the former. Their longest common prefix is then necessarily $\lambda_a(u)a$ for a suitable $u \in \mathbb{A}^*$. Hence there exist letters $b < c$ such that $\lambda_a(u)ab$ and $\lambda_a(u)ac$ are respectively prefixes of $\lambda_a(x)a$ and $\lambda_a(y)a$; therefore $x < y$, as x begins with ub and y with uc . \square

For $c = \max \mathbb{A}$ we need the following slight variation:

Lemma 3.11. *Let $c = \max \mathbb{A}$ and $x, y \in \mathbb{A}^*$. Then $x < y \iff \lambda_c(x) < \lambda_c(y)$.*

Proof. If y is a proper prefix of x , then $\lambda_c(y)$ is a proper prefix of $\lambda_c(x)$. Conversely, if $\lambda_c(y)W = \lambda_c(x)$ for some nonempty W , then either y is a proper prefix of x , or $y = uc$ and $x = uax'$ for some $u, x' \in \mathbb{A}^*$ and a letter $a < c$. Hence $x < y$ anyway.

If $x = uav$ and $y = ubw$ for suitable $u, v, w \in \mathbb{A}^*$ and $a, b \in \mathbb{A}$ with $a < b$, then either $c \notin \{a, b\}$ or $b = c$. In both cases $\lambda_c(x)$ begins with $\lambda_c(u)ca$. As for $\lambda_c(y)$, it equals $\lambda_c(u)c$ if $b = c$ and $w = \varepsilon$, otherwise it has $\lambda_c(u)cb$ as a prefix. Conversely, if $\lambda_c(x) < \lambda_c(y)$ and their longest common prefix is shorter than $\lambda_c(y)$, then it necessarily ends in c . In other words, there exist $u \in \mathbb{A}^*$ and letters $a < b$ such that $\lambda_c(u)ca$ and $\lambda_c(u)cb$ are prefixes of $\lambda_c(x)$ and $\lambda_c(y)$ respectively. Again, it follows that x begins with ua , and y with ub . \square

Lemma 3.12. *Let $a = \min \mathbb{A}$ and $x \in \mathbb{A}^*$. Then x is singular if and only if $\lambda_a(x)a$ is singular.*

Proof. Equivalently, it suffices to show that x is reversible if and only if $\lambda_a(x)a$ is reversible. Fix a factorization $x = \bar{u}vw$ with $v \neq \bar{v}$ and $u \neq w$; this is equivalent to

$$\lambda_a(x)a = \overline{\lambda_a(u)a} \cdot a^{-1}\lambda_a(v) \cdot \lambda_a(w)a \quad (5)$$

since eq. (4) implies $\lambda_a(\bar{u})a = a\overline{\lambda_a(u)} = \overline{\lambda_a(u)a}$. Again by eq. (4) we have $\overline{a^{-1}\lambda_a(v)} = a^{-1}\lambda_a(\bar{v})$. Since $|a^{-1}\lambda_a(v)| = |a^{-1}\lambda_a(\bar{v})|$, we obtain

$$a^{-1}\lambda_a(v) < \overline{a^{-1}\lambda_a(v)} \iff \lambda_a(v)a < \lambda_a(\bar{v})a$$

as well as the same equivalence for the opposite inequality. By applying Lemma 3.10 to u, w and to v, \bar{v} , it follows that $x = \bar{u}vw$ is a reversible factorization if and only if the one in eq. (5) is reversible too.

It remains to show that if $\lambda_a(x)a$ has a reversible factorization, then it has one of the form shown in eq. (5). Let then $\lambda_a(x)a = \bar{U}VW$ be a reversible factorization. We may assume that the first letter of V differs from its last; in particular, by symmetry we may assume that the first letter of V is not a , in which case U must begin with a . Now, W cannot be empty, otherwise V would end in a and the factorization would not be reversible, as $\bar{V} < V$ and $U < W$; for the same reason, W must begin with a . It follows that there exist $u, v, w \in \mathbb{A}^*$ such that the factorization $\lambda_a(x)a = \bar{U}VW$ coincides with the one in eq. (5), as desired. \square

Lemma 3.13. *Let $c = \max \mathbb{A}$ and $x \in \mathbb{A}^+$. Then x is singular if and only if $\rho_c(x)c^{-1}$ is singular.*

Proof. Once again, we prove the contrapositive, i.e., x is reversible if and only if $\rho_c(x)c^{-1}$ is reversible. Let $x = \bar{u}vw$ for some $u, v, w \in \mathbb{A}^*$ with $v \neq \varepsilon$, which is equivalent to

$$\rho_c(x)c^{-1} = c^{-1}\lambda_c(x) = \overline{\lambda_c(u)} \cdot c^{-1}\lambda_c(v) \cdot \lambda_c(w) \quad (6)$$

in view of eq. (4), which also implies $\overline{c^{-1}\lambda_c(v)} = c^{-1}\lambda_c(\bar{v})$. Since clearly $c^{-1}\lambda_c(v)$ is less (resp. greater) than $c^{-1}\lambda_c(\bar{v})$ if and only if the same relation holds between $\lambda_c(v)$

and $\lambda_c(\bar{v})$, applying Lemma 3.11 to the pairs u, w and v, \bar{v} we obtain that $x = \bar{u}vw$ is reversible if and only if so is the factorization in eq. (6).

It remains to show that if $\rho_c(x)c^{-1}$ has a reversible factorization, then it has one like in eq. (6). Indeed, if $\rho_c(x)c^{-1} = \bar{U}VW$ is reversible, we may assume that V begins and ends with distinct letters, and by symmetry that V does not begin with c . It follows that U is either empty or begins with c . Moreover, if W is nonempty then it also must begin with c , since otherwise V would end in c , yielding $W < U$ and $V < \bar{V}$, a contradiction. It follows that there exist $u, v, w \in \mathbb{A}^*$ such that $\bar{U} \cdot V \cdot W$ coincides with the factorization in eq. (6). \square

Since Christoffel words are exactly the images of a, b under compositions of λ_a and ρ_b (see for instance [6, 12]), an alternative proof of Theorem 3 can easily be obtained from Lemmas 3.12 and 3.13.

We now focus on a ternary alphabet. In the following, we let $\mathbb{A} = \{a, b, c\}$ with $a < b < c$.

Remark 3.14. Let $x \in \mathbb{A}^*$. If $ab, cb \in L(x)$, or if $ba, bc \in L(x)$, then x is not singular. Indeed, $\bar{u}a \cdot bvc \cdot bw$, $\bar{u}c \cdot bva \cdot bw$ and their reverses are all reversible factorizations.

Lemma 3.15. Let $x \in \mathbb{A}^*$ be a singular word. If ab and bc (resp. cb and ba) occur in x , then $x = ab^n(ca)^m$ (resp. $\bar{x} = ab^n(ca)^m$) for some $n, m \geq 1$.

Proof. Suppose $ab, bc \in L(x)$. As $ab \in L(x)$, it follows that $\{cb, cc\} \cap L(x) = \emptyset$. Similarly, $bc \in L(x)$ implies $\{aa, ba\} \cap L(x) = \emptyset$. Write $x = \bar{u} \cdot c \cdot z$ where z follows the last occurrence of c in x . Then $|u|_b > 0$ and by Lemma 3.1, z is nonempty and hence begins with a . We claim that $|z|_b = 0$; indeed, x cannot end in b by Remark 3.2, and the last b in x can only be followed by c . It follows that $z = a$ and hence ca is a suffix of x . Thus $x = wab^n(ca)^m$ for some $n, m \geq 1$, which implies $w = \varepsilon$ otherwise the factorization $w \cdot ab^n(ca)^m \cdot \varepsilon$ would be reversible. \square

Proposition 3.16. Let $x \in \mathbb{A}^*$ be a singular word. If $|x|_a = |x|_c + 1$, then $x = ab^n(ca)^m$ or $\bar{x} = ab^n(ca)^m$ for some $n, m \geq 0$.

Proof. By Lemmas 3.8 and 3.9, $aa, cc \notin L(x)$. Hence $|x|_b = 0$ if and only if $x = a(ca)^m$ for some $m \geq 0$. Let then $|x|_b \geq 1$. If $|x|_a = 1$, then $x = ab^n$ with $n = |x|_b$ and the assertion is again verified. Otherwise, x begins and ends with a by Lemma 3.1. Since $|x|_a = |x|_c + 1$ and $aa, cc \notin L(x)$, it follows that ab and ba are both factors of x if and only if so are cb and bc . Since this is impossible in view of Remark 3.14, the only remaining options are $ab, bc \in L(x)$ or $cb, ba \in L(x)$. The assertion then follows from Lemma 3.15. \square

Lemma 3.17. Let $x \in \mathbb{A}^*$ be a singular word such that $|x| - |x|_c > 1$, and let $\delta = |x|_c - |x|_a + 1$. The following hold:

1. If $\delta > 0$ (resp. $\delta < 0$), then ab and ba (resp. bc and cb) do not occur in x .
2. If $|x|_b \geq |\delta| > 0$, then x has exactly $|\delta|$ runs of consecutive occurrences of b .

Proof. Assume $\delta > 0$ first, that is, $|x|_a < |x|_c + 1$. Then $|x|_b < |\delta|$ is equivalent to $|x|_c > |x|_a + |x|_b - 1$, and then to $cc \in L(x)$ by Lemma 3.9. In such a case, c is separating for x , so that $ab, ba \notin L(x)$. So assume that $|x|_b \geq |\delta|$, in which case $cc \notin L(x)$. By Lemma 3.1, c is neither a prefix nor a suffix of x . By contradiction, suppose $ab \in L(x)$, so that $cb \notin L(x)$ in view of Remark 3.14. Thus all occurrences of c would be followed by a . As $ab \in L(x)$, a occurs in x not only as a suffix; by Lemma 3.1, it must occur as a prefix too, so that $|x|_a \geq |x|_c + 1$, contradicting $\delta > 0$. Thus $ab \notin L(x)$, and $ba \notin L(x)$ by a symmetric argument. Hence, a can be followed (and preceded) only by c within x . A simple counting argument then shows that x has exactly $|x|_c - |x|_a + 1 = \delta$ runs of b .

Now let $\delta < 0$, so that $|x|_a > |x|_c + 1$, and x begins and ends with a by Lemma 3.1. By a similar argument as before, we obtain $cb, bc \notin L(x)$, so that c can be preceded and followed only by a . If $|x|_b \geq |\delta|$, that is, if $|x|_a \leq |x|_b + |x|_c + 1$, we have $aa \notin L(x)$ by Lemma 3.8. Therefore, we can count $|x|_a - |x|_c - 1 = |\delta|$ runs of b in x . \square

Let $\xi : \mathbb{A}^* \rightarrow \mathbb{A}^*$ be the map defined as follows: for all $x \in \mathbb{A}^*$, $\xi(x)$ is obtained by adding an occurrence of b to all existing runs of consecutive b in x , as well as in the middle of any occurrence of aa or cc . Unlike the maps we used for adding occurrences of a and c , this ξ cannot be realized via episturmian morphisms, but it is *sequential*, i.e., obtained as the output of a sequential transducer (cf. [23]), as shown in Figure 1. We remark that ξ commutes with reversal, that is, for all $x \in \mathbb{A}^*$,

$$\overline{\xi(x)} = \xi(\bar{x}).$$

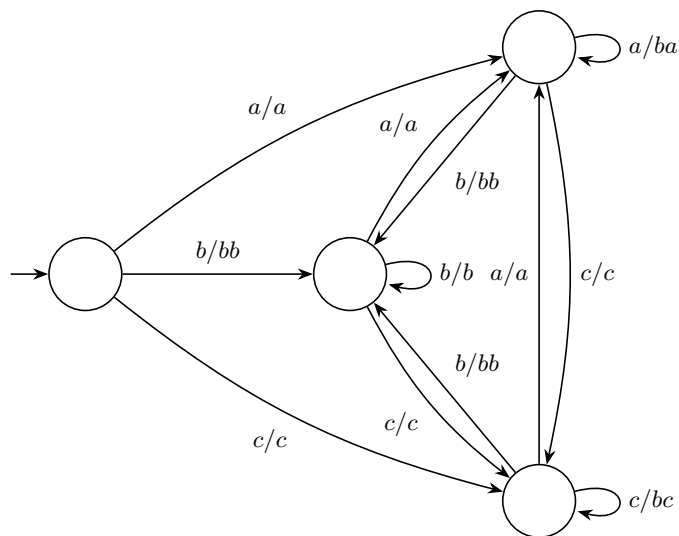


Figure 1: Diagram of a transducer realizing the ξ map. Labels show input/output.

In the following results, we will often need to add an occurrence of b at the end of

$\xi(x)$, when x ends in c . This can be expressed as $\xi(xc)c^{-1}$, i.e.,

$$\xi(xc)c^{-1} = \begin{cases} \xi(x)b & \text{if } x \text{ ends in } c, \\ \xi(x) & \text{otherwise.} \end{cases} \quad (7)$$

Similarly, $c^{-1}\xi(cx)$ adds a b before a possible leading c , and $c^{-1}\xi(cxc)c^{-1}$ deals with both ends (but note that $c^{-1}\xi(cc)c^{-1} = b$).

Remark 3.18. The mapping on \mathbb{A}^* given by $y \mapsto c^{-1}\xi(cyc)c^{-1}$ is injective. Its image is the regular language of words $x \in \mathbb{A}^+$ satisfying all of the following conditions:

1. $aa, abc, cba, cc \notin L(x)$,
2. c is neither a prefix nor a suffix of x ,
3. x does not begin with ba or end with ab .

Hence, for each x satisfying such conditions there exists a unique $y \in \mathbb{A}^*$ such that $x = c^{-1}\xi(cyc)c^{-1}$. This y is obtained from x by simply deleting an occurrence of b from each run.

Lemma 3.19. *Let $x, y \in \mathbb{A}^*$. The following are equivalent:*

1. $x < y$,
2. $\xi(x) < \xi(y)$,
3. $\xi(xc)c^{-1} < \xi(yc)c^{-1}$.

Proof. Suppose $x < y$. If y is a proper prefix of x , then $\xi(y)$ is a proper prefix of $\xi(x)$ since ξ is sequential. Otherwise, let $x = ua'v$ and $y = ub'w$ for some $u, v, w \in \mathbb{A}^*$ and $a', b' \in \mathbb{A}$ with $a' < b'$. If u ends in b or is empty, then $\xi(x)$ and $\xi(y)$ begin respectively in $\xi(u)a'$ and $\xi(u)b'$; this also occurs if u ends in a and $a' \neq a$, or if u ends in c and $b' \neq c$. If we have $a' = a$ with u ending in a , then $\xi(x)$ begins with $\xi(u)ba$ while $\xi(y)$ begins with $\xi(u)bb$ or $\xi(u)c$; the case where $b' = c$ and u ends in c is similar. Thus $1 \Rightarrow 2$.

Next, assume $\xi(x) < \xi(y)$. If $\xi(y)$ is not a prefix of $\xi(x)$, inequality 3 follows in view of eq. (7); the same happens if $\xi(y)$ does not end in c , since in this case $\xi(xc)c^{-1} \leq \xi(x) < \xi(y) = \xi(yc)c^{-1}$. Let then $\xi(y)$ be a proper prefix of $\xi(x)$, with $\xi(y)$ ending in c . Now, $\xi(x)$ cannot begin with $\xi(y)c$, since by definition cc cannot occur in an image under ξ . Hence $\xi(x)$ has either $\xi(y)a$ or $\xi(y)b$ as a prefix. In both cases we have $\xi(xc)c^{-1} \leq \xi(x) < \xi(y)b = \xi(yc)c^{-1}$ (note that $\xi(xc)c^{-1} \neq \xi(y)b$, since $\xi(x) \neq \xi(y)$). Hence $2 \Rightarrow 3$ in all cases.

Finally, suppose inequality 3 from the statement holds. If $\xi(yc)c^{-1}$ is a proper prefix of $\xi(xc)c^{-1}$, then so is $\xi(y)$ in particular, and this implies that y is a proper prefix of x . If $\xi(xc)c^{-1} = Ua'V$ and $\xi(yc)c^{-1} = Ub'W$ for some $U, V, W \in \mathbb{A}^*$ and $a', b' \in \mathbb{A}$ with $a' < b'$, then there exist $u \in \mathbb{A}^*$ such that either $U = \xi(u)b$ or $U = \xi(u)$. In the first case, it is easy to see that x and y respectively begin with ua' and ub' , so that $x < y$. The

same happens when $U = \xi(u)$ ends in b . If U ends in c , then $a' = a$ and $b' = b$ since cc cannot appear in an image under ξ ; hence x begins with ua while y either equals u , or it begins with ub or uc . The case where U ends in a is symmetric, except for the $x = u$ option which cannot occur. In all cases, we get $3 \Rightarrow 1$ as desired. \square

We can now prove the analogue of Lemmas 3.12 and 3.13 for the letter b .

Lemma 3.20. *A word $x \in \mathbb{A}^*$ is singular if and only if $X = c^{-1}\xi(cxc)c^{-1}$ is singular.*

Proof. Assume $|X|_a = |X|_c + 1$. By Proposition 3.16, X is singular if and only if either X or \bar{X} is $ab^n(ca)^m$ for some $m \geq 0$ and $n \neq 1$ (as $abc, cba \notin L(x)$); equivalently, x or \bar{x} is $ab^{n-1}(ca)^m$ (or $a(ca)^m$ when $n = 0$), which happens if and only if x is singular, as $|x|_a = |X|_a$ and $|x|_c = |X|_c$.

Now suppose $|X|_a \neq |X|_c + 1$. We may also assume that X contains all three letters. Indeed, if a (resp. c) does not occur, then $X = \lambda_b(x)b$ (resp. $X = \rho_b(x)b^{-1}$) and the assertion follows from Lemma 3.12 (resp. Lemma 3.13). If X that does not contain b , then X is singular only if $X = a(ca)^m$ for some $m \geq 0$, which contradicts $|X|_a \neq |X|_c + 1$.

Let X be singular. We need to show that no factorization $x = \bar{u} \cdot v \cdot w$ is reversible; without loss of generality, we may assume $v = a'v'b'$ for some letters $a' < b'$. If $u = \varepsilon$, then $w \leq u$ and the factorization is not reversible, as desired; let then u_1 be the first letter of u . We have three options for a', b' :

1. $a' = a, b' = b$.

If $w = \varepsilon$, then X ends in $\xi(av'b)$; by Lemma 3.1, this is impossible if $u \neq \varepsilon$.

Let then w begin with $w_1 \in \mathbb{A}$. If $w_1 < u_1$, then $w < u$ and we are done, so we only need to check the cases where $u_1 \leq w_1$. By Lemma 3.17, $L(X) \cap \mathbb{A}^2$ is contained in $\{ab, ac, ba, bb, ca\}$ if $|X|_a > |X|_c + 1$, or in $\{ac, bb, bc, ca, cb\}$ if the opposite inequality holds. This excludes the sub-cases where $u_1 \neq c$ and $w_1 = c$.

- If $u_1 = w_1 = a$, then in X a single b is inserted between u_1 and a' . Since the factorization

$$X = c^{-1}\xi(c\bar{u})b \cdot \xi(v)b^{-1} \cdot b\xi(wc)c^{-1} \quad (8)$$

cannot be reversible, we have $\xi(wc)c^{-1} \leq \xi(uc)c^{-1}$, so that $w \leq u$ by Lemma 3.19.

- If $u_1 = a$ and $w_1 = b$, then

$$X = c^{-1}\xi(c\bar{u})b \cdot \xi(v)b^{-1} \cdot \xi(wc)c^{-1} \quad (9)$$

would always be reversible; hence this case cannot happen.

- If $u_1 = w_1 = b$, then as

$$X = c^{-1}\xi(c\bar{u}) \cdot \xi(v)b^{-1} \cdot \xi(wc)c^{-1} \quad (10)$$

cannot be reversible, we again obtain $w \leq u$ by Lemma 3.19.

- Finally, if $u_1 = w_1 = c$, the non-reversibility of

$$X = c^{-1}\xi(c\bar{u}) \cdot \xi(v) \cdot \xi(wc)c^{-1} \quad (11)$$

again implies $w \leq u$.

2. $a' = a, b' = c$.

If $w = \varepsilon$, then X ends in $\xi(av'c)b$; once again, this is impossible if $u \neq \varepsilon$, by Lemma 3.1. Let w begin with $w_1 \in \mathbb{A}$ such that $u_1 \leq w_1$, again. As in case 1, the possible factors of length 2 in X exclude some options for u_1 and w_1 . We only need to examine the following.

- If $u_1 = w_1 = a$, then as

$$X = c^{-1}\xi(c\bar{u}) \cdot b\xi(v) \cdot \xi(wc)c^{-1} \quad (12)$$

cannot be reversible, we obtain $w \leq u$ by Lemma 3.19.

- If $u_1 = w_1 = c$, then as

$$X = c^{-1}\xi(c\bar{u}) \cdot \xi(v)b \cdot \xi(wc)c^{-1} \quad (13)$$

is not reversible, it follows that $w \leq u$.

3. $a' = b, b' = c$.

If $w = \varepsilon$, then X ends in $V = \xi(bv'c)b$, which in turn begins with bb , so that $V < \bar{V}$. Since a factorization $X = \bar{U} \cdot V \cdot \varepsilon$ with $U \neq \varepsilon$ (as $u \neq \varepsilon$) is reversible, we obtain $w \neq \varepsilon$ also in this case. If w_1 is its first letter and $u_1 \leq w_1$, the following sub-cases are left to examine after factors of length 2 in X are considered.

- If $u_1 = w_1 = a$, then we obtain $w \leq u$ from the factorization in eq. (11).
- If $u_1 = w_1 = b$, then considering the factorization

$$X = c^{-1}\xi(c\bar{u}) \cdot b^{-1}\xi(v) \cdot \xi(wc)c^{-1} \quad (14)$$

leads to the conclusion $w \leq u$ as above.

- If $u_1 = b$ and $w_1 = c$, then the factorization

$$X = c^{-1}\xi(c\bar{u}) \cdot b^{-1}\xi(v) \cdot b\xi(wc)c^{-1} \quad (15)$$

is always reversible; therefore this cannot occur.

- If $u_1 = w_1 = c$, then we get $w \leq u$ from

$$X = c^{-1}\xi(c\bar{u})b \cdot b^{-1}\xi(v) \cdot b\xi(wc)c^{-1}. \quad (16)$$

This concludes the proof that if X is singular then so is x .

Conversely, let us suppose that x is singular with $|x|_a \neq |x|_c + 1$, and prove the same for X . We need to show that no factorization $X = \bar{U} \cdot V \cdot W$ is reversible, where $V = a'V'b'$ for some $a', b' \in \mathbb{A}$ with $a' < b'$, without loss of generality.

If $U = \varepsilon$, there is nothing to prove as $W \leq U$, so let U_1 be the first letter of U . If W were empty, then since X cannot end in c , we would have $a' = a$ and $b' = b$. Hence x would not end in a ; by Lemma 3.1, $a' = a$ would then be a prefix of x , and then of X , against $U \neq \varepsilon$. Let then W begin with $W_1 \in \mathbb{A}$, with $U_1 \leq W_1$ (otherwise $W < U$ and there is nothing to prove).

By Lemma 3.17, the set $L(x) \cap \mathbb{A}^2$ is contained in either $\{ac, bb, bc, ca, cb, cc\}$ or $\{aa, ab, ac, ba, bb, ca\}$, depending on the sign of $|x|_c - |x|_a + 1$. This implies that $L(X) \cap \mathbb{A}^2$ is contained in $\{ac, bb, bc, ca, cb\}$ or $\{ab, ac, ba, bb, ca\}$, respectively. Hence, the only cases left to examine are the following:

1. $U_1 = a$, $a' = b$, $b' = c$, and $W_1 = a$.

Then V begins with either ba or bb . In the first case, there exist $u, v, w \in \mathbb{A}^+$ such that $x = \bar{u}vw$ and our factorization $X = \bar{U}VW$ coincides with eq. (12); as x is singular, we have $w \leq u$ and then $W \leq U$ by Lemma 3.19. In the second case, the same argument applied to eq. (11) leads to $W \leq U$ as well.

2. $U_1 = b$, $a' = a$, $b' = b$, and $W_1 = b$.

By Remark 3.18, X cannot begin with ba , so that U begins with ba or bb . The same is true for W , for otherwise x would end with b and have an internal occurrence of a , against Lemma 3.1.

- If U and W both begin with ba , there exist u, v, w such that $x = \bar{u}vw$, and eq. (8) is $X = \bar{U} \cdot V \cdot W$. Then $w \leq u$, which implies $W \leq U$ by Lemma 3.19.
- If U began with ba , but W with bb , we would obtain eq. (9) and $x = \bar{u}vw$ for some $u < w$, which is impossible.
- If U begins with bb and W with ba , we have $W \leq U$ as desired.
- Finally, if both U and W begin with bb , eq. (10) and $x = \bar{u}vw$ describe the situation; again $w \leq u$ follows, so that $W \leq U$.

3. $U_1 = b$, $a' = b$, $b' = c$, and $W_1 = b$.

If $U = b$, then $W \leq U$ and we are done. If $U \neq b$ and $W = b$ instead, x would end with c , against Lemma 3.1. Hence we can assume U and W begin in either bb or bc .

- If U and W both begin with bb , eq. (14) applies and yields $W \leq U$.
- If U began with bb while W began with bc , eq. (15) would apply for some $u < w$, a contradiction.
- If U begins with bc and W begins with bb , there is nothing to prove.
- If U and W both begin with bc , eq. (16) describes the situation and implies $W \leq U$.

4. $U_1 = c$, $a' = a$, $b' = b$, and $W_1 = c$.

Then V ends in either bb or cb , leading to eqs. (11) and (13) respectively, and then to $W \leq U$ in both cases.

The proof is now complete. \square

We now prove one of the main results of this section.

Theorem 3.21. *Let $\mathbb{A} = \{a, b, c\}$ with $a < b < c$. Every abelian class of \mathbb{A}^* contains exactly one pair $\{x, \bar{x}\}$ of singular words.*

Proof. Let $\mathbf{v} = (n_a, n_b, n_c) \in \mathbb{N}^3$. We need to show that up to reversal, there exists a unique singular word x with Parikh vector \mathbf{v} , i.e., such that $|x|_a = n_a$, $|x|_b = n_b$, and $|x|_c = n_c$. If $n_a n_b n_c = 0$, this follows from Theorem 3, since there exists a unique power of a Christoffel word for every non-zero Parikh vector. In particular, this proves the assertion for $n_a + n_b + n_c = |x| \leq 2$.

Let then $n_a n_b n_c > 0$, and assume that the result holds for all vectors (p, q, r) with $p + q + r < n_a + n_b + n_c$. We can identify three cases:

1. If $n_a \geq n_b + n_c + 1$, then by induction there exists a unique pair of singular words $\{x', \bar{x}'\}$ with Parikh vector $(n_a - n_b - n_c - 1, n_b, n_c)$. Then $x = \lambda_a(x')a$ and \bar{x} have vector \mathbf{v} , and are singular by Lemma 3.12. Any other singular word y with vector \mathbf{v} begins and ends with a by Lemma 3.1, and has a as a separating letter by Lemma 3.8; hence $y = \lambda_a(y')a$ for some y' with vector $(n_a - n_b - n_c - 1, n_b, n_c)$. Such a y' is necessarily singular by Lemma 3.12, so that $y' \in \{x', \bar{x}'\}$. This case is therefore settled.
2. If $n_c \geq n_a + n_b - 1$, then by induction there exists a unique pair of singular words $\{x', \bar{x}'\}$ with vector $(n_a, n_b, n_c - n_a - n_b + 1)$ (note that $n_a + n_b - 1 \geq 1$ since $pq > 0$). Then $x = \rho_c(x')c^{-1}$ and \bar{x} have vector \mathbf{v} , and are singular by Lemma 3.13. By Lemma 3.9, any singular word y with vector \mathbf{v} has c as a separating letter, so that $y = \rho_c(y')c^{-1}$ for some word y' , which is singular by Lemma 3.13 and has vector $(n_a, n_b, n_c - n_a - n_b + 1)$. Thus $y' \in \{x', \bar{x}'\}$, as desired.
3. If $n_a < n_b + n_c + 1$ and $n_c < n_a + n_b - 1$, it follows $n_b > |\delta|$, with $\delta = n_c - n_a + 1$. By Proposition 3.16, if $\delta = 0$ then $x = ab^{n_b}(ca)^{n_c}$ and \bar{x} are the only singular words with vector \mathbf{v} . Let us then assume $\delta \neq 0$.

By induction, there exists a unique pair of singular words $\{x', \bar{x}'\}$ with vector $(n_a, n_b - |\delta|, n_c)$. Let $x = c^{-1}\xi(cx'c)c^{-1}$. Then x and \bar{x} are singular by Lemma 3.20. Since $aa, cc \notin L(x)$, by Lemmas 3.8 and 3.9 we obtain $|x|_b \geq |\delta|$. Lemma 3.17 then implies that x and \bar{x} have exactly $|\delta|$ runs of b , and hence Parikh vector \mathbf{v} . If y is any singular word with vector \mathbf{v} , then $aa, cc \notin L(y)$ by Lemmas 3.8 and 3.9. Furthermore, by Lemma 3.1, y cannot begin with c or ba , and it cannot end with c or ab . Finally, we have $abc, cba \notin L(y)$ by Lemma 3.15, as $\delta \neq 0$. In view of Remark 3.18, this implies the existence of a unique word y' such that $y = c^{-1}\xi(cy'c)c^{-1}$. By Lemma 3.17, y' has vector $(n_a, n_b - |\delta|, n_c)$, and by Lemma 3.20 it is singular. Hence we once again obtain $y' \in \{x', \bar{x}'\}$. \square

Behind induction, the above proof hides the following algorithm for determining the unique (up to reversal) singular word with a given Parikh vector (n_a, n_b, n_c) :

1. Starting from the vector (n_a, n_b, n_c) , we iterate the following rule:
 - If $n_a \geq n_b + n_c + 1$, the next vector is $(n_a - n_b - n_c - 1, n_b, n_c)$;
 - If $n_c \geq n_a + n_b - 1$, the subsequent vector is $(n_a, n_b, n_c - n_a - n_b + 1)$;
 - Otherwise, the next vector is $(n_a, n_b - |n_c - n_a + 1|, n_c)$.
2. Repeat step 1 until a vector (p, q, r) is reached with $pqr = 0$ or $p = r + 1$ is reached.
3. Use Theorem 3 or Proposition 3.16, respectively, to find the unique (up to reversal) singular word with vector (p, q, r) .
4. Go back through the previous vectors, using the appropriate result (Lemma 3.12, Lemma 3.13, or Lemma 3.20) to construct the corresponding singular word.

Example 3.22. Let us show that the only singular words with Parikh vector $(3, 5, 7)$ are $x = acbcbcbcbcbca$ and its reverse. Step 1 yields vector $(3, 5, 0)$, and since the only power of a Christoffel word with $3 - 1$ occurrences of a and $5 + 1$ of b is $abbbabbb$, Theorem 3 implies that $x' = abbbabba$ is singular. Hence $x = \rho_c(x')c^{-1}$ is singular too, by Lemma 3.13.

The singular words with vector $(3, 7, 5)$ are $y = acbbcbcbcbcbca$ and \bar{y} . Indeed, the above algorithm gives the sequence of vectors $(3, 4, 5) \mapsto (3, 1, 5) \mapsto (3, 1, 2)$; by Proposition 3.16, $y_0 = abcaca$ is singular, whence so are $y_1 = \rho_c(y_0)c^{-1} = acbccacca$, $y_2 = c^{-1}\xi(cy_1c)c^{-1} = acbbcbcbcbca$, and $y = c^{-1}\xi(cy_2c)c^{-1}$.

We observe that Theorem 3.21 is essentially a restatement of the Theorem 1 given in the introduction. The next example shows that Theorem 3.21 does not extend to larger alphabets.

Example 3.23. Consider the word $y = abcbdd$ on the ordered alphabet $\mathbb{A} = \{a, b, c, d\}$ with $a < b < c < d$. Then the abelian class of y contains two singular words (up to reversal), namely $x = bcd bda$ and $x' = bdb cda$. Thus relative to any order preserving assignment $\phi : \{a, b, c, d\} \rightarrow \{2, 3, 4, \dots\}$, the maximum of $\dot{K}(\cdot)$ will be attained at either x or x' . Now, one can check that for the assignment $(a, b, c, d) \mapsto (3, 4, 5, 6)$ one finds $\dot{K}(x) = 6827 > 6825 = \dot{K}(x')$ and hence amongst all permutations of 344566 the maximum of $\dot{K}(\cdot)$ is attained uniquely at x (or \bar{x}). In contrast, if $(a, b, c, d) \mapsto (3, 4, 15, 16)$ then $\dot{K}(x) = 171127 < 171135 = \dot{K}(x')$, whence the maximum of $\dot{K}(\cdot)$ is attained uniquely at x' . This shows that in this case the maximizing arrangement depends on the actual values assigned to each of a, b, c and d . Finally, relative to the assignment $(a, b, c, d) \mapsto (3, 4, 7, 8)$ one finds that $\dot{K}(x) = \dot{K}(x') = 18247$ which shows that the maximizing arrangement need not be unique.

4 Infinite singular words

Let \mathbb{A} be an ordered set. For $x \in \mathbb{A}^{\mathbb{N}} \cup \mathbb{A}^{\mathbb{Z}}$, let $L(x)$ denote the set of all factors $u \in \mathbb{A}^+$ occurring in x . We do not assume that each $a \in \mathbb{A}$ occurs in x . We say $L(x)$ is *symmetric* if $L(x)$ is closed under reversal, i.e., if $u \in L(x)$ then $\bar{u} \in L(x)$.

We begin by investigating infinite binary singular words.

Proposition 4.1. *Let $x \in \mathbb{A}^{\mathbb{Z}}$ be a bi-infinite word over an ordered binary alphabet $\mathbb{A} = \{a, b\}$. Then x is singular if and only if x is balanced.*

Proof. By Lemma 3.3, if x is singular then x is balanced. Conversely, if x is not singular, then x admits a reversible factorization $x = \bar{u}vw$. Thus we may write $v = ra'v'b'\bar{r}$, $u = sa'u'$ and $w = sb'w'$ with $r, s, v' \in \mathbb{A}^*$, $u', w' \in \mathbb{A}^{\mathbb{N}}$ and $\{a', b'\} = \{a, b\}$. It follows that $a'\bar{s}ra'$ and $b'\bar{r}sb'$ are each factors of x , whence x is not balanced. \square

As an immediate corollary:

Corollary 4.2. *Let $x \in \mathbb{A}^{\mathbb{Z}}$ be a bi-infinite word over a binary alphabet $\mathbb{A} = \{a, b\}$. Then x verifies the Markoff property (M) if and only if x is singular for every linear order $<$ on \mathbb{A} .*

Proof. Fix a linear order $<$ on \mathbb{A} . Then by Proposition 4.1, x is singular if and only if x is balanced. The result now follows from Proposition 3.1 in [34]. \square

In order to characterize one sided infinite binary singular words, we first establish the following general lemma:

Lemma 4.3. *Let \mathbb{A} be any ordered alphabet. Let $x \in \mathbb{A}^{\mathbb{N}}$ and assume $L(x)$ is symmetric. If x is singular, then $x \leq x'$ for each suffix x' of x . In particular, if x is not (purely) periodic, then x is Lyndon.*

Proof. Assume to the contrary that $x' < x$ for some proper suffix x' of x . Then there exist $z \in \mathbb{A}^*$, $a, b \in \mathbb{A}$ with $a < b$ such that zb is a prefix of x and za a prefix of x' . Let v be a prefix of x beginning in zb and ending in $a\bar{z}$. Then we have $x = vw$ for some $w \in \mathbb{A}^{\mathbb{N}}$ and $\bar{v} < v$. It follows that the factorization $x = \bar{u}vw$ with $u = \varepsilon$ is reversible, whence x is not singular, a contradiction. Finally, if x is not purely periodic, then $x \neq x'$ for each proper suffix x' of x . It follows that $x < x'$ for each proper suffix x' of x and hence x is infinite Lyndon. \square

Theorem 4. *Let $x \in \{a, b\}^{\mathbb{N}}$ be an aperiodic binary (one sided) infinite word. Then x is singular if and only if x is a Sturmian Lyndon word.*

Proof. Without loss of generality we may assume that $a < b$. First assume x is singular. Then x is balanced by Lemma 3.3. It follows that x is Sturmian (see Theorem 2.1.5 in [23]). Since $L(x)$ is symmetric (see Proposition 2.1.19 in [23]), it follows from Lemma 4.3 that x is Lyndon.

For the converse, assume x is a Sturmian Lyndon word, and suppose to the contrary that x admits a reversible factorization $x = \bar{u}vw$. Of all such factorizations, pick one

with the length of v minimal. It follows that the first and last letter of v are distinct. Thus, assume v begins in c and ends in d with $\{c, d\} = \{a, b\}$. If u is a prefix of w , then $w < u$ and hence $\bar{v} < v$ which implies that $c = b$ and $d = a$. It follows that au is a factor of x and hence so is $\bar{u}a$. But x begins in $\bar{u}b$ which contradicts the fact that x is Lyndon. Thus u is not a prefix of w . In this case we have $u = zeu'$ and $w = zfw'$ with $z, u' \in \mathbb{A}^*$, $w' \in \mathbb{A}^{\mathbb{N}}$ and e and f distinct letters. In particular z is a right special factor of x . But since $\bar{z}c$ and $\bar{z}d$ are also factors of x , it follows that \bar{z} is also right special, whence $z = \bar{z}$. Thus ezc and dzf are each factors of x . If $v < \bar{v}$ (i.e., $c < d$) then $u < w$ (i.e., $e < f$) whence $a = c = e$ and $b = d = f$ from which it follows that aza and bzb are each factors of x , a contradiction. Similarly, if $v > \bar{v}$ then $u > w$ whence $b = c = e$ and $a = d = f$ which again leads to the contradiction that aza and bzb are both factors of x . This concludes our proof of Theorem 4. \square

Corollary 4.4. *Let $x \in \mathbb{A}^{\mathbb{N}}$ be an aperiodic word over an ordered binary alphabet $\mathbb{A} = \{a, b\}$. If x is singular then x is uniformly recurrent.*

Proof. This follows immediately from Theorem 4 together with the fact that every Sturmian word is uniformly recurrent (see for instance Proposition 2.1.25 in [23]). \square

Corollary 4.5. *Let $x \in \mathbb{A}^{\mathbb{N}}$ be a uniformly recurrent aperiodic word over an ordered binary alphabet $\mathbb{A} = \{a, b\}$. Then the shift orbit closure of x contains a singular word if and only if x is Sturmian. Furthermore, this singular word is unique.*

Proof. If x is Sturmian, then the unique Lyndon word in the shift orbit closure of x is singular by Theorem 4. Conversely, assume y is a singular word in the shift orbit closure of a uniformly recurrent aperiodic binary word x . Then y is also uniformly recurrent, aperiodic and binary, whence y is Sturmian Lyndon by Theorem 4. It follows that x is also Sturmian. \square

The binary case is quite special as already on a ternary alphabet infinite singular words display a much different behavior. As we saw an infinite singular aperiodic word over a binary alphabet is necessarily uniformly recurrent and its set of factors is closed under reversal. Furthermore, a uniformly recurrent word x over a binary alphabet contains a singular word in its shift orbit closure if and only if x is Sturmian, and moreover, this singular word is unique. This is in general not the case on alphabets of cardinality greater than 2. For example, it is easy to see that over the ternary alphabet $\mathbb{A} = \{a, b, c\}$ with $a < b < c$, any infinite concatenation of ac and abc is singular. This implies in particular that there exist non recurrent singular words or recurrent aperiodic singular words which are not uniformly recurrent. It also shows that in general the set of factors of an infinite singular word need not be closed under reversal.

We next investigate the structure of infinite singular words whose set of factors is closed under reversal. In what follows, let $\mathbb{A}_k = \{1, 2, \dots, k\}$ be ordered by $1 < 2 < \dots < k$.

Definition 4.6. Let $L \subseteq \mathbb{A}_k^*$. We say that L satisfies the *symmetric order condition* if whenever

$$asd, bsc \in L \text{ with } a \neq b \text{ and } c \neq d \text{ (} a, b, c, d \in \mathbb{A}_k \text{), then } a < b \Leftrightarrow c < d \quad (17)$$

for each $s \in \mathbb{A}_k^*$.

Theorem 4.7. Let $x \in \mathbb{A}_k^{\mathbb{N}} \cup \mathbb{A}_k^{\mathbb{Z}}$. Assume $L(x)$ is symmetric.

1. If $x \in \mathbb{A}_k^{\mathbb{Z}}$, then x is singular if and only if $L(x)$ satisfies the symmetric order condition.
2. If $x \in \mathbb{A}_k^{\mathbb{N}}$, then x is singular if and only if $L(x)$ satisfies the symmetric order condition and $x \leq x'$ for each suffix x' of x .

Proof. We begin by showing that if $x \in \mathbb{A}_k^{\mathbb{N}} \cup \mathbb{A}_k^{\mathbb{Z}}$ is singular, then $L(x)$ verifies the symmetric order condition. So assume that $asd, bsc \in L(x)$ with $a \neq b$ and $c \neq d$. Since $L(x)$ is symmetric both $d\bar{s}a, bsc \in L(x)$. Furthermore, these two words cannot overlap one another. Thus there exists $r \in \mathbb{A}_k^*$ such that $d\bar{s}arb\bar{s}c \in L(x)$ or $b\bar{s}c\bar{s}a \in L(x)$. If $d\bar{s}arb\bar{s}c \in L(x)$, then we can write $x = \bar{u}vw$ with $v = arb$, and where w begins in sc and u begins in sd . Then $a < b \Leftrightarrow v < \bar{v} \Leftrightarrow w < u \Leftrightarrow c < d$. Similarly, if $b\bar{s}c\bar{s}a \in L(x)$ then we can write $x = \bar{u}vw$ with $v = crd$, and where w begins in $\bar{s}a$ and u begins in $\bar{s}b$. Then $c < d \Leftrightarrow v < \bar{v} \Leftrightarrow w < u \Leftrightarrow a < b$. Also, if $x \in \mathbb{A}_k^{\mathbb{N}}$, then by Lemma 4.3 we have $x \leq x'$ for each suffix x' of x .

For the converse, first assume that $x \in \mathbb{A}_k^{\mathbb{Z}}$. We will show that if $x = \bar{u}vw$ with $v \in \mathbb{A}_k^+$ and $v \neq \bar{v}$ and $u \neq w$ then $v < \bar{v}$ if and only if $w < u$. Without loss of generality we may assume that v begins and ends in distinct letters c and d . Thus fix a factorization $x = \bar{u}vw$ with $u \neq w$ and with $v = cyd$ with $y \in \mathbb{A}_k^*$ and $c, d \in \mathbb{A}_k$ distinct. Let us write $u = sbu'$ and $w = saw'$ with $s \in \mathbb{A}_k^*$, $u', w' \in \mathbb{A}_k^{\mathbb{N}}$ and $a, b \in \mathbb{A}_k$ distinct. Since $L(x)$ is symmetric, both $a\bar{s}d$ and $b\bar{s}c$ belong to $L(x)$. It follows from the symmetric order condition that if $a < b \Leftrightarrow c < d$. In other words, if $w < u \Leftrightarrow v < \bar{v}$ as required.

Next assume that $x \in \mathbb{A}_k^{\mathbb{N}}$ and $L(x)$ satisfies the symmetric order condition and $x \leq x'$ for every suffix x' of x . Fix a factorization $x = \bar{u}vw$ with $v = cyd$ with $y \in \mathbb{A}_k^*$ and $c, d \in \mathbb{A}_k$ distinct and $u \neq w$. Then, the same proof as in the case of $x \in \mathbb{A}_k^{\mathbb{Z}}$ shows that if u is not a proper prefix of w , then $v < \bar{v} \Leftrightarrow w < u$. So it remains to consider the case when u is a proper prefix of w in which case $w < u$. As $L(x)$ is symmetric and $du \in L(x)$ it follows that $\bar{u}d$ is a factor of x . Let x' be a (proper) suffix of x beginning in $\bar{u}d$. Since $\bar{u}c$ is a prefix of x and $x \leq x'$, it follows that $c < d$ and hence $v < \bar{v}$ as required. \square

We will now use Theorem 4.7 to show that infinite singular words $x \in \mathbb{A}_k^{\mathbb{Z}}$, with $L(x)$ symmetric, arise as natural codings of symmetric k -interval exchange transformations. In fact, the symmetric order condition is precisely the combinatorial criterion which distinguishes the language of symmetric interval exchange transformations from other symmetric languages of the same factor complexity including Arnoux-Rauzy subshifts or more generally Episturmian subshifts.

Interval exchange transformations were originally introduced by Oseledec [28], following an idea of Arnold [1], see also [20]. A k -interval exchange transformation \mathcal{I} is given by a probability vector $(\alpha_1, \alpha_2, \dots, \alpha_k)$, $0 < \alpha_i < 1$, together with a permutation π of $\{1, 2, \dots, k\}$. The unit interval $[0, 1]$ is partitioned into k sub-intervals of lengths $\alpha_1, \alpha_2, \dots, \alpha_k$ labeled $1, 2, \dots, k$ which are then rearranged according to the permutation π^{-1} . (Note: In some definitions, the intervals are rearranged according to the permutation π .) We will only be interested here in symmetric interval exchanges, that is, where the permutation π is given by $\pi(i) = k + 1 - i$:

Definition 4.8. A *symmetric k -interval exchange transformation* \mathcal{I} is a k -interval exchange transformation with probability vector $(\alpha_1, \dots, \alpha_k)$, and permutation $\sigma(i) = k + 1 - i$, $1 \leq i \leq k$ defined by

$$\mathcal{I}(x) = x + \sum_{\pi^{-1}j < \pi^{-1}i} \alpha_j - \sum_{j < i} \alpha_j$$

when x belongs to the (half open) interval

$$\mathcal{I}_i = \left[\sum_{j < i} \alpha_j, \sum_{j \leq i} \alpha_j \right).$$

We denote by β_i ($1 \leq i \leq k - 1$), the i -th point of discontinuity of \mathcal{I}^{-1} , namely $\beta_i = \sum_{j=k+1-i}^k \alpha_j$ and by γ_i is the i -th discontinuity of \mathcal{I} , namely $\gamma_i = \sum_{j=1}^i \alpha_j$. Then $\mathcal{I}_1 = [0, \gamma_1)$, $\mathcal{I}_i = [\gamma_{i-1}, \gamma_i)$, $2 \leq i \leq k - 1$ and $\mathcal{I}_k = [\gamma_{k-1}, 1)$.

Two points $x, y \in [0, 1]$ are said to belong to the same \mathcal{I} -orbit if $\mathcal{I}^n(x) = y$ for some $n \in \mathbb{Z}$. This defines an equivalence relation on $[0, 1]$ and the equivalence classes are called *orbits*. To each point $\gamma \in [0, 1]$, one associates a bi-infinite word $(x_n)_{n \in \mathbb{Z}} \in \mathbb{A}_k^{\mathbb{Z}}$, called the *natural coding* of γ under \mathcal{I} , where $x_n = i$ whenever $\mathcal{I}^n(\gamma) \in \mathcal{I}_i$. We define the language of \mathcal{I} , denoted $L(\mathcal{I})$, to be the language generated by all natural codings, i.e., $w \in L(\mathcal{I})$ if and only if w is a factor of the natural coding of some point γ under \mathcal{I} .

Via a decomposition result due to D. Gaboriau, G. Levitt and F. Paulin which applies generally to all systems of partial isometries (see Theorem 3.1 in [18]), every symmetric k -interval exchange transformation \mathcal{I} decomposes canonically into a finite number of invariant sub-systems \mathcal{J}_i . Moreover on each \mathcal{J}_i , either every orbit is finite, meaning each corresponding natural coding is periodic, or each orbit is dense, in which case \mathcal{J}_i is said to be *minimal*. In particular, the closure of an orbit is not a Cantor set and every natural coding under \mathcal{I} of a point $\gamma \in [0, 1]$ is uniformly recurrent.

We will make use of the following recent result due to S. Ferenczi, P. Hubert and the third author [14] characterizing symmetric k -interval exchange transformations languages (see the proof of Theorem 13 and Lemma 11 in [14] or Proposition 4 in [15]):

Theorem 4.9. [Theorem 13 in [14]] *A language $L \subseteq \mathbb{A}_k^*$ is the language of a symmetric k -interval exchange transformation \mathcal{I} with interval lengths $(\alpha_1, \alpha_2, \dots, \alpha_k)$ if and only if the following two conditions are satisfied:*

- L satisfies the symmetric order condition
- *measure condition*: there exists an invariant probability measure μ on the symbolic dynamical system (X_L, S) generated by L such that $\mu([w]) > 0$ for each $w \in L$ and $\mu([i]) = \alpha_i$ for each $i \in \mathbb{A}_k \cap L$.

The language L in Theorem 4.9 is assumed to be factorial and extendable. That is, writing $L = \bigcup_{i \geq 0} L_i$ with $L_0 = \{\varepsilon\}$ and $L_n \subseteq \mathbb{A}_k^n$ for all n , we have that for each $v \in L_n$ there exists $a, b \in \mathbb{A}_k$ with $av, vb \in L_{n+1}$ and each $v \in L_{n+1}$ may be written as $v = au = u'b$ with $a, b \in \mathbb{A}_k$ and $u, u' \in L_n$. A language L is *minimal* if for each $v \in L$ there exists n such that v is a factor of each word $w \in L_n$. The *symbolic dynamical system* (X_L, S) generated by a language L is the two-sided shift $S : X_L \rightarrow X_L$ where X_L consists of all bi-infinite words $x \in \mathbb{A}_k^{\mathbb{Z}}$ such that $L(x) \subseteq L$ and where the shift operator S is defined by $S((x_i)_{i \in \mathbb{Z}})_n = x_{n+1}$. Finally, by $[w]$ we mean the *cylinder set* defined by $w \in L$, i.e., $[w] = \{x \in X_L : x_0 x_1 \cdots x_{|w|-1} = w\}$.

Proposition 4.10. *Let $x \in \mathbb{A}_k^{\mathbb{Z}}$ be uniformly recurrent and assume that each $i \in \mathbb{A}_k$ occurs in x . If $L(x)$ satisfies the symmetric order condition, then $L(x)$ is symmetric and hence x is singular.*

Proof. Since x is uniformly recurrent, it follows that $L(x)$ is minimal. Minimality of $L(x)$ in turn implies the measure condition given in Theorem 4.9. In fact, as in [7], let μ be any invariant probability measure on the shift orbit closure of x , which is the same as the symbolic system generated by $L(x)$. Then for each positive integer n there is at least one word $v(n) \in L(x)$ of length n with $\mu([v(n)]) > 0$. Now for each $w \in L(x)$, as x is uniformly recurrent, it follows that w is a factor of $v(n)$ for all n sufficiently large. Hence $\mu([w]) \geq \mu([v(n)]) > 0$ for all n sufficiently large. It follows from Theorem 4.9 (applied to $L(x)$) that $L(x) = L(\mathcal{I})$ for some minimal symmetric k -interval exchange transformation \mathcal{I} with interval lengths $(\mu([1]), \mu([2]), \dots, \mu([k]))$.

Now consider $\bar{x} \in \mathbb{A}_k^{\mathbb{Z}}$. Then $L(\bar{x}) = \{w \in \mathbb{A}_k^* : \bar{w} \in L(x)\}$. Then $L(\bar{x})$ also verifies the symmetric order condition. Furthermore, we can define an invariant probability measure μ' on the shift orbit closure of \bar{x} by $\mu'([w]) = \mu([\bar{w}])$ for each $w \in L(\bar{x})$. It follows that $L(\bar{x})$ also satisfies the measure condition and hence by Theorem 4.9, $L(\bar{x}) = L(\mathcal{I}')$ where \mathcal{I}' is a minimal symmetric k -interval exchange transformation with interval lengths $(\mu'([1]), \mu'([2]), \dots, \mu'([k]))$. Since $\mu([i]) = \mu'([i])$ for each $i \in \mathbb{A}_k$, it follows that $\mathcal{I} = \mathcal{I}'$ and hence $L(x) = L(\mathcal{I}) = L(\mathcal{I}') = L(\bar{x})$. This proves that $L(x)$ is symmetric. Finally, that x is singular now follows from Theorem 4.7. \square

Theorem 5. *Let $\mathbb{A}_k = \{1, 2, \dots, k\}$ ($k \geq 2$) and let $x \in \mathbb{A}_k^{\mathbb{Z}}$ be uniformly recurrent and assume that each $i \in \mathbb{A}_k$ occurs in x . Then the following are equivalent:*

1. $L(x)$ is the language of a symmetric k -interval exchange transformation.
2. x is singular and $L(x)$ is symmetric.

Proof. Let $x \in \mathbb{A}_k^{\mathbb{Z}}$ and assume $L(x) = L(\mathcal{I})$ for some symmetric k -interval exchange transformation \mathcal{I} . We will show that x is singular and $L(x)$ symmetric. By Theorem 4.9,

$L(x)$ satisfies the symmetric order condition. As x is uniformly recurrent, it follows from Proposition 4.10 that $L(x)$ is symmetric and x singular.

For the converse, let $x \in \mathbb{A}_k^{\mathbb{Z}}$ be uniformly recurrent. Assume x is singular and $L(x)$ is symmetric. It follows from Theorem 4.7 that $L(x)$ satisfies the symmetric order condition. Also, as x is uniformly recurrent, it follows (as in the proof of Proposition 4.10) that $L(x)$ satisfies the measure condition. Hence by Theorem 4.9, we have that $L(x) = L(\mathcal{I})$ for some minimal k -interval exchange transformation \mathcal{I} . \square

We now give a characterization of natural codings of symmetric k -interval exchange transformations satisfying Keane's infinite distinct orbit condition [21]:

Definition 4.11. A k -interval exchange transformations \mathcal{I} satisfies the *infinite distinct orbit condition* (or *i.d.o.c.* for short) if the $k - 1$ negative trajectories $\{\mathcal{I}^{-n}(\gamma_i)\}_{n \geq 0}$ ($1 \leq i \leq k - 1$) of the discontinuities of \mathcal{I} are infinite disjoint sets.

If \mathcal{I} satisfies i.d.o.c., then \mathcal{I} is minimal but not conversely. A complete characterization of languages of interval exchange transformations satisfying i.d.o.c. was obtained by S. Ferenczi and the third author in [15] (see Theorem 4.13 below). It is based on Kerckhoff's definition of k -interval exchange transformations which involves two permutations (π_0, π_1) in which the unit interval $[0, 1]$ is partitioned into k sub-intervals of lengths $\alpha_1, \alpha_2, \dots, \alpha_k$ ordered according to the permutation π_0^{-1} and then rearranged according to the permutation π_1^{-1} (see [22]). We first need to recall some terminology:

Definition 4.12. For a permutation π of $\{1, 2, \dots, k\}$, we define the π -order by $a <_{\pi} b$ whenever $\pi(a) < \pi(b)$. A π -interval is a nonempty set of consecutive integers in the π -order.

Let L be a language. For $w \in L$, we define *arrival* set of w , denoted $A(w)$, as the set of all letters a such that aw is in L , and the *departure* set of w , denoted $D(w)$, as the set of all letters a such that $wa \in L$.

The following theorem gives a characterization of languages generated by a k -interval exchange transformation satisfying i.d.o.c.:

Theorem 4.13. [Theorem 2 in [15]] A language L is the language of a k -interval exchange transformation \mathcal{I} , defined by permutations (π_0, π_1) such that $\pi_0^{-1}(\{1, \dots, j\}) \neq \pi_1^{-1}(\{1, \dots, j\})$ for every $1 \leq j \leq k - 1$, and satisfying i.d.o.c., if and only if L satisfies

(H0) $L_1 = \{1, \dots, k\}$,

(H1) L is minimal,

(H2) if w is a bispecial word, $A(w)$ is a π_1 -interval,

(H3) if w is a bispecial word and $a \in A(w)$, $D(aw)$ is a π_0 -interval,

(H4) if $a, b \in A(w)$ with $a <_{\pi_1} b$, $c \in D(aw)$, $d \in D(bw)$, then $c \leq_{\pi_0} d$,

(H5) if $a, b \in A(w)$ are consecutive in the π_1 order, $D(aw) \cap D(bw)$ is a singleton.

We will also be needing the following lemma:

Lemma 4.14. *[Lemma 6 in [15]] If L satisfies (H0) to (H5) for $\pi_0 = Id$, $\pi_1 = \sigma : i \mapsto k + 1 - i$, then L is symmetric.*

As observed in [15], condition (H5) precludes the existence of weak bispecial factors (see [8]). It is implied by i.d.o.c.. In general, a natural coding x of a symmetric k -interval exchange transformation may contain weak bispecial factors as the following example illustrates:

Example 4.15. Let $y = 01001010010 \dots$ be the Fibonacci word fixed by the morphism $0 \mapsto 01$, $1 \mapsto 0$. Let $x \in \{1, 2, 3\}^{\mathbb{N}}$ be the image of $0y$ under the morphism $0 \mapsto 1213$, $1 \mapsto 12213$.

$$x = 1213121312213121312131221312131221312131221312131221312131 \dots$$

Then it is readily verified that x is an aperiodic uniformly recurrent singular word and $L(x)$ is symmetric (in fact, x begins in infinitely many palindromes). It follows that $L(x)$ satisfies the symmetric order condition and the measure condition, whence $L(x) = L(\mathcal{I})$ for some symmetric 3-interval exchange transformation \mathcal{I} . However, \mathcal{I} does not satisfy i.d.o.c. since $L(x)$ does not verify (H5). In fact, consider the bispecial factor $w = 1$. Then $2, 3 \in A(1)$ are consecutive in the π_1 -order. However, $D(21) = \{3\}$ while $D(31) = \{2\}$ whence $D(21) \cap D(31) = \emptyset$.

Theorem 4.16. *Let $x \in \mathbb{A}_k^{\mathbb{Z}}$ be uniformly recurrent and assume each $i \in \mathbb{A}_k$ occurs in x . Assume that for each $w \in L(x)$ there exists $a \in \mathbb{A}$ such that $D(aw) = D(w)$. Then the following are equivalent*

1. x is singular and $L(x)$ is symmetric.
2. $L(x)$ is the language of a symmetric k -interval exchange transformation satisfying i.d.o.c..

Proof. That 2. implies 1. follows from Theorem 5. To see that 1. implies 2. we begin with the following lemma:

Lemma 4.17. *Let $x \in \mathbb{A}_k^{\mathbb{Z}}$. Assume that $L(x)$ is symmetric and that each $i \in \mathbb{A}_k$ is recurrent in x . If x is singular, then $A(s)$ and $D(s)$ are both intervals for each $s \in L(x)$.*

Proof. Fix $s \in L(x)$. It suffices to show that $D(s)$ is an interval. In fact, since $L(x)$ is symmetric it follows that $A(s) = D(\bar{s})$ for each $s \in L(x)$. So assume that there exist $a < b < c$ in \mathbb{A}_k with $a, c \in D(s)$. We will show that $b \in D(s)$. Since b is recurrent in x we may write $x = \bar{u}bw$ with $u, w \in \mathbb{A}_k^{\mathbb{N}}$ and with sa and sc each occurring in \bar{u} . Thus we may write $x = \bar{u}_1v_1w$ where v_1 begins in a and ends in b and u_1 begins in \bar{s} . Since $v_1 < \bar{v}_1$ and x is singular, it follows that $w \leq u_1$. Similarly, we may write $x = \bar{u}_2v_2w$ where v_2 begins in c and ends in b and u_2 begins in \bar{s} . Since $\bar{v}_2 < v_2$ we have that $u_2 \leq w$. Since \bar{s} is a prefix of both u_1 and u_2 it follows that \bar{s} is a prefix of w , whence $b\bar{s} \in L(x)$ from which it follows that $sb \in L(x)$ as required. \square

We now prove that 1. implies 2. So assume that $x \in \mathbb{A}_k^{\mathbb{Z}}$ satisfies the hypotheses of Theorem 4.16, x is singular and that $L(x)$ is symmetric. We now show that $L(x)$ verifies each of the conditions in Theorem 4.13. Condition (H0) is immediate since each $i \in \mathbb{A}_k$ occurs in x . Condition (H1) follows from the fact that x is uniformly recurrent. Conditions (H2) and (H3) follow immediately from Lemma 4.17. Condition (H4) applied to $\pi_0 = Id$ and $\pi_1 = \sigma$ is merely a reformulation of the symmetric order condition. Thus (H4) follows from Theorem 4.7. To show (H5), suppose $a, b \in A(w)$ are consecutive. Without loss of generality, we may assume that $a < b$. Let $c, d \in D(aw) \cap D(bw)$. We will show that $c = d$. We have $awc, awd, d\bar{w}b, c\bar{w}b \in L(x)$. Considering the factors awc and $d\bar{w}b$, since $a < b$ it follows that $wc \geq wd$ and hence $c \geq d$. Similarly, considering the factors awd and $c\bar{w}b$, since $a < b$ we get $wd \geq wc$ and hence $d \geq c$. This proves that $c = d$ and hence that $D(aw) \cap D(bw)$ is at most a singleton. To see that $D(aw) \cap D(bw) \neq \emptyset$, pick $c \in \mathbb{A}_k$ such that $D(c\bar{w}) = D(\bar{w})$. As $a, b \in D(\bar{w})$ we get that $c\bar{w}a, c\bar{w}b \in L(x)$. It follows that $awc, bwc \in L(x)$ and hence $c \in D(aw) \cap D(bw)$. This concludes our proof of Theorem 4.16. \square

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