Standard words and solutions of the word equation $X_1^2 \cdots X_n^2 = (X_1 \cdots X_n)^2$

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Abstract We consider solutions of the word equation $X_1^2 \cdots X_n^2 = (X_1 \cdots X_n)^2$ such that the squares X_i^2 are minimal squares found in optimal squareful infinite words. We apply a method developed by the second author for studying word equations and prove that there are exactly two families of solutions: reversed standard words and words obtained from reversed standard words by a simple substitution scheme. A particular and remarkable consequence is that a word w is a standard word if and only if its reversal is a solution to the word equation and $gcd(|w|, |w|_1) =$ 1. This result can be interpreted as a yet another characterization for standard Sturmian words.

We apply our results to the symbolic square root map $\sqrt{\cdot}$ studied by the first author and M. A. Whiteland. We prove that if the language of a minimal subshift Ω contains infinitely many solutions to the word equation, then either Ω is Sturmian and $\sqrt{\cdot}$ -invariant or Ω is a so-called SL-subshift and not $\sqrt{-}$ -invariant. This result is progress towards proving the conjecture that a minimal and $\sqrt{-}$ invariant subshift is necessarily Sturmian.

Keywords: word equation, symbolic square root map, standard word, Sturmian word, optimal squareful word

Introduction 1

Recently the second author of this paper solved a long-standing open problem by proving that if the equality of words $X^k = X_1^k \cdots X_n^k$ holds for three positive values of k, then the words X_1, \ldots , X_n commute [8, 10]. If the equation is satisfied for at most two values of k, then noncommuting, or nonperiodic, solutions can exist. In relation to Sturmian words, it was shown by the first author and M. A. Whiteland in [6] (see also [5]) that reversed standard words form a large nonperiodic solution class when k = 1, 2. More precisely, the research of [6] concerns solutions of the word equation

$$X_1^2 \cdots X_n^2 = (X_1 \cdots X_n)^2 \tag{1}$$

such that the words X_i are among the following six words for some fixed integers $\mathfrak{a} \geq 1$ and $\mathfrak{b} \geq 0$:

$$S_{1} = 0, \qquad S_{4} = 10^{a},$$

$$S_{2} = 010^{a-1}, \qquad S_{5} = 10^{a+1}(10^{a})^{b},$$

$$S_{3} = 010^{a}, \qquad S_{6} = 10^{a+1}(10^{a})^{b+1}.$$
(2)

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For example, the word 01010010 is a solution when $\mathfrak{a} = 1$ and $\mathfrak{b} = 0$ because $(S_2S_1S_6)^2 = (01010010)^2 = (01)^2 \cdot 0^2 \cdot (10010)^2 = S_2^2S_1^2S_6^2$.

Let us define standard words. Let (d_k) be a sequence of positive integers, and define a sequence (s_k) of words as follows:

$$s_{-1} = 1$$
, $s_0 = 0$, $s_1 = s_0^{d_1 - 1} s_{-1}$, $s_k = s_{k-1}^{d_k} s_{k-2}$ for $k \ge 2$.

The words s_k obtained in this manner are called *standard words*. If $(d_k) = (2, 1, 1, 1, ...)$, then the words of the sequence (s_k) are called *Fibonacci words*. Notice that the word 01010010 above is a reversed Fibonacci word (i.e., a Fibonacci word read from right to left). Notice also that the words (2) are reversed standard words (see Section 2 for additional details).

One of the main results of [6] is that reversed standard words are solutions to (1). Another related solution class was also determined in [6]: words obtained from reversed standard words by a certain substitution scheme. For example, consider the word *LSS* and substitute *S* by a reversed standard word *w* and *L* by the word obtained from *w* by exchanging its first two letters. If w = 01010010, then the resulting word 10010010010010010010010010 is no longer a reversed standard word, but it is nevertheless a solution to (1). The main result of this paper is that there is no third solution type, that is, if we insist that the words X_i in (1) are among the words (2), then a solution to (1) is either

- a reversed standard word (a solution of type I) or
- obtained from a reversed standard word by a substitution scheme (a solution of type II).

For the precise statement, see Theorem 3.1. The essential component in our proofs is the method of assigning numerical values to letters and studying sums of letters geometrically developed by the second author in [8, 10]. See also [9] and especially [3, 4] where the method was used to solve long-standing open problems on word equations.

Our main result Theorem 3.1 has the following surprising corollary.

Theorem 1.1. A word is standard if and only if its reversal is a type I solution to (1). In other words, a word w is standard if and only if its reversal is a solution to (1) and $gcd(|w|, |w|_1) = 1$.

This is indeed remarkable given how strikingly different the definition of standard words is compared to (1).

Standard words are the building blocks of the important and widely studied Sturmian words. Sturmian words are often defined as the infinite words having n + 1 factors of each length n, but a more useful definition is that a Sturmian word is an infinite word that shares a language with a standard Sturmian word, and a standard Sturmian word is simply a limit of a sequence of standard words [2, Proposition 2.2.24]. Hence Theorem 1.1 can be reinterpreted as follows.

Theorem 1.2. An infinite word is a standard Sturmian word if and only if it is a limit of the reversals of solutions w to (1) such that $gcd(|w|, |w|_1) = 1$.¹

This is a surprising connection between a priori unrelated objects: standard Sturmian words can be characterized as the infinite words having n + 1 factors of each length n that are left-special [2, Proposition 2.1.22]. An infinite word **w** is *left-special* if a**w** has the same language as **w** for all letters a in the alphabet of **w**.

The specific solutions to (1) considered in this paper were originally considered as a tool to construct fixed points for the symbolic square root map acting on optimal squareful words. An *optimal squareful word* \mathbf{w} is an aperiodic word such that each position of \mathbf{w} begins with a square

¹A tidier statement would be obtained if we reversed the words (2), but then the interpretation of (2) as minimal squares appearing in optimal squareful words is lost; see one paragraph below.

and the number of minimal squares occurring in **w** is the least possible. K. Saari proves in [11] that an optimal squareful word **w** contains exactly six minimal squares and there exists $\mathfrak{a} \ge 1$ and $\mathfrak{b} \ge 0$ such that each minimal square X^2 in **w** is such that X is among the words (2). Let **w** be an optimal squareful word and write it as a product of minimal squares: $\mathbf{w} = X_1^2 X_2^2 \cdots$. The square root $\sqrt{\mathbf{w}}$ of **w** is the word $X_1 X_2 \cdots$ obtained by removing half of each square X_i^2 .

Saari showed that Sturmian words are optimal squareful [11, Thm. 20], and the first author and Whiteland showed in [6, Thm. 9] that the square root map preserves the language of Sturmian words: if **s** is a Sturmian word, then typically $\mathbf{s} \neq \sqrt{\mathbf{s}}$, but **s** and $\sqrt{\mathbf{s}}$ have the same set of factors. This raised the question if other, non-Sturmian, and optimal squareful words with such a peculiar property exist. Clearly words having arbitrarily long prefixes that are squares of solutions to (1) are fixed points of the square root map. The type II solutions of (1) give in this way rise to non-Sturmian fixed points. If **u** is such a fixed point and **v** has the same language as **u**, then typically $\sqrt{\mathbf{v}}$ has the same language as **v**. Therefore the solutions of (1) can be used to construct infinite words having interesting dynamics with respect to the square root map. The dynamics of these non-Sturmian words is further studied in [7].

While non-Sturmian words whose language is preserved by the square root map exist, Sturmian words satisfy a strong property: a Sturmian subshift is $\sqrt{\cdot}$ -invariant (a subshift is Sturmian if it consists of Sturmian words). This property is not satisfied by the minimal subshifts related to the infinite words constructed from type II solutions (see Proposition 5.5), and no further examples are known. We formulate a question of [6] as the following conjecture stating a characterization of Sturmian subshifts.

Conjecture 1.3. *Let* Ω *be a minimal optimal squareful subshift. Then* Ω *is a Sturmian subshift if and only if* $\sqrt{\Omega} \subseteq \Omega$ *.*

We apply our main result Theorem 3.1 and make progress towards this conjecture by proving the following result.

Theorem 1.4. Let Ω be a minimal subshift whose language contains infinitely many solutions to (1) such that $\sqrt{\Omega} \subseteq \Omega$. Then Ω is Sturmian.

See Theorem 5.6 for a slightly more general result. We leave Conjecture 1.3 open in the case that the language of Ω contains finitely many solutions to (1).

The structure of the paper is as follows. The next section recalls preliminary notions and needed results. After this, we prove the main result Theorem 3.1 in Section 3. In the following Section 4, we provide a formula for counting solutions to (1) of length n. In Section 5, we apply the main results to the study of the square root map and prove Theorem 5.6. We end the paper by Section 6 which contains additional results concerning the square root map.

2 Preliminaries

We use standard definitions and notation in combinatorics on words. The book [2] is a standard reference for these concepts, and its second chapter is a standard reference for Sturmian words. Let *A* be an *alphabet*, i.e., a finite set of *letters*, or *symbols*. By concatenating the letters of *A*, we obtain the set of *words* over *A* denoted by A^* . The set A^* contains the empty word ε , and we set $A^+ = A^* \setminus {\varepsilon}$. The length |w| of a word *w* is the number of letters in *w*, and by $|w|_a$ we mean the number of occurrences of the letter *a* in *w*. A word *w* is *primitive* if $w = u^n$ only when n = 1. We often use the synchronization property of primitive word which states that a primitive word *w* occurs in w^2 exactly twice: as a prefix and as a suffix. By a *language* we simply mean a set of words, and by a language of a word we mean its set of factors. If *w* is a word such that $|w| \ge 2$, then by L(w) we mean the word obtained from *w* by exchanging its first two letters. A word *u* is *conjugate* to *v* if there exists words *x* and *y* such that u = xy and v = yx.

We also consider infinite words over A which are simply mappings $\mathbb{N} \to A$. An infinite word is *purely periodic* if it is of the form v^{ω} and *ultimately periodic* if it is of the form uv^{ω} . An infinite word that is not ultimately periodic is called *aperiodic*. If $\mathbf{w} = a_0 a_1 a_2 \cdots, a_i \in A$, is an infinite word, then the *shift* $T\mathbf{w}$ of \mathbf{w} is the infinite word $a_1 a_2 \cdots$. Let \mathcal{L} be an extendable and factor-closed language. The set Ω of infinite words having language \mathcal{L} is a *subshift* with language \mathcal{L} . If \mathcal{L} is the language of an infinite word \mathbf{w} , then we say that Ω is the subshift generated by \mathbf{w} , and we write $\Omega = \sigma(\mathbf{w})$. If every word in a subshift is aperiodic, then we call the subshift *aperiodic*. A subshift is *minimal* if it does not contain nonempty subshifts as proper subsets. A subshift is *Sturmian* if all words in it are Sturmian words.

We repeat the definition of optimal squareful words from the introduction. A square w^2 is *minimal* if for each square prefix u^2 of w^2 it follows that u = w. Next we give the definition of squareful words; see [11] for the more general definition of an everywhere α -repetitive word.

Definition 2.1. An infinite word **w** is *squareful* if each position of **w** begins with a square and the number of minimal squares occurring in **w** is finite. An infinite word **w** is *optimal squareful* if it is aperiodic, squareful, and the number of distinct minimal squares in **w** is the least possible among aperiodic and squareful words.

Saari proves in [11, Thm. 16] that if **w** is optimal squareful, then the minimal squares occurring in **w** are (up to renaming of letters) the squares of the words (2) for some fixed $a \ge 1$ and $b \ge 0$. In particular, a squareful word containing at most five distinct minimal squares is necessarily ultimately periodic. Saari characterizes optimal squareful words in [11, Thm. 17] as follows.

Proposition 2.2. An aperiodic infinite word **w** is optimal squareful if and only if (up to renaming of letters) there exist integers $a \ge 1$ and $b \ge 0$ such that **w** is an element of the language²

$$0^{*}(10^{\mathfrak{a}})^{*}(10^{\mathfrak{a}+1}(10^{\mathfrak{a}})^{\mathfrak{b}}+10^{\mathfrak{a}+1}(10^{\mathfrak{a}})^{\mathfrak{b}+1})^{\omega}=S_{1}^{*}S_{4}^{*}(S_{5}+S_{6})^{\omega}.$$

Here the symbols S_i refer to the words (2), and we assume this throughout the paper. Similarly we always use \mathfrak{a} and \mathfrak{b} to refer to the parameters of (2); the parameters are assumed to be fixed. Moreover, we often write "minimal square" to mean a square of one of the words (2). We refer to the words (2) themselves as *minimal square roots*.

By Proposition 2.2, optimal squareful words may initially contain arbitrarily high powers of S_1 and S_4 . In the setting of the papers [6, 7] this does not happen, and we continue this tradition.

Definition 2.3. The language $\mathcal{L}(\mathfrak{a}, \mathfrak{b})$ consists of all factors of the infinite words in the language

$$(10^{\mathfrak{a}+1}(10^{\mathfrak{a}})^{\mathfrak{b}} + 10^{\mathfrak{a}+1}(10^{\mathfrak{a}})^{\mathfrak{b}+1})^{\omega} = (S_5 + S_6)^{\omega}.$$

Definition 2.4. The language $\Pi(\mathfrak{a}, \mathfrak{b})$ consists of all nonempty words in $\mathcal{L}(\mathfrak{a}, \mathfrak{b})$ that are products of the squares of the words (2).

Recall the word equation (1):

$$X_1^2 X_2^2 \cdots X_n^2 = (X_1 X_2 \cdots X_n)^2.$$

We define specific solutions to this equation with respect to the language $\Pi(\mathfrak{a}, \mathfrak{b})$.

Definition 2.5. A nonempty word w is a *solution to* (1) if $w^2 \in \Pi(\mathfrak{a}, \mathfrak{b})$ and w can be written as a product of minimal square roots $w = X_1 X_2 \cdots X_n$ which satisfy the word equation (1). The solution w is *primitive* if w is a primitive word.

Notice that the factorization of a square of a solution as a product of minimal squares is unique because none of the minimal squares is a prefix of another minimal square.

²The language $(u + v)^{\omega}$ consists of the infinitely long concatenations of the words *u* and *v*.

Example 2.6. Let w be the word 01010010, $\mathfrak{a} = 1$, and $\mathfrak{b} = 0$. Then $w^2 = 0101001001010010 = 010S_5S_6^2$, so w^2 is a suffix of $S_6S_5S_6^2$ meaning that $w^2 \in \mathcal{L}(\mathfrak{a}, \mathfrak{b})$. Moreover, we have $w^2 = S_2^2S_1^2S_6^2$, so $w^2 \in \Pi(\mathfrak{a}, \mathfrak{b})$. Since $w = S_2S_1S_6$, we see that $S_1^2S_1^2S_6^2 = (S_2S_1S_6)^2$. Thus w is a solution to (1). In fact, the word w is a primitive solution to (1) since w is a primitive word.

Let us then define the symbolic square root map defined in the introduction.

Definition 2.7. Factorize a word w in $\Pi(\mathfrak{a}, \mathfrak{b})$ as a product of minimal squares: $w = X_1^2 \cdots X_n^2$. The *square root* \sqrt{w} of w is defined as the word $X_1 \cdots X_n$.

In other words, a word *w* is a solution to (1) if and only if $\sqrt{w^2} = w$.

Next we introduce the substitution scheme mentioned in the introduction as a means to build new solutions out of known solutions.

Definition 2.8. Let $u = a_0 \cdots a_{n-1}$ with $a_i \in \{S, L\}$ be a nonempty word over the alphabet $\{S, L\}$. We say that the word u is a *pattern word* if $a_i = a_j$ whenever i and j are in the same orbit³ of the mapping $x \mapsto 2x \mod n$. We say that u is *nontrivial* if |u| > 1.

If *w* is a nonempty binary word and *u* is a word over $\{S, L\}$, then by $\mathcal{P}_w(u)$ we mean the word obtained from *u* by replacing *S* by *w* and *L* by L(w).

Example 2.9. If u = LSS or u = SLLSLSS, then u is a pattern word. Whenever w is a suitable solution to (1), then $\mathcal{P}_w(u)$ is also a solution to (1) for a pattern word u (see Proposition 3.5 below). For example, when u = LSS and w = 01010010, then $\mathcal{P}_w(u) = 1001001001001001001010010$ is a solution.

In what follows, we often use the symbol *S* and the word *w* interchangeably, but it will always be clear if *S* stands for the letter *S* or a binary word. Notice that the map P_S is injective when the first two letters of *S* are distinct.

The definition of standard words was already given in the introduction. By a *reversed* standard word, we mean a standard word read from right to left. Standard words are primitive; see [2, Lemma 2.2.3]. Consider then an integer sequence (d_k) and the corresponding sequence (s_k) of standard words. Replacing (d_k) by $(d_2 + 1, d_3, d_4, ...)$ if necessary, we may assume that $d_1 \ge 2$ so that 11 does not occur in the words s_k . It is not difficult to see that d_1 (resp. $d_1 - 1$) is the maximum (resp. minimum) number of occurrences of the letter 0 between two letters 1 in the corresponding standard words s_k . Similarly d_2 (resp. $d_2 - 1$) indicates the maximum (resp. minimum) number of occurrences of 10^{d_1-1} between two occurrences of 10^{d_1} . Hence we see that the words s_k belong to the language $\mathcal{L}(\mathfrak{a}, \mathfrak{b})$ with $\mathfrak{a} = d_1 - 1$ and $\mathfrak{b} = d_2 - 1$. The limit **s** of (s_k) is a standard Sturmian word, and it is an optimal squareful word with parameters \mathfrak{a} and \mathfrak{b} . Whenever we mention the words S_i of (2) in relation to a standard word w, we understand that the parameters \mathfrak{a} and \mathfrak{b} related to S_i and w are the same. Given an integer sequence $(\mathfrak{a} + 1, \mathfrak{b} + 1, \ldots)$, the corresponding sequence of standard words begins as follows:

$$s_{-1} = 1,$$

 $s_0 = 0,$
 $s_1 = 0^{a}1,$
 $s_2 = (0^{a}1)^{b+1}0$

Notice that the reversals of s_0 and s_1 equal the words S_1 and S_4 of (2). Moreover, we have $S_2 = L(S_4)$, but S_2 is also a reversed standard word corresponding to $(\mathfrak{a}, 1, \ldots)$. The word S_3 is a reversed standard word corresponding to $(\mathfrak{a} + 1, 1, \ldots)$, and the word $L(S_3)$ is a standard word corresponding to $(\mathfrak{a} + 2, \ldots)$. Similarly reversals of the words S_5 and S_6 correspond to standard

³The numbers *i* and *j* are in the same orbit if there exists k_1 and k_2 such that $2^{k_1}i \equiv 2^{k_2}j \pmod{n}$.

words in the sequences $(\mathfrak{a} + 1, \mathfrak{b}, 1, ...)$ and $(\mathfrak{a} + 1, \mathfrak{b} + 1, 1, ...)$. Moreover, the words $L(S_5)$ and $L(S_6)$ are standard words. Therefore the words (2) found in a standard Sturmian word with parameters \mathfrak{a} and \mathfrak{b} are all reversals of standard words and some of them are related by the mapping *L*. It is straightforward to see that all reversed standard word of length at least 2 begin with two distinct letters.

3 Characterization of Solutions

We can now formulate the following theorem which is the main result of this paper.

Theorem 3.1. Let w be a primitive solution to (1). Then

- (I) w is a reversed standard word or
- (II) there exists a reversed standard word S with $|S| > |S_6|$ and a nontrivial and primitive pattern word u such that $w = \mathcal{P}_S(u)$.

Conversely, if (I) or (II) holds for a word w, then w is a primitive solution to (1). Moreover, if w is a nonprimitive solution to (1), then w is a power of a primitive solution to (1).

We respectively call the two solution types of Theorem 3.1 solutions of type I and type II. Observe also that a primitive pattern word always has odd length.

Theorem 3.1 implies the remarkable characterization of standard words stated in Theorem 1.1.

Proof of Theorem 1.1. If *w* is a standard word, then its reversal is a solution to (1) by Theorem 3.1. It is a well-known property of standard words (see, e.g., the proof of [2, Lemma 2.2.3]) that $gcd(|w|, |w|_1) = 1$. Suppose on the other hand that *w* is a solution to (1) and $gcd(|w|, |w|_1) = 1$. Then *w* must be primitive for otherwise $gcd(|w|, |w|_1) > 1$. If *w* is a solution of type II, then Theorem 3.1 implies that there exists a reversed standard word *S* and a nontrivial and primitive pattern word *u* such that $w = \mathcal{P}_S(u)$. Since $|S|_1 = |L(S)|_1$, we see that |w| = |u||S| and $|w|_1 = |u||S|_1$, so $gcd(|w|, |w|_1) \ge |u|$. Thus it must be that |u| = 1, but this contradicts the fact that *u* is nontrivial. Hence *w* cannot be of type II, so it is of type I, that is, *w* is a reversed standard word.

Notice that the preceding proof also shows that the sets of type I solutions and type II solutions are disjoint.

Before showing that solutions to (1) are of the claimed form, we present results showing that words satisfying (I) or (II) of Theorem 3.1 are indeed solutions. The case (I) is handled by the following result.

Proposition 3.2. [6, Proposition 23] If w is a reversed standard word, then w is a solution to (1).

For the case (II) (see Proposition 3.5), we need the following lemmas.

Lemma 3.3. [6, Lemma 22] Let S be a reversed standard word such that $|S| > |S_6|$, and set L = L(S). Then SS, SL, LS, $LL \in \Pi(\mathfrak{a}, \mathfrak{b}), \sqrt{SS} = \sqrt{SL} = S$, and $\sqrt{LL} = \sqrt{LS} = L$.

Lemma 3.4. Let u be a primitive word over $\{S, L\}$ and w a reversed standard word such that |w| > 1. Then $\mathcal{P}_w(u)$ is primitive.

Proof. Let $\mathcal{P}_w(u) = v^k$ for a primitive word v and integer $k \ge 1$. From |w| = |L(w)| and $|w|_1 = |L(w)|_1$, it follows that $|\mathcal{P}_w(u)| = |u| \cdot |w|$ and $|\mathcal{P}_w(u)|_1 = |u| \cdot |w|_1$. Because w is a reversed standard word, we have $gcd(|w|, |w|_1) = 1$, and therefore

$$\gcd(|\mathcal{P}_w(u)|, |\mathcal{P}_w(u)|_1) = \gcd(|u| \cdot |w|, |u| \cdot |w|_1) = |u| \gcd(|w|, |w|_1) = |u|.$$

On the other hand,

$$\gcd(|\mathcal{P}_w(u)|, |\mathcal{P}_w(u)|_1) = \gcd(|v^k|, |v^k|_1) = \gcd(k|v|, k|v|_1) = k \gcd(|v|, |v|_1)$$

Thus |u| is a multiple of *k*, and we can write $u = u_1 \cdots u_k$ with $|u_1| = \ldots = |u_k|$. Then

$$v^k = \mathcal{P}_w(u) = \mathcal{P}_w(u_1) \cdots \mathcal{P}_w(u_k)$$
 and $|\mathcal{P}_w(u_1)| = \ldots = |\mathcal{P}_w(u_k)|$,

and therefore $v = \mathcal{P}_w(u_i)$ for all *i*. By the injectivity of \mathcal{P}_w , we see that $u_1 = \ldots = u_k$ and $u = u_1^k$. Because *u* is primitive, it must be that k = 1. Since $\mathcal{P}_w(u) = v^k$, we conclude that $\mathcal{P}_w(u)$ is primitive.

Parts of the following result and its proof appear in less general form in [6, Lemma 39], [6, Lemma 40], and [7, Lemma 2.8].

Proposition 3.5. Let *S* be a reversed standard word such that $|S| > |S_6|$. Then $\mathcal{P}_S(u)$ is a solution to (1) for any pattern word *u*. Moreover, if *u* is primitive, then $\mathcal{P}_S(u)$ is primitive.

Proof. Let *u* be a pattern word. Write u^2 as blocks of two letters: $u^2 = A_0 B_0 \cdot A_1 B_1 \cdots A_{|u|-1} B_{|u|-1}$. Then $\sqrt{\mathcal{P}_S(A_i B_i)} = \mathcal{P}_S(A_i)$ for all *i* by Lemma 3.3. Consequently

$$\sqrt{\mathcal{P}_{S}(u^{2})} = \sqrt{\mathcal{P}_{S}(A_{0}B_{0}\cdots A_{i}B_{i}\cdots A_{|u|-1}B_{|u|-1})} = \mathcal{P}_{S}(A_{0}\cdots A_{i}\cdots A_{|u|-1}).$$
(3)

The letter A_i is the 2*i*th letter of u^2 . Since u is a pattern word, it follows that A_i equals the *i*th letter of u. Thus (3) states that $\sqrt{\mathcal{P}_S(u^2)} = \mathcal{P}_S(u)$. This means that $\mathcal{P}_S(u)$ is a solution to (1).

If *u* is primitive, then $\mathcal{P}_{S}(u)$ is primitive by Lemma 3.4.

Let us then begin proving the converse of Proposition 3.2 and Proposition 3.5. The method used is to assign numerical values to letters as mentioned in the introduction.

If we assign distinct real weights to the letters 0 and 1, say ω_0 and ω_1 , then we may define the sum $\Sigma(u)$ of $u = a_1 \cdots a_n \in \{0, 1\}^*$ to be the real number

$$\Sigma(u) = \omega_{a_1} + \dots + \omega_{a_n} = |u|_0 \cdot \omega_0 + |u|_1 \cdot \omega_1.$$
(4)

Different weights ω_0 and ω_1 obviously give different sum functions Σ . We want to choose the weights ω_0 and ω_1 so that $\Sigma(w) = 0$ for a certain fixed word w containing both letters 0 and 1. Moreover, we want to normalize the weights so that $\omega_1 - \omega_0 = 1$. Both of these conditions are satisfied if we choose

$$\omega_0 = -\frac{|w|_1}{|w|} \quad \text{and} \quad \omega_1 = \frac{|w|_0}{|w|}.$$
(5)

In what follows, we fix a word w that is a solution to (1), and then assume that ω_0 , ω_1 , and Σ have been defined as in (5) and (4).

The *slope* of $u \in \{0,1\}^+$ is $\pi(u) = |u|_1/|u|$. We can represent Σ also with the help of the function π :

$$\Sigma(u) = |u|(\pi(u) - \pi(w)). \tag{6}$$

This is shown by the following computation:

$$\begin{split} \Sigma(u) &= -|u|_0 \cdot \frac{|w|_1}{|w|} + |u|_1 \cdot \frac{|w|_0}{|w|} = -|u|_0 \pi(w) + |u|_1 \cdot \frac{|w| - |w|_1}{|w|} \\ &= -|u|_0 \pi(w) + |u|_1 - |u|_1 \pi(w) = |u|_1 - (|u|_0 + |u|_1)\pi(w) = |u|\pi(u) - |u|\pi(w). \end{split}$$

Let $u = a_1 \cdots a_n$ be a word over $\{0, 1\}$. We define the *prefix sum word* psw(u) of u to be the word $psw(u) = b_1 \cdots b_n$, where $b_i = \Sigma(a_1 \cdots a_i)$ for all i. This is a word over some alphabet that is a subset of the rational numbers. Naturally, we can denote the largest and smallest letters in psw(u) by max(psw(u)) and min(psw(u)), respectively. The word u has a graphical representation as a plane curve that we get by connecting the points (0,0), $(1,b_1)$, \ldots , (n,b_n) .

Example 3.6. Let w = 01010010. Then $\omega_0 = -3/8$, $\omega_1 = 5/8$, and

$$psw(w) = \frac{-3}{8}, \frac{2}{8}, \frac{-1}{8}, \frac{4}{8}, \frac{1}{8}, \frac{-2}{8}, \frac{3}{8}, \frac{0}{8}, \frac{-2}{8}, \frac{3}{8}, \frac{0}{8}, \frac{-2}{8}, \frac{3}{8}, \frac{0}{8}, \frac{-2}{8}, \frac{-2$$

where we have used commas between the letters and the same denominator 8 in every letter for clarity. See Figure 1 for a graphical representation.

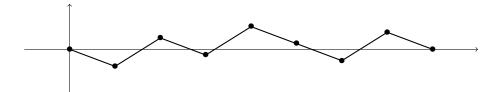


Figure 1: The curve of the word 01010010.

Lemma 3.7. Let $x \in \{S_1, S_2, S_3, S_4, S_5, S_6\}$.

- 1. If x = y10z and $y \neq \varepsilon$, then $\pi(y) < \pi(10z)$.
- 2. If x = y01z and $y \neq \varepsilon$, then $\pi(y) > \pi(01z)$.

Proof. In the first case, either y = 0 and $10z = 10^i$ for some i or $y = 10^{\mathfrak{a}+1}(10^\mathfrak{a})^i$ and $10z = (10^\mathfrak{a})^j$ for some i, j. The former option is clear: $\pi(y) = 0 < \pi(10z)$. In the latter case, we have $\pi(10z) = 1/(\mathfrak{a}+1) > (i+1)/((i+1)(\mathfrak{a}+1)+1) = \pi(y)$.

In the second case, the only possibility is $y \in \{10^{\mathfrak{a}}, 10^{\mathfrak{a}+1}(10^{\mathfrak{a}})^i 10^{\mathfrak{a}-1}\}$ and $01z = 0(10^{\mathfrak{a}})^j$ for some *i*, *j*, and then $\pi(y) = 1/(\mathfrak{a}+1) = \pi(1z) > \pi(01z)$.

The following lemma states that the curve of a solution *w* is contained in the rather small space between the lines $y = \omega_0$ and $y = \omega_1$.

Lemma 3.8. Let w be a solution to (1) containing both letters 0 and 1. Then $\omega_0 \leq \min(\text{psw}(w)) \leq \max(\text{psw}(w)) \leq \omega_1$.

Proof. Write w^2 as a product of minimal squares: $w^2 = X_1^2 \cdots X_n^2$. First we want to argue that if the maximum of psw(w) occurs at a position between $|X_1 \cdots X_r|$ and $|X_1 \cdots X_r X_{r+1}|$, then $\Sigma(X_1 \cdots X_r) \leq 0$ and $\Sigma(X_1 \cdots X_{r+1}) \leq 0$. Say $max(psw(w)) = \Sigma(X_1 \cdots X_r u)$ and $X_{r+1} = uv$ (we allow here r = 0, and then $X_1 \cdots X_r = \varepsilon$). Assume for a contradiction that $\Sigma(X_1 \cdots X_r) > 0$. Since w is zero-sum, we have $max(psw(w^2)) = max(psw(w))$. The word $X_1^2 \cdots X_r^2 u$ is a prefix of w^2 . Now

$$\Sigma(X_1^2 \cdots X_r^2 u) = 2\Sigma(X_1 \cdots X_r) + \Sigma(u) > \Sigma(X_1 \cdots X_r) + \Sigma(u) = \max(\operatorname{psw}(w)),$$

which contradicts the fact that $\max(psw(w^2)) = \max(psw(w))$. Hence $\Sigma(X_1 \cdots X_r) \le 0$. Suppose then that $\Sigma(X_1 \cdots X_{r+1}) > 0$. The word $X_1^2 \cdots X_r^2 X_{r+1} u$ is a prefix of w^2 . We compute:

$$\Sigma(X_1^2 \cdots X_r^2 X_{r+1} u) = \Sigma(X_1 \cdots X_{r+1}) + \Sigma(X_1 \cdots X_r u) > \Sigma(X_1 \cdots X_r u) = \max(\operatorname{psw}(w)).$$

This is impossible, so $\Sigma(X_1 \cdots X_{r+1}) \leq 0$.

A symmetric argument shows that if psw(w) attains its minimum value at $X_1 \cdots X_r u$, then $\Sigma(X_1 \cdots X_r) \ge 0$ and $\Sigma(X_1 \cdots X_{r+1}) \ge 0$ when *r* and *u* are defined like above.

Let us proceed to consider the case of the maximum value $\max(psw(w))$. Let $\max(psw(w)) = \Sigma(X_1 \cdots X_r u)$ and $X_{r+1} = uv$. We have shown above that $\Sigma(X_1 \cdots X_r) \leq 0$ and $\Sigma(X_1 \cdots X_{r+1}) \leq 0$. If $|u| \in \{0, 1, |X_{r+1}|\}$, then it is easy to see that $\max(psw(w)) \leq \omega_1$. Otherwise, we can write u = ya and v = bz, where $a, b \in \{0, 1\}$ and $y \neq \varepsilon$. If a = 0, then

$$\Sigma(X_1\cdots X_r u) = \Sigma(X_1\cdots X_r y) + \omega_0 < \Sigma(X_1\cdots X_r y),$$

which contradicts $\max(psw(w)) = \Sigma(X_1 \cdots X_r u)$, so it must be a = 1. Similarly, if b = 1, then

$$\Sigma(X_1\cdots X_r u 1) = \Sigma(X_1\cdots X_r u) + \omega_1 > \Sigma(X_1\cdots X_r u)$$

contradicts $\max(psw(w)) = \Sigma(X_1 \cdots X_r u)$, so it must be b = 0. By Lemma 3.7, we have $\pi(y) < \pi(10z)$. Therefore, both $\pi(w) < \pi(y)$ and $\pi(10z) < \pi(w)$ cannot hold. In other words, at least one of $\pi(y) \le \pi(w)$ and $\pi(10z) \ge \pi(w)$ is true. In the former case, $\Sigma(y) \le 0$ by (6), and thus

$$\max(\operatorname{psw}(w)) = \Sigma(X_1 \cdots X_r) + \Sigma(y_1) \le \omega_1.$$

In the latter case, $\Sigma(10z) \ge 0$ by (6), and so

$$\max(\mathrm{psw}(w)) = \Sigma(X_1 \cdots X_{r+1}) - \Sigma(0z) \le \omega_1.$$

Consider then the minimum min(psw(w)). Using the above notation, we have shown that $\Sigma(X_1 \cdots X_r) \ge 0$ and $\Sigma(X_1 \cdots X_{r+1}) \ge 0$. If $|u| \in \{0, 1, |X_{r+1}|\}$, then it is again easy to see that min(psw(w)) $\ge \omega_0$. Otherwise, we can write u = y0 and v = 1z, where $y \ne \varepsilon$. Again Lemma 3.7 implies that $\pi(y) \ge \pi(w)$ or $\pi(01z) \le \pi(w)$. In the former case, $\Sigma(y) \ge 0$ by (6), and hence

$$\min(\mathsf{psw}(w)) = \Sigma(X_1 \cdots X_r) + \Sigma(y_0) \ge \omega_0.$$

In the latter case, $\Sigma(01z) \leq 0$ by (6), and thus

$$\max(\operatorname{psw}(w)) = \Sigma(X_1 \cdots X_{r+1}) - \Sigma(1z) \ge \omega_0.$$

Lemma 3.9. Let w be a solution to (1) containing both letters 0 and 1. Let $\pi(w) = c/d$, where c and d are relatively prime positive integers. Then $w \in \{01u, 10u\}^+$, where $u = a_1 \cdots a_{d-2}$ and

$$a_j = \left\lfloor \frac{c(j+1)}{d} \right\rfloor - \left\lfloor \frac{cj}{d} \right\rfloor \tag{7}$$

for all j.

Proof. The point of the proof is that after the initial letter of w is chosen, the remaining letters are uniquely determined by the number $\pi(w)$. Indeed, if v is a prefix of w and $\Sigma(v) > 0$, then v0 is a prefix of w or otherwise Lemma 3.8 is violated. If $\Sigma(v) < 0$, then v1 is a prefix of w.

Write $w = z_1 \cdots z_m$ where for all *i* we have $\Sigma(z_i) = 0$ and $\Sigma(p) \neq 0$ for all nonempty proper prefixes *p* of z_i . We are going to show that every z_i is in $\{01u, 10u\}$, which proves the theorem. By Lemma 3.8, $\omega_0 \leq \Sigma(p) \leq \omega_1$ for all prefixes *p* of z_i . By (6), $\Sigma(z_i) = 0$ is equivalent to $\pi(z_i) = \pi(w)$ which implies $|z_i| \geq d \geq 2$. Because $\Sigma(00) < \omega_0$ and $\Sigma(11) > \omega_1$, z_i must begin with either 01 or 10. Let the following letters after that be b_1, \ldots, b_{d-2} . Let $k_j = |b_1 \cdots b_j|_1$ for all *j*. Then

$$\begin{split} \omega_0 &\leq \Sigma(01b_1\cdots b_j) \leq \omega_1 \\ \Longleftrightarrow &\omega_0 \leq (j-k_j+1)\omega_0 + (k_j+1)\omega_1 \leq \omega_1 \\ \Leftrightarrow &-(j+1)\omega_0 + \omega_0 - \omega_1 \leq k_j(\omega_1 - \omega_0) \leq -(j+1)\omega_0 \\ \Leftrightarrow &(j+1)\frac{c}{d} - 1 \leq k_j \leq (j+1)\frac{c}{d}. \end{split}$$

Here we have used the facts $\omega_1 - \omega_0 = 1$ and $\omega_0 = -\pi(w) = -c/d$. If $j \le d-2$, then (j+1)c/d is not an integer, and thus $k_j = \lfloor (j+1)c/d \rfloor$. It follows that $b_j = k_j - k_{j-1} = a_j$ for all $j \in \{1, \ldots, d-2\}$. Consequently, we have shown that z_i begins with either 01u or 10u. Further, we have

$$\pi(01u) = \frac{1 + k_{d-2}}{d} = \frac{1 + \lfloor (d-1)c/d \rfloor}{d} = \frac{c}{d},$$

so $\Sigma(01u) = \Sigma(10u) = 0$ by (6). Because z_i does not have nonempty proper prefixes with zero sum, it must be that $z_i \in \{01u, 10u\}$.

The formula (7) for the word u of Lemma 3.9 matches exactly the construction of so-called central words. Usually it is defined that a binary word w is *central* if w01 and w10 are standard words. In [2, Ch. 2.2.1], a central word of length d containing c occurrences of 1 with c, d relatively prime is constructed. This construction uses the same formula as (7), so [2, Prop. 2.2.12], which proves the validity of the construction, shows that the word u of Lemma 3.9 is a central word. Thus u01 and u10 are standard words. Since central words are palindromes (see [2, Thm. 2.2.4]), it follows that the words 01u and 10u are reversed standard words. We have thus proved the following result.

Proposition 3.10. Let w be a solution to (1) containing both letters 0 and 1. Then there exists a unique reversed standard word S such that $w \in \{S, L(S)\}^+$.

We need one small result before we can prove Theorem 3.1. When we use this result in the proof of Theorem 3.1, the word w' will actually be w^2 .

Lemma 3.11. Let w' in $\Pi(\mathfrak{a}, \mathfrak{b})$ be a word such that $\sqrt{w'}$ is a prefix of w'. If u^2 is a prefix of w', then u is a solution to (1).

Proof. Write w' as a product of minimal squares: $w' = X_1^2 \cdots X_n^2$, and let m be the largest index such that $X_1^2 \cdots X_m^2$ is a prefix of u^2 . Write $u^2 = X_1^2 \cdots X_m^2 z$ for a prefix z of X_{m+1}^2 . It follows that |z| is even, so we may write z = xy with |x| = |y|. Since u and $X_1 \cdots X_m X_{m+1}$ are prefixes of w', x is a prefix of X_{m+1} , and $|u| = |X_1 \cdots X_m x|$, we see that $u = X_1 \cdots X_m x$. Hence x is a suffix of u and y = x, that is, $z = x^2$. Since the square X_{m+1} is minimal and the index m is maximal, the only option is that z is empty. Thus $u^2 = X_1^2 \cdots X_m^2$ and $u = X_1 \cdots X_m$. In other words, the word u is a solution to (1).

Proof of Theorem 3.1. Let *w* be a primitive solution to (1). If |w| = 1, then w = 0 and *w* is a reversed standard word. We may thus suppose that |w| > 1. Since *w* is primitive, this means that both letters 0 and 1 occur in *w*. By Proposition 3.10, there exists a reversed standard word *S* such that $w \in \{S, L\}^+$ where L = L(S). The word *w* can be understood as a word over the alphabet $\{S, L\}$; we denote this word by *u*. If |u| = 1, then the case (I) applies, so assume that |u| > 1. For the claim, it suffices to establish that *u* is a primitive pattern word and $|S| > |S_6|$. Suppose first that

 $|S| > |S_6|$. Group the letters of u^2 as blocks of two: $u^2 = A_0 B_0 \cdot A_1 B_1 \cdots A_{|u|-1} B_{|u|-1}$. If *AB* is such a block, then $\sqrt{\mathcal{P}_S(AB)} = \mathcal{P}_S(A)$ by Lemma 3.3. Then

$$\sqrt{\mathcal{P}_S(A_0B_0\cdots A_iB_i)}=\mathcal{P}_S(A_0\cdots A_i)$$

for all *i*. Since *w* is a solution, the word $\mathcal{P}_S(A_0 \cdots A_i)$ is a prefix of *w*. Since \mathcal{P}_S is injective, we conclude that the *i*th letter of *u* equals its 2*i*th letter when the indices are understood modulo |u|. Therefore *u* is a pattern word. The word *u* must be primitive because otherwise $\mathcal{P}_S(u)$ is not primitive.

The next part of the proof consists of showing that w^2 is not in $\Pi(\mathfrak{a}, \mathfrak{b})$ if $|S| \leq |S_6|$ meaning that w is not a solution. Recall from Section 2 the construction of reversed standard words having parameters \mathfrak{a} and \mathfrak{b} and the fact that the words (2) are reversed standard words. It is straightforward to see that if *S* is a reversed standard word having parameters \mathfrak{a} and \mathfrak{b} and containing both letters 0 and 1 and $|S| \leq |S_6|$, then *S* is of the form

10^{*a*}, $0(10^{a})^{\ell}$ with $1 \le \ell \le \mathfrak{b} + 1$, $10^{\mathfrak{a}+1}(10^{\mathfrak{a}})^{\mathfrak{b}+1}$

up to an application of the mapping *L*.

Since the word *u* is primitive and |u| > 1, both letters *S* and *L* occur in *u*. It follows that both *SL* and *LS* occur in u^2 . If $S = 10^{\mathfrak{a}}$, then $L = 010^{\mathfrak{a}-1}$ and *LS* contains the factor $010^{\mathfrak{a}-1}1$ showing that $\mathcal{P}_S(LS) \notin \mathcal{L}(\mathfrak{a}, \mathfrak{b})$. By symmetry, the same happens if $S = 010^{\mathfrak{a}-1}$. Similar reasoning in the remaining cases shows that *LS* or *SL* must contain a factor that contradicts with $w^2 \in \mathcal{L}(\mathfrak{a}, \mathfrak{b})$. Consequently $w^2 \notin \Pi(\mathfrak{a}, \mathfrak{b})$.

If (I) or (II) holds for w, then Proposition 3.2 and Proposition 3.5 respectively imply that w is a primitive solution to (1). Let finally w be a nonprimitive solution to (1), and write $w = v^k$ for a primitive word v and integer $k \ge 2$. By Lemma 3.11, the word v is a solution to (1). Thus w is a power of a primitive solution to (1).

4 Enumeration of Solutions

In this section, we give a formula for counting solutions to (1) of length n for all possible values of a and b.

As before, we assume that a solution never contains the factor 11, that is, we count the solutions up to the isomorphism $0 \mapsto 1, 1 \mapsto 0$. Since L(w) is a solution whenever w is a solution and $|w| \ge 2$, we may count the solutions up to the application of the mapping L as well. Let us first recall an important result.

Proposition 4.1. [2, Cor. 2.2.16] The number of standard words of length n up to the isomorphism $0 \mapsto 1$, $1 \mapsto 0$ is given by $\varphi(n)$, where φ is Euler's totient function.

Before counting the number of solutions, we need to count the number of pattern words of length ℓ that begin with the letter *S*. From the definition of a pattern word, it is clear that this number is $2^{\mathcal{O}(\ell)-1}$ where $\mathcal{O}(\ell)$ is the number of orbits of the mapping $x \mapsto 2x \mod \ell$. The number $\mathcal{O}(\ell)$ depends heavily on the arithmetic nature of ℓ , and we do not study it in more detail in this paper. Suffice it to say that the first values of $\mathcal{O}(\ell)$ are 1, 1, 2, 1, 2, 2, 3, 1, 3, 2, 2, 2, 2, 3, 5, 1, 3, 3, 2, 2, 6 (see the entry A000374 in Sloane's *On-Line Encyclopedia of Integer Sequences* [12]), and the following lemma provides a formula for $\mathcal{O}(\ell)$.

Lemma 4.2. Let ℓ be a positive integer and 2^i the largest power of 2 dividing ℓ , and set $\ell' = \ell/2^i$. We have

$$\mathcal{O}(\ell) = \sum_{d|\ell'} \frac{\varphi(d)}{\operatorname{ord}(2,d)}$$

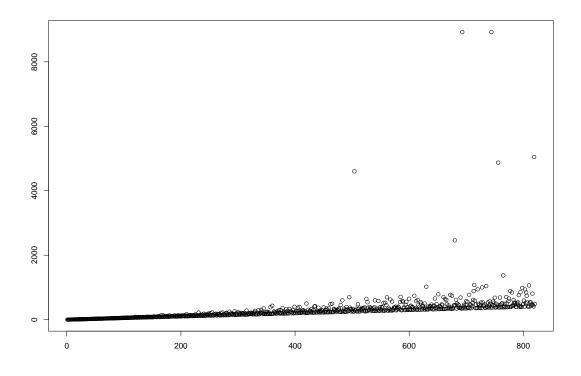


Figure 2: Plot of the number of solutions to (1) of length *n*.

where $\operatorname{ord}(2, d)$ is the order of the element 2 in the group \mathbb{Z}_d^* .

Proof. Each orbit of the mapping $x \mapsto 2x \mod \ell$ contains a unique cycle, so it suffices to compute the number of cycles. If $x, 2x, \ldots, 2^k x$ is a cycle (that is, $2^{k+1}x = x$), then $(2^{k+1}-1)x \equiv 0 \pmod{\ell}$, and it must be that 2^i divides x. By dividing x by 2^i , we thus obtain a cycle of length k + 1 modulo $\ell/2^i$. Conversely every cycle modulo $\ell/2^i$ produces a cycle of the same length modulo ℓ so, in order to count the cycles, it suffices to consider the case i = 0.

Let $d = \operatorname{gcd}(x, \ell)$. Then x/d, 2x/d, ..., $2^k x/d$ is a cycle of length k + 1 modulo ℓ/d , and it corresponds to a coset of the subgroup $\langle 2 \rangle$ generated by 2. Thus $k + 1 = \operatorname{ord}(2, \ell/d)$. Conversely every coset of $\langle 2 \rangle$ yields a cycle of length $\operatorname{ord}(2, \ell/d)$ modulo ℓ . The number of such cosets is $|\mathbb{Z}_{\ell/d}^*| / \operatorname{ord}(2, \ell/d)$. As $|\mathbb{Z}_{\ell/d}^*| = \varphi(\ell/d)$, the claim follows by summing over the divisors of the number ℓ .

The sequence $(ord(2, 2n + 1))_n$ is given as the sequence A002326 in the OEIS [12]; see also A037226.

Let *n* be an integer such that n > 2 and *w* be a solution of (1) of length *n* for some values of a and b such that 11 is not a factor of *w* and *w* begins with 0. The main message of Theorem 3.1 is that for each solution to (1) there exists a pattern word (perhaps a trivial one) *u* and a reversed standard word *v* such that $w = \mathcal{P}_v(u)$. The word *w* can be constructed in this manner in two ways. Indeed, if we denote by L(u) the word we obtain from the pattern word *u* by exchanging the letters *S* and *L*, then clearly $w = \mathcal{P}_{L(v)}(L(u))$. However, there is no third possibility since **Proposition** 3.10 ensures that *v* is unique up to an application of *L*. Our conclusion is that *u* and *v* are unique if we insist that *w* begins with 0 and *u* begins with *S*.

Therefore in order to find all solutions of length n, we need to find all reversed standard

п	S(n)	n	S(n)								
1	1	7	4	13	7	19	10	25	13	31	16
2	2	8	5	14	8	20	11	26	14	32	17
3	2	9	5	15	8	21	11	27	14	33	19
4	3	10	6	16	9	22	12	28	15	34	18
5	3	11	6	17	9	23	12	29	15	35	18
6	4	12	7	18	10	24	14	30	16	36	20

Table 1: Number of solutions of length *n*, denoted by S(n), for n = 1, ..., 36.

words v of length d that begin with 0 and all pattern words u of length n/d that begin with S for all divisors d of n. By Theorem 3.1, we also need to require that the reversed words v satisfy $|v| > |S_6|$ whenever the pattern word is nontrivial and primitive. Say v is a reversed standard word such that v has length d, v begins with 0, and v has parameters \mathfrak{a} and \mathfrak{b} . Then $|v| \le |S_6|$ if and only if $v = 0(10^{\mathfrak{a}})^{\ell}$ for some ℓ such that $0 \le \ell \le \mathfrak{b} + 2$. The conclusion is that $|v| \le |S_6|$ if and only if v = 0 or $\mathfrak{a} + 1$ and ℓ are divisors of d - 1. There is thus a total of $\sigma(d - 1) - 1$ reversed standard words we need to exclude ($\sigma(k)$ is the number of distinct divisors of k with 1 and k included). The preceding arguments and Proposition 4.1 together now show that if d is a divisor of n and d > 2, then the contribution of reversed standard words of length d to the total number of solutions of length n is

$$\frac{\varphi(d)}{2} + \mathcal{H}(n,d),\tag{8}$$

where

$$\mathcal{H}(n,d) = (2^{\mathcal{O}(n/d)-1} - 1) \left(\varphi(d)/2 - \sigma(d-1) + 1\right)$$
(9)

Here the first summand of (8) represents the contribution of all reversed standard words of length d that begin with 0 applied to the pattern word $S^{n/d}$.

If d = 1 or d = 2, then there is only a single reversed standard word that has prefix 0. Overall, we have that the number of solutions to (1) of length n, n > 2, is given by

$$\sum_{\substack{d|n\\2$$

By recalling the well-known identity $\sum_{d|n} \varphi(d) = n$, we obtain the following result.

Theorem 4.3. The number of solutions to (1) of length n up to isomorphism and application of L is

$$\left\lfloor \frac{n}{2} \right\rfloor + 1 + \sum_{\substack{d \mid n \\ 2 < d \le n}} \mathcal{H}(n, d)$$

where \mathcal{H} is given by (9).

Clearly the value of the formula of Theorem 4.3 is always at least $\lfloor n/2 \rfloor + 1$, and this lower bound is attained infinitely often (for example when *n* is a prime). It seems that typically the value is close to $\lfloor n/2 \rfloor + 1$ (see Figure 2), but for a suitable *n* the difference can be large: the value is 1050644 when n = 1736, for example. The explanation is that 217 is a factor of 1736 and O(217) = 21. Some additional values are given in Table 1. The values are recorded as the sequence A330878 in the OEIS [12].

5 Application to the Square Root Map

The original reason why the specific solutions to the equation (1) were studied was to construct fixed points of the square root map and large sets of words whose language is preserved by this mapping. In this section, we continue this study and apply Theorem 3.1 to obtain a characterization of minimal subshifts whose languages contain arbitrarily long solutions to (1) (Theorem 5.6).

Recall that if **w** is an optimal squareful word with parameters \mathfrak{a} and \mathfrak{b} written as a product of the minimal squares, $\mathbf{w} = X_1^2 X_2^2 \cdots$, then $\sqrt{\mathbf{w}} = X_1 X_2 \cdots$. An infinite word **w** is a *fixed point* if $\sqrt{\mathbf{w}} = \mathbf{w}$.

In the paper [6], the first author and Whiteland showed that Sturmian words have the curious property that the square root map preserves their language. Alternatively phrased, we have the following result.

Theorem 5.1. [6, Thm. 9] Let **w** be a Sturmian word and Ω be the Sturmian subshift generated by it. Then the subshift is invariant, that is, $\sqrt{\Omega} \subseteq \Omega$.

Remark 5.2. Optimal squareful words are by definition aperiodic. Many periodic words nevertheless have a well-defined square root. For instance, any periodic word in $(S_5 + S_6)^{\omega}$ is expressible as a product of minimal squares. Another example is the class of so-called periodic Sturmian words. An infinite word **w** is a *periodic Sturmian word* if it equals a shift of S^{ω} for a reversed standard word *S*. Theorem 5.1 is in fact true for periodic Sturmian words as well. If $|S| > |S_6|$, then the claim follows by [7, Remark 2.4]. If $|S| \le |S_6|$ then, strictly speaking, the parameters a and b might not exist as S^{ω} can contain arbitrarily large powers of 0 or 10^{a} , but Theorem 5.1 still holds. To see this, we can adapt the proof of [6, Lemma 11] appropriately or use a case-by-case analysis. For example, if $S = 10^{a}$ and $\mathbf{w} \in \sigma(S^{\omega})$, then $\mathbf{w} = 0^{\ell}(10^{a})^{\omega}$ for ℓ such that $0 \le \ell \le a$. If ℓ is even, then $\sqrt{\mathbf{w}} = 0^{\ell/2}\sqrt{(10^{a})^{\omega}} = 0^{\ell/2}(10^{a})^{\omega}$. If ℓ is odd, then $\sqrt{\mathbf{w}} = 0^{(\ell-1)/2}\sqrt{(010^{a-1})^{\omega}} = 0^{(\ell-1)/2}0(10^{a})^{\omega}$. Thus $\sqrt{\mathbf{w}}$ has the same language as \mathbf{w} .

Extending the results of this section to allow periodic words is mostly a matter of minor adjustments to details and definitions, so we focus only on the aperiodic case.

Theorem 5.1 is somewhat unexpected as intuitively it could be expected that the square root map changes the language of a typical optimal squareful word. This raised the question if there are other large sets or subshifts than Sturmian subshifts that are invariant under the square root map. A natural way to find candidates of such sets is to pick a fixed point of the square root map and study the dynamics of the square root map in the subshift generated by this word. This is what was done in [6, 7] for fixed points that are so-called SL-words (see below).

How to find fixed points then? One way is to use solutions to (1). Suppose that w is a solution to (1), that is, suppose that $\sqrt{w^2} = w$. Therefore if (Z_n) is a sequence of solutions to (1) such that its limit **w** has infinitely many squares Z_n^2 as prefixes, then $\sqrt{\mathbf{w}} = \mathbf{w}$. If solutions of type I are used, then **w** and the subshift generated by **w** are Sturmian. In [6, 7], specific type II solutions were considered resulting in the following theorem.

Theorem 5.3. [7, Thm. 2.10] Let S be a reversed standard word with $|S| > |S_6|$ and c a positive integer. Let (Z_n) be the sequence defined by setting $Z_0 = S$ and $Z_{n+1} = L(Z_n)Z_n^{2c}$ for $n \ge 0$. Let w be a limit of (Z_n) and Ω the subshift generated by w. Then w is a fixed point, Ω is aperiodic, and for all $\mathbf{u} \in \Omega$ either $\sqrt{\mathbf{u}} \in \Omega$ or $\sqrt{\mathbf{u}}$ is purely periodic with minimum period conjugate to S.

Theorem 5.3 means that at least certain subshifts Ω obtained from type II solutions fail to be invariant. This applies even more generally; see Proposition 5.5.

Definition 5.4. Let *S* be a reversed standard word with $|S| > |S_6|$, and let L = L(S). An infinite word **w** is an *SL*-word if $\mathbf{w} \in \{S, L\}^{\omega} \setminus \sigma(S^{\omega})$. A subshift Ω is an *SL*-subshift if there exist fixed *S* and *L* such that for each **w** in Ω there exists an SL-word **u** in Ω such that **w** is a shift of **u**.

Notice that if S is a reversed standard word, then S and L(S) are conjugate [6, Proposition 6].

Proposition 5.5. [7, Thm. 2.11], [6, Lemma 48] Let \mathbf{w} be an SL-word. Then there exists a shift \mathbf{u} of \mathbf{w} such that $\sqrt{\mathbf{u}}$ is purely periodic with minimum period conjugate to S.

The above proposition states that if Ω is an aperiodic SL-subshift, then it cannot be invariant. The solutions of type II give rise to SL-subshifts, so type II solutions do not help to find non-Sturmian invariant subshifts. This led the authors of [6, 7] to formulate Conjecture 1.3 stating that a minimal and invariant subshift is necessarily Sturmian. Notice that it was observed in [6, Proposition 60] that without the assumption that Ω is minimal the claim is false.

Using Theorem 3.1, we prove Conjecture 1.3 for a natural class of subshifts.

Theorem 5.6. Let Ω be a minimal and aperiodic subshift whose language contains infinitely many solutions to (1). Then either

- (*i*) Ω *is Sturmian and* $\sqrt{\Omega} \subseteq \Omega$ *or*
- (*ii*) Ω *is an SL-subshift and* $\sqrt{\Omega} \not\subseteq \Omega$.

Proof. If the language of Ω contains infinitely many reversed standard words, then there exists an infinite word **u** in Ω having arbitrarily long reversed standard words as prefixes. In other words, the word **u** is a standard Sturmian word. Then the subshift Ω is Sturmian because the subshift generated by **u** equals Ω by minimality. Then $\sqrt{\Omega} \subseteq \Omega$ by Theorem 5.1. Thus we may suppose that the language of Ω contains only finitely many reversed standard words.

Since the language of Ω contains infinitely many solutions to (1), we can find a sequence (Z_n) of solutions converging to a word \mathbf{w} in Ω . Since the language of Ω contains only finitely many reversed standard words and Ω is aperiodic, all but finitely many solutions in the sequence (Z_n) are powers of type II solutions by Theorem 3.1. There must exist a fixed reversed standard word S such that $Z_n \in \{S, L(S)\}^+ \setminus (S^+ \cup L(S)^+)$ for all n large enough; otherwise there exists infinitely many reversed standard words in the language of Ω . It follows that $\mathbf{w} \in \{S, L(S)\}^{\omega} \setminus \sigma(S^{\omega})$, that is, the word \mathbf{w} is an SL-word. Hence minimality implies that Ω is an SL-subshift. Then by Proposition 5.5, there exists a word \mathbf{v} in Ω such that $\sqrt{\mathbf{v}}$ is purely periodic. Thus $\sqrt{\mathbf{v}} \notin \Omega$ since Ω is aperiodic by assumption. In other words, we see that $\sqrt{\Omega} \not\subseteq \Omega$.

Let us end this section by making a few remarks on attacking the remaining cases of Conjecture 1.3. One of the first things that comes to mind is to ask if an invariant subshift Ω must necessarily contain a fixed point. So far our only method for constructing fixed points is to use solutions to (1), so if a fixed point exists and a fixed point must be constructed in this way, Theorem 5.6 would show that Conjecture 1.3 is true. Moreover, we show in the next lemma that every square prefix of a fixed point must correspond to a solution to (1). However, below in Proposition 5.8, we construct an aperiodic fixed point having finitely many square prefixes, which casts some doubt on the workability of these ideas.

Lemma 5.7. Let **w** an optimal squareful word that is a fixed point. If X^2 is a prefix of **w**, then X is a solution to (1).

Proof. This follows immediately from Lemma 3.11.

Proposition 5.8. *There exists an optimal squareful word* **w** *that is a fixed point and has exactly one square prefix.*

Proof. Let b = 0, and define an infinite word **w** as follows:

$$\mathbf{w} = S_5^2 S_6^2 \cdot \prod_{i=0}^{\infty} (S_3^{2^i} S_6^{2^i})^2.$$

We show that **w** has the claimed properties. First of all, we have $S_5^2 S_6^2 (S_3 S_6)^2 \in \Pi(\mathfrak{a}, \mathfrak{b})$, and

$$\sqrt{S_5^2 S_6^2 S_3 S_6 S_3 S_6} = S_5 S_6 \cdot \sqrt{010^{\mathfrak{a}} 10^{\mathfrak{a}+1} 10^{\mathfrak{a}} 010^{\mathfrak{a}} 10^{\mathfrak{a}+1} 10^{\mathfrak{a}}} = S_5 S_6 \cdot S_2 S_1 S_6 = S_5^2 S_6^2.$$

Clearly $(S_3^{2i}S_6^{2i})^2 \in \Pi(\mathfrak{a},\mathfrak{b})$ when $i \ge 1$, and then

$$\sqrt{(S_3^{2^i}S_6^{2^i})^2} = (S_3^{2^{i-1}}S_6^{2^{i-1}})^2.$$

Therefore **w** is optimal squareful and $\sqrt{\mathbf{w}} = \mathbf{w}$. Let u^2 be a prefix of **w** with $|u| \ge 2|S_5S_6S_3S_6|$. In particular, the word $S_5^2S_6^20$ is a prefix of u. The suffix u of u^2 occurs in **w** in some concatenation $(S_3^{2i}S_6^{2i})^2(S_3^{2i+1}S_6^{2i+1})^2$ of two blocks for some $i \ge 1$. Let $z = (10^{a+1})^310^a$. Now u has prefix z. No word of the form S_6^{2j} with $j \ge 1$ contains $(10^{a+1})^21$, so either z is a suffix of S_3^{2i} or S_3^{2i+1} or the prefix $10^{a+1}10^a$ of z is a suffix of S_6^{2i} . The prefix z is followed in u by S_60 . Since S_60 is not a prefix of S_6^2 , it follows that the latter option is true: the prefix $10^{a+1}10^a$ of z is a suffix of S_6^{2i} . This in turn means that S_6^{2i} is followed by $010^{a+1}10^{a}10^{a+1}10^{a+1}$. This word is not a prefix of $S_3^2S_6^2$ or S_3^4 , so we obtain a contradiction. The conclusion is that u does not exist, and for each square prefix v^2 of \mathbf{w} , we have $|v| < 2|S_5S_6S_3S_6|$. It is a straightforward task to verify that \mathbf{w} has exactly one square prefix.

Notice that the word **w** of the proof of Proposition 5.8 is not a counterexample to Conjecture 1.3. First of all, the subshift generated by **w** is not minimal. Secondly, the subshift generated by Ω is not invariant. Indeed, consider the square root of the word **z** obtained from **w** by removing its first $|S_6|$ letters. We have

$$\sqrt{z} = 010^{\mathfrak{a}}10^{\mathfrak{a}+1}10^{\mathfrak{a}+1}10^{\mathfrak{a}}10^{\mathfrak{a}+1}10^{\mathfrak$$

Similar to the proof of Proposition 5.8, it is straightforward to verify that this visible prefix is not a factor of **w**.

We considered above only square prefixes, but arbitrary positions could be considered as well. While an optimal squareful word contains an occurrence of a square at each position, it is unclear if long squares need to appear. Every position of a Sturmian word begins with arbitrarily long squares [1, Lemma 8], and the language of the word **w** constructed in the proof of Proposition 5.8 contains infinitely many squares.

Question. Does there exist an optimal squareful word whose language contains only finitely many squares?

6 Remark on Periodic Points

The results presented in this paper concern fixed points of the square root map, but other periodic points could be considered as well. Clearly solutions to (1) are not helpful in constructing *p*-periodic points when p > 1. We are not aware of a general construction method, but we show next that aperiodic proper 2-periodic points exist. By $\sqrt[2]{\mathbf{w}}$ we mean the second iterate of \mathbf{w} .

Proposition 6.1. There exists an optimal squareful word **w** such that $\sqrt{\mathbf{w}} \neq \mathbf{w}$ and $\sqrt[2]{\mathbf{w}} = \mathbf{w}$.

Proof. Define two integer sequences $(r(n))_n$ and $(s(n))_n$ as follows: r(1) = s(1) = 2, r(2) = 6, s(2) = 8 and r(n+1) = 4r(n), s(n+1) = 4s(n) for all $n \ge 2$. Let $\mathfrak{b} = 0$, and define

$$\mathbf{w} = S_2^2 S_1^2 \cdot \prod_{n=1}^{\infty} (S_6^2)^{r(n)} (S_3^2)^{s(n)},$$

so that

$$\sqrt{\mathbf{w}} = S_2 S_1 \cdot \prod_{n=1}^{\infty} S_6^{r(n)} S_3^{s(n)} = S_2 S_1 S_6^2 S_3^2 \cdot \prod_{n=2}^{\infty} S_6^{r(n)} S_3^{s(n)} = S_2^2 S_1^2 S_4^2 S_3^2 S_3 \cdot \prod_{n=2}^{\infty} S_6^{r(n)} S_3^{s(n)}.$$

Since $S_2^2 S_1^2 S_4^2$ is not a prefix of **w**, we see that $\sqrt{\mathbf{w}} \neq \mathbf{w}$. Notice that the word $S_2 S_1 S_4$ is a solution to (1). Since $S_3 S_6^2 = S_2^2 S_1^2 S_4^2 S_3$, we see that $S_3 (S_6^2)^i = (S_2^2 S_1^2 S_4^2)^i S_3 = (S_2 S_1 S_4)^{2i} S_3$ for all *i*. It follows that

$$S_2^2 S_1^2 S_4^2 S_3^2 S_3 \cdot S_6^6 S_3^8 = S_2^2 S_1^2 S_4^2 S_3^2 \cdot (S_2^2 S_1^2 S_4^2)^3 S_3 \cdot S_3^8,$$

so

$$\begin{split} & \sqrt[2]{\mathbf{w}} = S_2 S_1 S_4 S_3 (S_2 S_1 S_4)^3 S_3^4 \cdot \sqrt{\prod_{n=3}^{\infty} S_3 S_6^{r(n)} S_3^{s(n)-1}} \\ & = S_2^2 S_1^2 (S_6^2)^2 S_3^3 \cdot \sqrt{\prod_{n=3}^{\infty} (S_2^2 S_1^2 S_4^2)^{r(n)/2} S_3^{s(n)}} \\ & = S_2^2 S_1^2 (S_6^2)^2 S_3^3 \cdot \prod_{n=3}^{\infty} (S_2 S_1 S_4)^{r(n)/2} S_3^{s(n)/2} \\ & = S_2^2 S_1^2 (S_6^2)^2 S_3^3 \cdot \prod_{n=3}^{\infty} (S_2^2 S_1^2 S_4^2)^{r(n)/4} (S_3^2)^{s(n)/4} \\ & = S_2^2 S_1^2 (S_6^2)^2 S_3^4 \cdot \prod_{n=3}^{\infty} (S_6^2)^{r(n)/4} (S_3^2)^{s(n)/4} \\ & = S_2^2 S_1^2 (S_6^2)^2 (S_3^2)^2 \cdot \prod_{n=2}^{\infty} (S_6^2)^{r(n)} (S_3^2)^{s(n)} \\ & = \mathbf{w}. \end{split}$$

Since the sequences $(r(n))_n$ and $(s(n))_n$ are increasing, the word **w** is aperiodic. It is straightforward to check that **w** is optimal squareful.

We do not how to produce *p*-periodic points for p > 2. Moreover, we are not completely satisfied with the word **w** of the proof of Proposition 6.1 because the subshift generated by **w** is not minimal, that is, the word **w** is not uniformly recurrent.

Question. Does there exist an optimal squareful word that is a proper *p*-periodic point for all p > 1? Can such words be taken as uniformly recurrent?

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