9. Infinite words generated by invertible substitutions

Combinatorial properties of finite and infinite words are of increasing importance in various fields of science (for a general reference, the reader should consult [271, 272] and the references therein). The combinatorial properties of the Fibonacci infinite word have been studied extensively by many authors (see for examples [65, 130, 176, 452]).

This chapter looks at infinite words generated by invertible substitutions. As we shall see, words of this family generalize the Fibonacci infinite word.

The combinatorial properties of those infinite words are of great interest in various fields of mathematics, such as number theory [10, 95, 164, 232], dynamical systems [331, 340, 350, 400], fractal geometry [43, 103, 222, 274], tiling theory [43, 409], formal languages and computational complexity [65, 67, 202, 201, 233, 295, 384, 385, 449], and also in the study of quasicrystals [82, 99, 257, 258, 274, 456, 454, 455, 459].

The purpose of this chapter is to study the properties of factors of infinite words generated by primitive invertible substitutions over a two-letter alphabet. It is deeply linked to Chap. 6: as we will see, all these words are Sturmian words. The chapter is organized as follows.

Section 9.1 is devoted to the introduction and preliminaries. Section 9.2 is concerned with the structure of the semigroup of invertible substitutions for which we give a set of generators; we derive various consequences from the structure theorem.

Section 9.3 lists properties of factors of the Fibonacci word. After recalling some basic facts, we introduce what we call the singular words of the Fibonacci word and give their properties. We then establish two decompositions of the Fibonacci word involving the singular words. Some applications are derived from those decompositions, describing combinatorial properties of the Fibonacci word related to powers of its factors, for example. We also prove local isomorphisms properties of the Fibonacci word and the overlap properties of the factors.

In Sec. 9.4, we consider more general invertible substitutions. We define singular factors of fixed points of invertible substitutions, and then give applications of decompositions associated with these singular words, after proving some general properties of factors of fixed points of invertible substitutions.

[1] This chapter has been written by Z. -Y. Wen

As we shall see, the general framework we introduce is at a much higher level of complexity than with the Fibonacci word.

9.1 Preliminary

Let us now introduce some definitions and notation (see also Chap. 1).

Free monoid and free group. Let $\mathcal{A}_n = \{a_1, a_2, \cdots, a_n\}$ be an alphabet with n letters. Let $\mathcal{A}_n^*$ and Γ_n respectively denote the free monoid with empty word ε as neutral element and the free group generated by $\mathcal{A}_n$. By a natural embedding, we can regard the set $\mathcal{A}_n^*$ as a subset of Γ_n, and consider any $W \in \mathcal{A}_n^*$ as a reduced element of Γ_n (see [331] and the references therein, see also [275, 278, 416]).

The canonical abelianization map on $\mathcal{A}_n^*$ is denoted by $\mathbf{l} : \mathcal{A}_n^* \to \mathbb{N}^n$, as defined in Chap. 1.

Factors. Let $V, W \in \mathcal{A}_n^*$.

- We write $V \prec W$ when the finite word V is a *factor* of the word W, that is, when there exist words $U, U' \in \mathcal{A}_n^*$ such that $W = UVU'$.
- We say that V is a *left* (respectively *right*) *factor* of a word W, and we write $V \triangleleft W$ (respectively $V \triangleright W$), if there exists a word $U' \in \mathcal{A}_n^*$ such that $W = VU'$ (respectively $W = U'V$).
- We denote by W^{-1} the *inverse word* of W, that is, $W^{-1} = w_p^{-1} \cdots w_2^{-1} w_1^{-1}$ if $W = w_1 w_2 \ldots w_p$. This only makes sense in Γ_n; but if V is a right factor of W, we can write $WV^{-1} = U$, with $W = UV$; this makes sense in $\mathcal{A}_n^*$, since the reduced word associated with WV^{-1} belongs to $\mathcal{A}_n^*$. This abuse of language will be very convenient in what follows.

Definition 9.1.1. *Let u and v be two infinite words over $\mathcal{A}_n$. We say that u and v are* locally isomorphic *if any factor of u is also a factor of v and vice versa. If u and v are locally isomorphic, we shall write $u \simeq v$.*

Remarks.

- This means that the dynamical systems associated with u and v under the action of the shift, in the sense of Chap. 1, are the same. If we are only interested in the language of factors of an infinite word, or in the system associated with this infinite word, we do not need to differentiate between locally isomorphic infinite words. We will use this remark several times.
- The notion of local isomorphism was first introduced in connection with quasicrystals, and for physical reasons, the definition was that each factor of u, or its mirror image, should also be a factor of v. Since however all the languages we will consider in this chapter are closed under mirror image, the definition we take here is equivalent in our case, and will allow simpler proofs.

Conjugation of a word. Let $W = w_1 w_2 \dots w_p \in \mathcal{A}_n^*$.

- The *reversed word* (or *mirror image*) of W, denoted $\overline{W}$, is defined as $\overline{W} = w_p \dots w_2 w_1$.
- A word W is called a *palindrome* if $W = \overline{W}$. We denote by $\mathcal{P}$ the set of palindromic words.
- For $1 \leq k \leq |W|$, we define the *k-th conjugation* of W as $C_k(W) = w_{k+1} \dots w_n w_1 \dots w_k$, and we denote by $C(W) = \{C_k(W);\ 1 \leq k \leq |W|\}$. By convention, $C_{-k}(W) = C_{|W|-k}(W)$. We will say that two words are *conjugate* if they belong to the same conjugacy class.

This may seem an abuse of language, since there is another notion of conjugacy, if we consider the two words as an element of the free group; in this sense, U and V are conjugate if there exist an element U' of the free group Γ_n such that $U = U'VU'^{-1}$. These two definitions turn out to be equivalent:

Lemma 9.1.2. *Two words U and V in $\mathcal{A}_n^*$ are conjugate as elements of the free monoid $\mathcal{A}_n^*$ if and only if they are conjugate as elements of the free group Γ_n; in that case, we can always find a conjugating element of length strictly less than $|U| = |V|$.*

Exercise 9.1.3. Give a proof of this lemma, and give the most general form for the conjugating word U' such that $U = U'VU'^{-1}$.

A word $W \in \mathcal{A}_n^*$ is called *primitive* if $W = U^p$, $U \in \mathcal{A}_n^*$, $p > 0$, implies $W = U$ (and thus $p = 1$). That is, W cannot be expressed as a proper power of any other word. Notice that the k-th conjugation C_k is an action from $\mathcal{A}_n^*$ to $\mathcal{A}_n^*$ preserving primitivity. That is, the word $C_k(W)$ is primitive if and only if W is itself a primitive word. We will use the following lemma.

Lemma 9.1.4. *A word $W \in \mathcal{A}_n^*$ is primitive if and only if the cardinality of $C(W)$ is $|W|$.*

Proof. If the cardinality is smaller, it means that we can find k, l distinct, $1 \leq k < l \leq n$, such that $C_k(W) = C_l(W)$. It is immediate to check that we can then find two nonempty words U, V such that $C_k(W) = UV$, $C_l(W) = VU$; since $UV = VU$, it is well known that they must be a power of the same word U', and $C_k(W)$ is not primitive. Hence W is not primitive. The reciprocal is trivial. ∎

There is a useful criterion of primitivity:

Lemma 9.1.5. *If the numbers $|W|_{a_1}, |W|_{a_2}, \dots, |W|_{a_n}$ are relatively prime, the word W is primitive.*

We leave the proof to the reader.

Substitution. Let us recall that a *substitution* (or a *morphism*) over $\mathcal{A}_n$ is a map $\sigma : \mathcal{A}_n^* \to \mathcal{A}_n^*$, such that for any two words U and V, one has $\sigma(UV) = \sigma(U)\sigma(V)$. The substitution σ is uniquely determined by the image of the elements of $\mathcal{A}_n$. We denote by $\sigma = (U_1, U_2, \cdots, U_n)$ the substitution defined by $\sigma(a_i) = U_i,\ 1 \le i \le n$.

The notions of incidence matrix and primitivity were introduced in Chap. 1. In this chapter, unless stated otherwise, all substitutions we consider are primitive.

If for some letter $a \in \mathcal{A}_n$, the word $\sigma(a)$ begins with a and has length at least 2, then the sequence of words $\sigma^n(a)$ converges to a fixed point $\sigma^\omega(a) \in \mathcal{A}_n^{\mathbb{N}}$. In this chapter, we shall only consider fixed points of a substitution that can be obtained by iterating a morphism in the above manner. We denote by u_σ any one of the fixed points of σ, if it exists.

Invertible substitution. Let $\sigma : \mathcal{A}_n^* \to \mathcal{A}_n^*$ be a substitution over $\mathcal{A}_n^*$. Then σ can be naturally extended to Γ_n by defining $\sigma(a_i^{-1}) = (\sigma(a_i))^{-1}$, $1 \le i \le n$. Denote by $\mathrm{Aut}(\Gamma_n)$ the *group of automorphisms* over Γ_n.

Definition 9.1.6. *A substitution σ is called an* invertible substitution *if it can be extended to all of Γ_n by an automorphism (also called σ), that is, if there exists a map $\eta : \Gamma_n \to \Gamma_n$ such that $\sigma\eta = \eta\sigma = Id$ on Γ_n (where Id is the substitution given by $Id = (a_1, a_2, \cdots, a_n)$). The set of invertible substitutions over $\mathcal{A}_n^*$ is denoted by* $\mathrm{Aut}(\mathcal{A}_n^*)$.

Remark. The set $\mathrm{Aut}(\mathcal{A}_n^*)$ is obviously a semigroup. Remark that its elements extend to automorphism of the free group, but they are not automorphisms of the free monoid $\mathcal{A}_n^*$ in the usual sense, since they are not onto, except for the trivial case of the permutations of the alphabet.

Example 9.1.7 (The Fibonacci substitution). Set $\mathcal{A}_2 = \{a, b\}$ for convenience. The *Fibonacci substitution* $\sigma = (ab, a)$ is an invertible substitution over $\mathcal{A}_2$: an easy computation shows that the map $\eta = (b, b^{-1}a)$ is its inverse.

REcall that the fixed point generated by the Fibonacci substitution $\sigma = (ab, a)$ (iterated over a) is called the *infinite Fibonacci word*;it is denoted by u_σ. We shall often simply call it the *Fibonacci word* when no confusion occurs.

General structure of $\mathrm{Aut}(\boldsymbol{\Gamma_n})$. The structure of $\mathrm{Aut}(\Gamma_n)$ is well known [278, 314, 331]. In particular, we have the following theorem, where, as usual, $\langle S \rangle$ denotes the group generated by a set S of generators.

Theorem 9.1.8. *Let $n > 0$. The number of generators of the group* $\mathrm{Aut}(\Gamma_n)$ *is $3n - 3$ and these generators can be determined explicitly.*

If $n = 2$, then

$$\mathrm{Aut}(\Gamma_2) = \langle \sigma, \quad \pi, \quad \psi \rangle,$$

where $\sigma = (ab, a)$, $\pi = (b, a)$ and $\psi = (a, b^{-1})$

In the following section, we will give a description in terms of generators of the related semigroup $\mathrm{Aut}(\mathcal{A}_2^*)$.

Inner automorphisms and conjugacy. Let $W \in \Gamma_n$. We denote by $i_W : \Gamma_n \to \Gamma_n$ the *inner automorphism* defined by $U \mapsto WUW^{-1}$, for any $U \in \Gamma_n$. The set of all inner automorphisms of Γ_n will be denoted by $\mathrm{Inn}(\Gamma_n)$.

For any substitution τ, the composition $i_W \circ \tau$ results in $U \mapsto W\tau(U)W^{-1}$; it is a morphism of the free group, but not a substitution in general. We have the following lemma:

Lemma 9.1.9. *Let τ be a substitution, and $W \in \Gamma_n$. The composition $i_W \circ \tau$ is a substitution if and only if: either $W \in \mathcal{A}_n^*$ and W is of the form $X_a\tau(a)^k$, where X_a is a suffix of $\tau(a)$, for any letter a , or $W^{-1} \in \mathcal{A}_n^*$ and W^{-1} is of the form $\tau(a)^k X_a$, where X_a is a prefix of $\tau(a)$, for any letter a.*

If $i_W \circ \tau$ is a substitution, then, for any letter a, $i_W \circ \tau(a)$ admits X_a as prefix in the first case, and X_a as suffix in the second.

Proof. This is an immediate consequence of Lemma 9.1.2; $i_W \circ \tau$ is a substitution if and only if, for all a, $W\tau(a)W^{-1}$ is an element of the free monoid; but this gives the necessary and sufficient condition for the form of W. ■

We will say that two substitutions σ, τ are *conjugate* if there exists a word $W \in \Gamma_n$ such that $\sigma = i_W \circ \tau$, which will be denoted as $\sigma \sim \tau$.

Note that the conjugating word W can be strictly longer than the images of some letters; for example, the two substitutions (aba, ba) and (aba, ab) are conjugate by the word aba. However, if σ and τ are two substitutions conjugate by a word W, that is $\sigma = i_W \circ \tau$, it is easy to check that, for any suffix V of W, $i_V \circ \tau$ is again a substitution. Considering the particular case where V is a letter, we see that the only way to conjugate a substitution is to suppress a common initial (or final) letter from the images of the letters, to replace it as a final (or initial) letter, and to iterate the operation; in particular, a substitution can be conjugate to another substitution if and only if all the images of letters have a common final or initial letter.

We can be more precise; we know that the word W or its inverse belong to $\mathcal{A}_n^*$. We will say that the substitution σ is a *left conjugate* of τ if there exists $W \in \mathcal{A}_n^*$ such that $\sigma = i_W \circ \tau$.

Exercise 9.1.10. 1. Prove that the conjugacy is an equivalence relation on the set of substitutions.
2. Prove that the left conjugacy induces a total order relation on each class.
3. Prove that an element is maximal (respectively minimal) for that order if the images of letters have no common prefix (respectively suffix).

Conjugacy has an interesting consequence:

Proposition 9.1.11. *Let τ, σ be two conjugate primitive substitutions. Let u_τ, u_σ be fixed points of τ and σ. Then u_τ and u_σ are locally isomorphic.*

Proof. We can suppose, by exchanging τ and σ if needed, that $\tau = i_W \circ \sigma$, with $W \in \mathcal{A}^*$. Then by induction we have

$$\tau^k = (i_W \sigma)^k = i_W i_{\sigma(W)} \cdots i_{\sigma^{n-1}(W)} \sigma^k.$$

Let $W_k = W\sigma(W) \cdots \sigma^{k-1}(W)$. We have $\tau^k = i_{W_k}\sigma^k$, that is, $\tau^k(a)W_k = W_k\sigma^k(a)$. Thus there exist U_k and V_k such that $\tau^k(a) = U_kV_k$, and $\sigma^k(a) = V_kU_k$. Since, by primitivity, $|\tau^k(a)|$ tends to infinity, so does $|U_k|$ or $|V_k|$.

Let U be a factor of u_τ, by minimality of the fixed words of primitive substitutions, $U \prec U_k$ or $U \prec V_k$ for k large enough, thus $U \prec u_\sigma$. The same argument proves that any factor of u_σ is a factor of u_τ. Hence $u_\tau \simeq u_\sigma$. ■

9.2 Structure of invertible substitutions

This section describes a set of generators for the semigroup $\mathrm{Aut}(\mathcal{A}_2^*)$, thus revealing part of its structure.

We will prove the following conclusion: *any invertible substitution over a three-letter alphabet can be written as a finite product of three special invertible substitutions.* This first result is a starting point for studying invertible substitutions, since many basic properties will be derived from it.

The proof we present here is borrowed from [450]. A geometrical proof of the same result is given in [158].

Theorem 9.2.1 ([450]). *Let* $\pi = (b,a)$, $\sigma = (ab,a)$, $\varrho = (ba,a)$, $\gamma = (ab,b)$, *and* $\delta = (ba,b)$. *We have,*

$$\mathrm{Aut}(\mathcal{A}_2^*) = \langle \pi, \varrho, \sigma \rangle = \langle \pi, \gamma, \delta \rangle.$$

The proof follows from the following lemmas.

Lemma 9.2.2. *An automorphism* $\tau \in \mathrm{Aut}(\Gamma_2)$ *is an inner automorphism if and only if its incidence matrix* $\mathbf{M}_\tau$ *is the identity matrix.*

Proof. This means that the kernel of the abelianization map: $\mathrm{Aut}(\Gamma_2) \to GL(2,\mathbb{Z})$ is exactly the group of inner automorphisms; it is clear that the matrix associated with an inner automorphism is the identity. To prove the converse, it suffices to give a presentation of $GL(2,\mathbb{Z})$ by generators and relations, to find generators of $\mathrm{Aut}(\Gamma_2)$ that project to the generators of $GL(2,\mathbb{Z})$, and to check that the combinations of these elements corresponding to the relations are inner automorphisms, see [275]. ■

Remark. This lemma does not generalize to more letters: the map (bab^{-1}, cbc^{-1}, c) gives an automorphism of the free group on three letters whose matrix is the identity, and which is not an inner automorphism.

Lemma 9.2.3. *Let* $\mathcal{M}$ *be the monoid of square matrices of size* 2 *with non-negative integer coefficients, and determinant* ± 1. *We have*

$$\mathcal{M} = \langle \mathbf{A},\ \mathbf{B} \rangle, \quad \text{where } \mathbf{A} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}.$$

Proof. Let

$$\mathbf{C} = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \quad \mathbf{D} = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}.$$

Let also $\mathbf{M} = \begin{pmatrix} p & r \\ q & s \end{pmatrix}$ be an element of $\mathcal{M}$ with at least one entry ≥ 1. Up to multiplication by $\mathbf{A}$, we can suppose $\det \mathbf{M} = 1$. It was proved in Chap. 6, by an easy induction using Euclidean divisions on the columns of the matrix, that the set of matrices with nonnegative coefficients and determinant 1 is the free monoid generated by $\mathbf{C}$ and $\mathbf{D}$ (see Lemma 6.5.14.). But one can easily check the following relations: $\mathbf{C} = \mathbf{BA}$, $\mathbf{D} = \mathbf{AB}$. This ends the proof. ∎

Proof of Theorem 9.2.1. Note that we have the trivial relations: $\sigma = \pi \circ \delta$, $\delta = \pi \circ \sigma$, $\varrho = \pi \circ \gamma$, $\gamma = \pi \circ \varrho$; hence, a substitution can be decomposed on $\{\pi, \sigma, \varrho\}$ if and only if it can be decomposed on $\{\pi, \gamma, \delta\}$. We will prove that this last set is a set of generators for $\mathrm{Aut}(\mathcal{A}_2^*)$.

The idea of the proof is, given an invertible substitution τ, to find, using Lemma 9.2.3, a substitution ϕ, written as a product of π and γ, with the same matrix as τ. Then, using Lemma 9.2.2, these two substitutions are conjugate; but then $\tau = i_W \circ \phi$ can be written as a product of π, γ and δ (this is a generalization of the easy relation $i_b \circ \gamma = \delta$).

Let $\tau \in \mathrm{Aut}(\mathcal{A}_2^*)$. Then $\mathbf{M}_\tau \in \mathcal{M}$. By Lemma 9.2.3, there exist $\mathbf{M}_1, \mathbf{M}_2, \ldots \mathbf{M}_k \in \{\mathbf{A}, \mathbf{D}\}$ such that $\mathbf{M}_\tau = \mathbf{M}_1 \cdots \mathbf{M}_k$. Note that $\mathbf{M}_\pi = \mathbf{A}$ and $\mathbf{M}_\gamma = \mathbf{D}$. Take $\phi = \phi_1 \cdots \phi_k$, with $\phi_i = \pi$ or $\phi_i = \gamma$, according to $\mathbf{M}_i = \mathbf{A}$ or $\mathbf{D}$. Then, we have $\mathbf{M}_\tau = \mathbf{M}_\phi$. Therefore Lemma 9.2.2 implies that $\tau \circ \phi^{-1}$ is an inner automorphism i_W. Hence we can write $\tau = i_W \circ \phi$, and the two substitutions τ, ϕ are conjugate; by Lemma 9.1.9, we have $W \in \mathcal{A}_2^*$ or $W^{-1} \in \mathcal{A}_2^*$. But it is clear that $\phi(a)$ and $\phi(b)$ have a different initial letter, since π and γ send words with different initial letters on words with different initial letters. Hence they have no common prefix, and $W \in \mathcal{A}_2^*$.

Thus we only need to prove the following claim: if $\phi \in \langle \pi, \ \gamma, \ \delta \rangle$ is such that $\phi(a) = UW$ and $\phi(b) = VW$ (with $U, V, W \in \mathcal{A}_2^*$), then $i_W \circ \phi \in \langle \pi, \ \gamma, \ \delta \rangle$. By induction, it is enough to prove it in the case where W is reduced to one letter $z \in \{a, b\}$.

First consider $z = b$. Since $i_b \circ \phi$, where $\phi = \phi_1 \phi_2 \ldots \phi_t$ ($\phi_j \in \{\pi, \ \gamma, \ \delta\}$), is a substitution, $\phi(a)$ and $\phi(b)$ must have b as last letter. This is only possible if one of the ϕ_i is equal to γ, since it is obvious that, for a product of π and δ, the images of a and b end with different letters. Let i be the first index such that $\phi_i = \gamma$, the proposition will follow if we can prove $i_b \phi_1 \phi_2 \ldots \phi_i \in \langle \pi, \ \gamma, \ \delta \rangle$.

Using the properties $\pi^2 = id$, $\gamma\delta = \delta\gamma$, we see that the product $\phi_1 \phi_2 \ldots \phi_i$ can be written $\delta^{e_1} \pi \delta^{e_2} \ldots \delta^{e_n} \pi \gamma$, with all the e_k strictly positive, except maybe the first, and n even (otherwise, $\tau(a)$ and $\tau(b)$ would end in a). A proof by induction, starting from the remark that $i_b \gamma = \delta$, shows that $i_b \phi_1 \phi_2 \ldots \phi_i \in \langle \pi, \ \gamma, \ \delta \rangle$.

A similar proof can be done for $z = a$, in which case n is odd. ∎

Corollary 9.2.4. *Let τ_1, τ_2 be two invertible substitutions and let u_{τ_1}, u_{τ_2} be the fixed points of τ_1 and τ_2 respectively. If there exist $m, n \in \mathbb{N}$ such that $\mathbf{M}_{\tau_1}^n = \mathbf{M}_{\tau_2}^m$, then $u_{\tau_1} \simeq u_{\tau_2}$.*

Proof. It is clear that a fixed point of a substitution is also a fixed point of all its powers; hence, by replacing τ_1, τ_2 by τ_1^n, τ_2^m, we can suppose that $\mathbf{M}_{\tau_1} = \mathbf{M}_{\tau_2}$. But in that case, $\tau_1 \circ \tau_2^{-1}$ is an automorphism of the free group whose matrix is the identity. By Lemma 9.2.2, it is an inner automorphism, hence the substitutions τ_1, τ_2 are conjugate; by Proposition 9.1.11, their fixed points are locally isomorphic. ∎

Exercise 9.2.5. The conjugacy class of a substitution is completely explicit: it is obtained by exchanging γ and δ, since this does not change the matrix. We know that left conjugacy defines a total order on this conjugacy class.

Find the maximal and the minimal element of a class, and explain how to find the successor and the predecessor (for this order) of an invertible substitution with given decomposition in the generators.

An interesting consequence of Corollary 9.2.4 is that fixed points of invertible substitutions are dense in the system generated by an invertible substitution:

Corollary 9.2.6. *Let ϕ be an invertible substitution. Let u_ϕ be a fixed point of ϕ, and let U be a factor of u_ϕ. Then there exists a substitution τ such that u_τ is locally isomorphic to u_ϕ, and admits U as prefix.*

Proof. The substitution ϕ is a product of π, ϱ and σ; we can replace all the ϱ by σ, this will change u_σ to a locally isomorphic word, and will not change the factors.

In that case, one of $\phi^n(a)$, $\phi^n(b)$ is a prefix of the other for all n; suppose it is $\phi^n(a)$. Then, by definition of U, it appears in $\phi^n(a)$, for n large enough, and we can find words W, A, B such that: $\phi^n(a) = WUA$, $\phi^n(b) = WUAB$. But then, $\tau = i_{W^{-1}} \circ \phi$ is a substitution, whose fixed point, by the preceding theorem, is locally isomorphic to u_ϕ and admits U as prefix. ∎

Another consequence of the proof of Theorem 9.2.1 is that any invertible substitution τ is conjugate to a substitution σ which is a product of π and γ. If we take the square, we can suppose that the number of π in the decomposition of σ is even, and an easy induction shows that σ can be written as a product of the substitutions γ and $\pi \circ \gamma \circ \pi$. But these are the two basic substitutions considered in Chap. 6, and from the results of this chapter, we obtain:

Corollary 9.2.7. *A fixed point of a primitive invertible substitution on two letters is Sturmian.*

Remarks.

- Observe that $\gamma \notin \langle \pi,\ \delta \rangle$ and $\delta \notin \langle \pi,\ \gamma \rangle$. Since the length of a substitution can only increase by composition, this proves that the minimal number of generators of $\mathrm{Aut}(\mathcal{A}_2^*)$ is exactly three.
- Brown [95], Kósa [254], Séébold [385], Mignosi and Séébold [296] have considered invertible substitutions in $\langle \pi, \pi_1, \pi_2 \rangle$, with $\pi_1 = (a, ab)$, $\pi_2 = (a, ba)$. They studied combinatorial and arithmetic properties of the infinite words generated by those invertible substitutions.
- Mignosi and Séébold [296] have considered Sturmian substitutions, that is, substitutions preserving all Sturmian sequences. They proved that a fixed point of a substitution over $\mathcal{A}_2$ is Sturmian if and only if the substitution is invertible [296, 450], giving a more precise form of the corollary 9.2.7 above. This motivates us to study the set of invertible substitutions.
- Let $n \geq 2$ and let $\mathcal{A}_n = \{a_1, \cdots, a_n\}$ be a n-letter alphabet. Invertible substitutions over $\mathcal{A}_n$ are defined in complete analogy with invertible substitutions over $\mathcal{A}_2$. The *Rauzy substitution*, $\varrho_n : \mathcal{A}_n^* \to \mathcal{A}_n^*$, is a typical invertible substitution and is defined as follows:

  $$\varrho_n(a_1) = a_1 a_2,\ \ \varrho_n(a_2) = a_2 a_3, \cdots, \varrho_n(a_{n-1}) = a_{n-1} a_n,\ \ \varrho_n(a_n) = a_1.$$

  From its definition, we see that the Rauzy substitution is a generalization of the Fibonacci substitution. This substitution has many remarkable properties and has some interesting relations with other domains; for more details, see Chap. 7. Other interesting invertible substitutions over $\mathcal{A}_n$ are described in [164].
- Theorems 9.1.8 and 9.2.1, bring us to naturally conjecture that the number of generators of $\mathrm{Aut}(\mathcal{A}_n^*)$ is $3n - 3$. However, authors in [453] have proved that the set of invertible substitutions over an alphabet of more than three letters is not finitely generated (their proof uses the notion of "prime substitution"). Also, they gave examples showing that, in that case, the structure of $\mathrm{Aut}(\mathcal{A}_n^*)$ is much more complex.
- Let τ be a substitution, we denote by Φ_τ the trace mapping induced from τ, see [331] and Chap. 10. Let $\tau_1, \tau_2 \in \mathrm{Aut}(\mathcal{A}_2^*)$, then u_{τ_1} and u_{τ_2} are locally isomorphic if and only $\Phi_{\tau_1} = \Phi_{\tau_2}$ [331].
- In [153], Durand has proved the following result: *If two primitive substitutions over $\mathcal{A}_n$ have the same nonperiodic fixed point, then they have some powers the incidence matrices of which have the same eigenvalues.*

9.3 Singular words of the Fibonacci word and applications

As we have seen in the last section, the Fibonacci substitution plays an important role in the study of the structure of the group of invertible substitutions. Our investigation of the properties of infinite words generated by invertible substitutions will be guided by the study of the factors of the Fibonacci word. Those factors have been studied in relation with mathematics and physics in theories such as number theory, fractal geometry, formal languages, computational complexity, quasicrystals, and so on; see for examples, [10, 82, 232, 340, 384, 449]. Moreover, the properties of the factors of the Fibonacci word have been studied extensively by many authors [65, 130, 233, 295, 384, 385, 452]. We give new properties of the factors of the Fibonacci word based on a new family of factors we call singular words. As we shall see, the most striking of those properties is that two distinct occurrences of a singular word never overlap.

This section is organized as follows. After making preliminary remarks on the Fibonacci word, we introduce the singular words and give elementary properties they satisfy. Then, we establish two decompositions of the Fibonacci word in terms of the singular words (Theorems 9.3.6 and 9.3.8), and describe some of their applications.

Those results (and, in particular, the positively separated property of the singular words) bring us in Sec. 9.3.2 to other combinatorial properties of the Fibonacci infinite word, such as local isomorphism, the overlap properties of the factors and the powers of factors of the Fibonacci word.

9.3.1 Singular words and their properties

As earlier, let $\sigma = (ab, a)$ be the Fibonacci substitution and u_σ denote the Fibonacci infinite word.

Two of the motivations we have are the following.

- The Fibonacci word is closely related to the Fibonacci numbers defined by the recurrence formula $f_{n+2} = f_{n+1} + f_n$, with the initial conditions $f_{-1} = f_0 = 1$, as shown in Chap. 2. Consider the following decomposition of the Fibonacci word

$$\underline{a}\,\underline{b}\,\underline{aa}\,\underline{bab}\,\underline{aabaa}\,\underline{babaabab}\,\underline{aabaababaabaa}\,\underline{babaababaabaababaabab}\cdots$$

  where the n-th block in the decomposition is of length f_n, $n \geq -1$. The question of whether those blocks share special properties naturally comes to mind. As we shall see, Theorem 9.3.6 will answer this question completely.
- As we know, the Fibonacci word is a Sturmian word, hence it has exactly $n+1$ factors of length n. It is also balanced (see Chap. 6), hence, for any n, there exists p such that each factor of length n has p or $p+1$ letters a. As we will see, for $n = f_k$ a Fibonacci number, there are n factors with f_{k-1} a's, all in the same conjugacy class, and one factor (the singular word) with $f_{k-1} \pm 1$ a's, depending on the parity. This only happens for special values of n, and is linked to the continued fraction expansion of the golden number.

We first need to state basic facts about the Fibonacci word, for which the reader is referred to [65, 130, 340, 384]; see also Chap. 6.

Proposition 9.3.1. *Let $F_n = \sigma^n(a)$, then*

1. $\mathbf{l}(F_n) = (f_{n-1}, f_{n-2})$;
2. F_n *is primitive;*
3. $|\sigma^n(a)| = \textit{Card } C(F_n) = f_n$, *that is, all conjugates of the word F_n are distinct. Moreover, $C(F_n) = \{\overline{W};\ W \in C(F_n)\}$.*
4. $F_{n+1} = F_n F_{n-1}$.
5. *For any $k \geq 1$, $\sigma^k(u_\sigma) = u_\sigma$, that is, $u_\sigma = F_k F_{k-1} F_k F_k F_{k-1} \cdots$.*
6. *The word ab is a suffix of F_n for odd positive n, and the word ba is a suffix of F_n for even strictly positive n.*
7. $b^2 \not\prec u_\sigma,\ a^3 \not\prec u_\sigma$.
8. *Any factor of u_σ appears infinitely many times in u_σ.*
9. *$W \prec u_\sigma$ if and only if $\overline{W} \prec u_\sigma$.*

Proof. The first statement is immediate by recurrence, or by computing the powers of the matrix of σ.

The second comes from the fact that consecutive Fibonacci numbers are relatively prime, which allows us to use Lemma 9.1.5; alternatively, one could use the fact that the matrix of σ^n has determinant 1 (the same argument shows that, for any substitution τ such that the associated matrix has determinant 1, $\tau^n(a)$ is primitive).

The third statement is a consequence of Lemma 9.1.4. The rest is easy to check. ■

Remark. No other results than those cited in Proposition 9.3.1 will be used.

A consequence of this proposition is that for any $n \geq 1$, the set $\mathcal{L}_{f_n}$ splits into two parts. The first part coincides with the conjugacy class of the word F_n, and the second part consists solely of some word W_n. We want to describe more precisely W_n.

Assume $\alpha, \beta \in \mathcal{A}_2$. Then $\alpha\beta \triangleright F_n$ implies $\alpha \neq \beta$, by virtue of Proposition 9.3.1.6. An induction using Proposition 9.3.1 proves the following lemma.

Lemma 9.3.2. *Let $n \geq 2$, and assume that $\alpha\beta$ is a suffix of F_n. Then*

$$F_n = F_{n-2} F_{n-1} \alpha^{-1} \beta^{-1} \alpha\beta,$$

Remark. Observe that $F_n = F_{n-1} F_{n-2}$. Using the preceding lemma, we see that the words $F_{n-1}F_{n-2}$ and $F_{n-2}F_{n-1}$ coincide except on the two last letters which are distinct. This remarkable property will be useful when studying the factors of the Fibonacci word.

Definition 9.3.3. *Let $\alpha\beta$ be a suffix of F_n. We denote by W_n the word $\alpha F_n \beta^{-1}$.*

The word W_n is called the n-th singular word *of the Fibonacci word u_σ. For convenience, we define $W_{-2} = \varepsilon$, $W_{-1} = a$ and $W_0 = b$. We denote by $\mathcal{S}$ the set of singular words of u_σ.*

Lemma 9.3.4. *We have:*

1. $W_n \notin C(F_n)$;
2. $\mathcal{L}_{f_n}(F_{n-1}F_n) = \{W_n\} \bigcup \{C_k(F_n);\ 0 \le k \le f_{n-1} - 2\}$. *In particular, as a factor,* W_n *appears only once in* $F_{n-1}F_n$.

Proof. Statement 1. follows from $\alpha \neq \beta$, so that $\mathbf{l}(W_n) \neq \mathbf{l}(F_n)$.

Lemma 9.3.2 implies that $F_{n-1}F_n = F_nF_{n-1}\alpha^{-1}\beta^{-1}\alpha\beta$ when $\alpha\beta \triangleright F_n$. Since $F_{n-1} \triangleleft F_n$, the first f_{n-1} factors of length f_n of the word $F_{n-1}F_n$ are exactly $C_k(F_n)$, $1 \le k \le f_{n-1} - 2$, and the last factor is $F_n = C_0(F_n)$. The $(f_{n-1} - 1)$-th factor is $\alpha F_n \beta^{-1} = W_n$, which ends the proof of 2. ■

We now describe properties of the singular words:

Proposition 9.3.5. *Let* $\{W_n\}_{n\ge -1}$ *be the singular words.*

1. *If* $n \ge 1$, *then*
$$\text{If } n \ge 0, \text{ then } \mathbf{l}(W_n) = \begin{cases} (f_{n-1} + 1, f_{n-2} - 1) & \text{if } n \text{ is odd;} \\ (f_{n-1} - 1, f_{n-2} + 1) & \text{if } n \text{ is even.} \end{cases}$$
2. $W_n \not\prec W_{n+1}$.
3. *If* $\alpha \triangleright W_{n+1}$, *then* $W_{n+2} = W_nW_{n+1}\alpha^{-1}\beta$.
4. $W_n = W_{n-2}W_{n-3}W_{n-2}$, $n \ge 1$.
5. *For* $n \ge 1$,
$$C_{f_{n-1}-1}(F_n) = W_{n-2}W_{n-1},$$
$$C_{f_n-1}(F_n) = W_{n-1}W_{n-2}.$$
In particular,
$$W_{n-2} \prec C_k(F_n) \text{ if and only if } 0 \le k \le f_{n-1} - 1;$$
$$W_{n-1} \prec C_k(F_n) \text{ if and only if } f_{n-1} - 1 \le k \le f_n - 1.$$
6. *For* $n \ge 1$, $W_{2n-1} = aaUaa$, $W_{2n} = bVb$, *where* $U, V \in \mathcal{A}_2^*$.
7. *For* $n \ge 2$, $1 < k < f_n$, *no proper conjugate of* W_n *is a subword of* F_∞.
8. *For* $n \ge 0$, $W_n^2 \not\prec F_\infty$.
9. *For* $n \ge -1$, W_n *is a palindrome.*
10. W_n *is not the product of two palindromes for* $n \ge 2$.
11. *If* $n \ge 2$, *then* W_n *is primitive.*
12. *For* $n \ge 1$, *let* $\alpha_n = a$ *if* n *is odd, and* $\alpha_n = b$ *if* n *is even. we have:*
$$W_n = \alpha_n \left(\prod_{j=-1}^{n-2} W_j \right) = \left(\prod_{j=-1}^{n-2} W_{n-j-3} \right) \alpha_n.$$
13. $W_n \not\prec \prod_{j=-1}^{n-1} W_j$.

14. Let $k \geq -1$ *and* $p \geq 1$*, and let* $U = \prod_{j=k}^{k+p} W_j$*. Then* $U \notin \mathcal{S}$*.*

The proofs are left to the readers as exercises (see also [452]).

The following theorem answers the question raised in the introductory part of this section.

Theorem 9.3.6. *We have* $u_\sigma = \prod_{j=-1}^{\infty} W_j$*.*

Proof. One easily checks that $F_n = abF_0F_1 \cdots F_{n-3}F_{n-2}$. By definition of the singular words W_n, we have $F_k = \alpha^{-1}W_k\beta$. Then by Proposition 9.3.1.4., we get

$$F_n = W_{-1}W_0 \cdots W_{n-2}\gamma_n,$$

where $\gamma_n = a$ if n is even, and b is n is odd. Letting $n \to \infty$ we obtain the conclusion of the theorem. ■

Some additional work [452] is needed to obtain an even more striking decomposition into singular words. In particular, this decomposition shows the non-overlapping property of the singular words and plays an important role in the study of the factors of the Fibonacci word.

Definition 9.3.7. *For every* $n \geq 1$*, we consider the set* $\Sigma_n = \{W_{n-1}, W_{n+1}\}$ *as a new alphabet of two letters, and we define a morphism* $\phi_n : \mathcal{A}_2 \to \Sigma_n$ *by setting* $\phi_n(a) = W_{n+1}, \phi_n(b) = W_{n-1}$*. We call the sequence* $Z = \phi_n(u_\sigma)$ *the* Fibonacci word over Σ_n*.*

By Proposition 9.3.1.6., the word W_n will appear in u_σ infinitely many times. We can now state the main result of this section:

Theorem 9.3.8. *For any* $n \geq 0$*, we have*

$$u_\sigma = \left(\prod_{j=-1}^{n-1} W_j\right) W_nZ_1W_nZ_2 \cdots W_nZ_kW_n \cdots$$

where $Z = Z_1Z_2 \cdots Z_n \cdots$ *is the Fibonacci word over* Σ_n*, and* W_n *has no other occurrences than the occurrences shown in the formula.*

For example, when $n = 2$, $W_2 = bab$ and the decomposition predicted by Theorem 9.3.8 is:

$$abaa(bab)\underline{aabaa}(bab)\underline{aa}(bab)\underline{aabaa}(bab)\underline{aabaa}(bab)\underline{aa}(bab)\underline{aabaa}(bab)\underline{aa}\cdots$$

Definition 9.3.9. *Let $v = v_1 v_2 \cdots v_n \cdots$ be an infinite word over $\mathcal{A}_2$. Let $X = v_k v_{k+1} \cdots v_{k+p}$ and $Y = v_l v_{l+1} \cdots v_{l+m}$ (with $l \geq k$) be two factors of v, then the distance between the occurrences of the factors X and Y is defined by*

$$d(X,Y) = \begin{cases} l-k-p & \text{if } l > k+p; \\ 0 & \text{otherwise.} \end{cases}$$

If $d(X,Y) > 0$, we say that the words X and Y are positively separated.

Let $W = v_k v_{k+1} \cdots v_{k+p}$ $(k, p \geq 1)$ be a factor of v. If there is an integer l, $1 \leq l \leq p$, such that $W = v_{k+l} v_{k+l+1} \cdots v_{k+l+p}$, then we say that W has an overlap over $p-l$ letters.

The following statement can be seen as equivalent to the above definition. Let $U \prec u_\sigma$ be a factor of the Fibonacci word. Then, the word U has an overlap if and only if there exist words X, Y and Z such that $U = XY = YZ$ and such that the word $UZ = XYZ$ is a factor of u_σ.

The next corollaries are consequences of Theorem 9.3.8.

Corollary 9.3.10. *Two adjacent occurrences of a singular word W_n, $n \geq 1$, are positively separated. More precisely, for any n and k, we have*

$$d(W_{n,k}, W_{n,k+1}) \in \{f_{n+1}, f_{n-1}\}.$$

Moreover, at least one of $d(W_{n,k}, W_{n,k+1})$ and $d(W_{n,k+1}, W_{n,k+2})$ is f_{n+1}.

In particular, for $n \geq 1$, W_n has no overlap, and the words of length f_{n-2k} adjacent to the word W_{n+1} on the left and on the right are precisely W_{n-2k}.

Corollary 9.3.11. *Let $U \prec u_\sigma$ and assume $f_n < |U| \leq f_{n+1}$. Let W be a singular word of maximal length contained in U. Then W appears only once in U. Moreover, W must be one of the three following singular words: W_{n-1}, W_n or W_{n+1}.*

9.3.2 Some applications of singular words

The results we will now describe follow from properties of singular words, and more particularly from the fact that two occurrences of a singular word are positively separated. Some of the results we give here are known (Example 1 and Example 3), but the proofs we provide are simpler.

Example 1. Power of factors [65, 233, 295, 384].

Theorem 9.3.12. *We have:*

1. *for any n, $W_n^2 \not\prec u_\sigma$;*
2. *for $0 \leq k \leq f_n - 1$, $\big(C_k(F_n)\big)^2 \prec u_\sigma$;*
3. *if $U \prec u_\sigma$, with $f_{n-1} < |U| < f_n$, then $U^2 \not\prec u_\sigma$;*
4. *if $0 \leq k \leq f_{n-1} - 2$, then $\big(C_k(F_n)\big)^3 \prec u_\sigma$;*
5. *if $f_{n-1} - 2 < k < f_n$, then $\big(C_k(F_n)\big)^3 \not\prec u_\sigma$;*
6. *for any $U \prec u_\sigma$, $U^4 \not\prec u_\sigma$.*

Proof.

1. The statement follows from Proposition 9.3.1.5. and 9.3.5.6.
2. Let $C_k(F_n) = UV$ with $F_n = VU$. Then $U \triangleright F_n$ and $V \triangleleft F_n$. The result follows from $F_n^3 \prec u_\sigma$, since $\big(C_k(F_n)\big)^2 = UVUV = UF_nV \prec (F_n)^3$.
3. Suppose that W_k is the largest singular word contained in U (as in Corollary 9.3.11), and let $U = V_1W_kV_2$. Assume that $U^2 = V_1W_kV_2V_1W_kV_2 \prec u_\sigma$. Then $W_k \not\prec V_2V_1$, otherwise Theorem 9.3.8 implies either that $W_{k+1} \prec V_1$, or $W_{k+1} \prec V_2$, which would contradict the hypothesis on W_k. But then these are consecutive occurrences, of W_k, so by Theorem 9.3.8 again, V_2V_1 must be either W_{k+1} or W_{k-1}. Hence, $U = V_1W_kV_2$ is conjugated to $W_kV_2V_1$, which is equal to W_kW_{k+1} or to W_kW_{k-1}, and by Proposition 9.3.5.5, U is conjugated either to F_{k+2}, or to F_{k+1}. But these two cases are impossible, since they violate the hypothesis made on U.
4. We have $F_nF_nF_{n-1}F_n \prec f_\infty$ since $aaba \prec f_\infty$. Let $\alpha\beta \triangleright F_{n-1}$. Then by Lemma 9.3.2, we have
$$F_n^2F_{n-1}F_n = F_n^2F_{n-1}F_{n-2}F_{n-1}\alpha^{-1}\beta^{-1}\alpha\beta = F_n^3F_{n-1}\alpha^{-1}\beta^{-1}\alpha\beta \prec u_\sigma.$$
Note that $F_{n-1} \triangleleft F_n$. Hence, if $0 \le k \le f_{n-1} - 2$, then
$$\big(C_k(F_n)\big)^3 \prec F_n^3F_{n-1}\alpha^{-1}\beta^{-1} \prec u_\sigma.$$
5. Now suppose that $f_{n-1} - 1 < k < f_n$. Then Proposition 9.3.5.5 implies $W_{n-1} \prec C_k(F_n)$. Let $C_k(F_n) = UW_{n-1}V$, so that $VU = W_{n-2}$. Thus
$$\big(C_k(F_n)\big)^3 = UW_{n-1}W_{n-2}W_{n-1}W_{n-2}W_{n-1}V.$$
Now, if $\big(C_k(F_n)\big)^3 \prec u_\sigma$, then the word $W_{n-1}W_{n-2}W_{n-1} = W_{n+1}$ would overlap itself which is impossible, by Corollary 9.3.11.
6. The statement is proved using an argument similar to that developed in statement 5. ■

Remark. From Theorem 9.3.12.2., we see that any two occurrences of a conjugate of F_n, $n \ge 0$, are not positively separated. This is a major difference between the conjugates of F_n and W_n.

Example 2. Local isomorphism.

Denote by $S^k = S(S^{k-1})$ the kth iteration of the shift S. Properties of the singular words of the Fibonacci word can be used to obtain the following results on the local isomorphism properties of the Fibonacci word.

Theorem 9.3.13. *1. An infinite word u'_σ obtained by changing a finite number of letters in u_σ is not locally isomorphic to u_σ.*

2. Let $U \in \mathcal{A}_2^*$. Then $u_\sigma \simeq Uu_\sigma$ if and only if there exists an integer $m > -1$ such that $U \triangleright W_m\alpha$, with $\alpha = a$ if m is odd, and $\alpha = b$ if m is even.

Proof.

1. Let $u_\sigma = \prod_{j=-1}^{\infty} W_j$ as in Theorem 9.3.6. Because only a finite number of letters are changed in u_σ, we can find an integer m and words $U, V \in \mathcal{A}_2^*$, such that
$$F'_\sigma = UV \prod_{j=m}^{\sigma} W_j,$$
where $|V| = f_{m-1}$, $V \neq W_{m-1}$. Therefore, $VW_m \not\prec u_\sigma$, that is, $u_\sigma \not\simeq F'_\sigma$.
2. From Theorem 9.3.6 and Proposition 9.3.5.12., for any $k > 0$ and $m \geq 0$,
$$\begin{aligned} W_{2m} a u_\sigma &= W_{2m} a \left(\prod_{j=-1}^{2m+2k-1} W_j \right) \left(\prod_{j=2m+2k}^{\infty} W_j \right) \\ &= W_{2m} W_{2m+2k+1} \left(\prod_{j=2m+2k}^{\infty} W_j \right). \end{aligned}$$
Then, $W_{2m} W_{2m+2k+1} \prec u_\sigma$. That is, for any $V \prec W_{2m} a u_\sigma$, we can find an integer k, such that $V \prec W_{2m} W_{2m+2k+1}$, so $V \prec u_\sigma$. The case dealing with $W_{2m+1} b$ can be proved similarly. That is, if $U \triangleright W_m \alpha$ for some m, then $u_\sigma \simeq U u_\sigma$. The case where U is not a right factor of any $W_m \alpha$, follows from an argument similar to that developed in the proof of statement 1. ∎

Example 3. Overlap of the factors of the Fibonacci word.

In this example, we shall determine the factors which have an overlap. First recall the notation we introduced earlier. We say that the word $U \prec u_\sigma$ *has an overlap* if there exist words X, Y and Z such that $U = XY = YZ$ and $XYZ \prec u_\sigma$. Write $\hat{U}(Y) = UZ = XYZ$. We shall say that the word U has an *overlap with overlap factor* Y (or overlap length $|Y|$). The word $\hat{U}(Y)$ is called the *overlap* of U with overlap factor Y. We denote by $\mathcal{O}(u_\sigma) = \mathcal{O}$ the set of factors which have an overlap. Obviously, if $U \in \mathcal{O}$, then
$$|U| + 1 \leq |\hat{U}(Y)| \leq 2|U| - 1, \tag{9.1}$$
where Y is any overlap factor of U.

Lemma 9.3.14. *Let $f_n < |U| \leq f_{n+1}$, and $U \neq W_{n+1}$. Then $U \in \mathcal{O}$ if and only if $W_n \not\prec U$.*

Proof. Let $W_n \prec U$ and write $U = SW_nT$. Note that $W_n \notin \mathcal{O}$, if $U \in \mathcal{O}$. Thus any overlap of U must be of the form SW_nVW_nT. Hence,
$$|SW_nvW_nT| \geq |S| + |T| + 2f_n + f_{n-1} = |U| + f_{n+1} \geq 2|U|,$$
which is in contradiction with (9.1).

Now suppose that $W_n \not\prec U$. We have

- either $U = SF_nT$, where $S, T \neq \varepsilon$, $|S| + |T| \leq f_{n-1}$, $S \triangleright F_n$, $T \triangleleft F_n$;
- or $U \prec F_n^2$.

In the first case, if $|T| = f_n - 1$, then $U = W_{n+1} \notin \mathcal{O}$. Now assume $|T| < f_n - 1$. We can write $F_n = TXS$, because $|S| + |T| \leq f_{n-1}$, with $S \triangleright F_n$, $T \triangleleft F_n$. Since $|T| < f_n - 1$, Theorem 9.3.12.4. implies

$$\left(C_{|T|}(F_n)\right)^3 = (XST)^3 = XSTXSTXST \prec u_\sigma.$$

That is, $U = SF_nT = STXST$ has an overlap with factor ST.

In the second case, observe that $U \prec F_n^2$ and $|U| > f_n$. Writing $U = ST$, with $|T| = f_n$, we get $T = C_k(F_n)$ for some k, and $S \triangleright T$, so $U = SXS$. On the other hand, since $U = SC_k(F_n) \prec F_n^2$, we have $SXSXS = S\left(C_k(F_n)\right)^2 \prec F_n^3 \prec u_\sigma$. That is, $U = SXS$ has an overlap with overlap factor S. ∎

Lemma 9.3.15. *If $U \in \mathcal{O}$, then U has a unique overlap factor.*

Proof. Let $f_n < |U| \leq f_{n+1}$, and let W be a singular word contained in U with maximal length. By Corollary 9.3.16, W is one of W_{n-1}, W_n and W_{n+1}. By virtue of Lemma 9.3.14, W must be W_{n-1} since $U \in \mathcal{O}$. So we can write $U = SW_{n-1}T$. Now suppose that U admits two different overlap factors. Then W_{n-1} will appear three times in one of these two overlap factors. Since $W_{n-1} \notin \mathcal{O}$, this overlap factor must be of the form $SW_{n-1}V_1W_{n-1}V_2W_{n-1}T$. An analogous argument to the one developed in Lemma 9.3.14 brings us to a contradiction with (9.1). ∎

The following corollary is immediate from Lemma 9.3.15 and the proof of Lemma 9.3.14.

Corollary 9.3.16. *Let $U \in \mathcal{O}$ be such that $f_n < |U| \leq f_{n+1}$. Then U can be decomposed under the form $U = VV'V$, the length of $|V|$ being the overlap length.*

The following theorem summarizes the results above.

Theorem 9.3.17. *Let U be a word such that $f_n < |U| \leq f_{n+1}$. Moreover assume that $U \neq W_{n+1}$ and $U \prec u_\sigma$. Then $U \in \mathcal{O}$ if and only if $W_n \not\prec U$. If $U \in \mathcal{O}$, then U has a unique overlap factor V satisfying $U = VV'V$ and $|V| = |U| - f_n$. In particular, $C_k(F_n) \in \mathcal{O}$ if and only if $0 \leq k \leq f_n - 2$.*

Remark. Note that:

1. $f_{n+1} < 2f_n < f_{n+2} < 3f_n < f_{n+3}$;
2. for any k, $W_{n+1} \not\prec \left(C_k(F_n)\right)^2$;
3. for any k, $W_{n+2} \not\prec \left(C_k(F_n)\right)^3$.

The following corollary is an immediate consequence of Theorem 9.3.17.

Corollary 9.3.18. *For any k, $\left(C_k(F_n)\right)^2 \in \mathcal{O}$, $\left(C_k(F_n)\right)^3 \in \mathcal{O}$.*

Remark. If $W^2 \not\prec u_\sigma$ and W has no overlap factor, then two consecutive occurrences of W are positively separated. Moreover, we can give for those words a decomposition similar to the one we gave for singular words.

For example, let $W = abab$, by Theorem 9.3.12.3. and Theorem 9.3.17, $W^2 \not\prec u_\sigma$ and $W \notin \mathcal{O}$, so W is positively separated. The following decomposition illustrates the remark above:

$$aba(abab)\underline{aaba}(abab)\underline{a}(abab)\underline{aaba}(abab)\underline{aaba}(abab)\underline{a}(abab)\underline{aaba}(abab)\cdots$$

We totally order $\mathcal{A}_2$ by setting $a < b$ and we extend this order to the set $\mathcal{A}_2^*$ of all words lexicographically. A *Lyndon word* is a word strictly smaller than its proper right factors. Melançon [287] established the factorization of the Fibonacci word into a nonincreasing product of Lyndon words. He also described the intimate links between the Lyndon factorization and the factorization into singular words, and also gave a self-similarity property of the Lyndon factorization. Those results enabled him to give new proofs for Theorems 9.3.6 and 9.3.8. He also introduced generalizations of singular words to the Sturmian words. Using another approach, Cao and Wen [104] generalized singular words and the corresponding factorizations to general Sturmian words and gave some applications to the studies of the factor properties of Sturmian words.

9.4 Properties of factors of the fixed points of invertible substitutions

In Sec. 9.3 we discussed some factor properties of the Fibonacci word. It is natural to seek for more general invertible substitutions based on the knowledge we developed on the Fibonacci substitution.

We will study some particular invertible substitutions; note that the matrices associated with σ and π generate the set of invertible nonnegative integral matrices, hence, for any invertible substitution, there is a conjugate substitution which is a product of σ and π.

Such a substitution can be written $\tau = \sigma^{n_k}\pi\sigma^{n_{k-1}}\pi\ldots\sigma^{n_2}\pi\sigma^{n_1}$, with $n_1 \geq 0$, $n_k \geq 0$, and $n_i > 0$ for $2 \leq i \leq k-1$. It is easy to check that the word appears in the fixed point u_τ if and only if $n_k > 0$, and that $\tau(b)$ is a prefix of $\tau(a)$ if $n_1 > 0$, $\tau(a)$ is a prefix of $\tau(b)$ if $n_1 = 0$. We see that we can define in this way four classes of substitutions. We will only study the substitutions such that $n_k > 0$, $n_1 > 0$, the other three classes have similar properties.

Definition 9.4.1. *We denote by $\mathcal{G}_\sigma$ the set of invertible substitutions that can be written as a product $\sigma^{n_k}\pi\sigma^{n_{k-1}}\pi\ldots\sigma^{n_2}\pi\sigma^{n_1}$, with $n_i > 0$ for $1 \leq i \leq k$.*

Section 9.4.1 is concerned with elementary factor properties for the fixed word of a substitution in $\mathcal{G}_\sigma$. Section 9.4.2 defines singular words for general invertible substitutions, and give some applications. These words are defined by using a substitution in $\mathcal{G}_\sigma$; however, as we will see, they have intrinsic properties which allow to define them just by considering the language associated with an invertible substitution.

9.4.1 Elementary properties of factors

Lemma 9.4.2. *Let τ be an invertible substitution. For all $\alpha \in \mathcal{A}_2$, the word $\tau(\alpha)$ is primitive.*

Proof. Suppose that $\tau(\alpha)$ is not primitive. Then there exist a word $W \in \mathcal{A}_2^*$ and an integer $p \geq 2$, such that $\tau(\alpha) = W^p$. Hence $\mathbf{l}(\tau(\alpha))) = (p|W|_a, p|W|_b)$. Thus $\det M_\tau$ will be divisible by p, which is in contradiction with the fact $\det M_\tau = \pm 1$. ■

We remark that, for any $\tau \in \mathcal{G}_\sigma$, we have $\tau(b) \triangleleft \tau(a)$. We remark also that, if $|\tau(b)| > 1$, the last two letters of $\tau(b)$ are distinct, and if we denote them by $\beta\alpha$, the last two letters of $\tau(a)$ are $\alpha\beta$; the proof is easy by induction.

We are now going to establish an important factorization of $\tau \in \mathcal{G}_\sigma$ which will be used in the sequel. We can write $\tau(a) = \tau(b)U^*$, by virtue of the remark. Let $U \triangleleft \tau(a)$ with $|U| = |U^*|$. We can also write $\tau(a) = UV$ with $|V| = |\tau(b)|$.

Lemma 9.4.3. *Let $\tau \in \mathcal{G}_\sigma$ with $|\tau(b)| \geq 2$ and let $\tau(a) = \tau(b)U^* = UV$ as above. If $\alpha\beta \triangleright \tau(a)$, then*

1. *$U = U^*$;*
2. *$\tau(b)\alpha^{-1}\beta^{-1} = V\beta^{-1}\alpha^{-1}$;*
3. *$\tau(a) = \tau(b)U = U\tau(b)\alpha^{-1}\beta^{-1}\alpha\beta$.*

Proof. Since $\alpha\beta \triangleright \tau(a)$, we have $\beta\alpha \triangleright \tau(b)$.

We prove the lemma by induction with respect to the length of τ in terms of $\mathcal{A}_\sigma := \{\sigma, \pi\}$.

1. The inequality $|\tau(b)| \geq 2$ holds only if τ has length at least 2; if this length is 2, then $\tau = \sigma^2$. In this case, $\tau(a) = \sigma^2(a) = aba = \tau(b)a$, $U^* = U = a$, and the statement is true.
   Suppose that for $\tau = \tau_n \cdots \tau_1$, we have
   $$\tau_n \cdots \tau_1(a) = \tau_n \cdots \tau_1(b)U_n^* = U_n V_n, \tag{9.2}$$
   with $U_n^* = U_n$ (so $|V_n| = |\tau_n \cdots \tau_1(b)|$).
   Let $\tau = \tau_{n+1}\tau_n \cdots \tau_1$. Write
   $$\tau(a) = \tau_{n+1}\tau_n \cdots \tau_1(a) = \tau_{n+1}\tau_n \cdots \tau_1(b)U_{n+1}^* = U_{n+1}V_{n+1},$$

with $|U^*_{n+1}| = |U_{n+1}|$. We will prove that $U^*_{n+1} = U_{n+1}$.
If $\tau_{n+1} = \pi$, the proof is trivial. Suppose now that $\tau_{n+1} = \sigma$. By virtue of (9.2), we have:

$$\sigma(\tau_n \cdots \tau_1(a)) = \sigma(U_n V_n) = \sigma(U_n)\sigma(V_n) = \sigma(\tau_n \cdots \tau_1(b))\sigma(U^*_n).$$

Thus $U^*_{n+1} = \sigma(U^*_n)$, $U_{n+1} = \sigma(U_n)$. So we get $U^*_{n+1} = U_{n+1}$, since $U^*_n = U_n$ by induction.

2. The case of $|\tau(b)| = 2$ can be checked directly. Let $\tau = \tau_n \cdots \tau_1$, then by statement 1. we have

$$\tau_{n+1}\tau_n \cdots \tau_1(a) = \tau_{n+1}\tau_n \cdots \tau_1(b)U_{n+1} = U_{n+1}V_{n+1}.$$

Let $\alpha\beta \triangleright \tau_n \cdots \tau_1(a)$ and suppose that $V_n\beta^{-1}\alpha^{-1} = \tau_n \cdots \tau_1(b)\alpha^{-1}\beta^{-1}$. We shall prove

$$V_{n+1}\alpha^{-1}\beta^{-1} = \tau_{n+1}\tau_n \cdots \tau_1(b)\beta^{-1}\alpha^{-1}.$$

As in the proof of statement 1., it suffices to consider $\tau_{n+1} = \sigma$. Since $\alpha\beta \triangleright \tau_{n+1}\tau_n \cdots \tau_1(b)$, $\beta\alpha \triangleright \sigma(V_{n+1})$, we have

$$\begin{aligned} V_{n+1} = \sigma(V_n) &= \sigma(\tau_n \cdots \tau_1(b)\alpha^{-1}\beta^{-1}\alpha\beta) \\ &= \sigma(\tau_n \cdots \tau_1(b))(\sigma(\beta\alpha))^{-1}\sigma(\alpha\beta). \end{aligned}$$

Notice that $\sigma(\alpha\beta) = a\beta\alpha$ for any $\alpha \neq \beta$, and therefore we obtain

$$V_{n+1}\alpha^{-1}\beta^{-1} = \tau_{n+1}\tau_n \cdots \tau_1(b)\beta^{-1}\alpha^{-1}.$$

3. The conclusion follows immediately from statements 1. and 2. ■

Lemma 9.4.4. *Let $W \in \mathcal{P}$, then $\sigma(W)a$, $a^{-1}\sigma(W) \in \mathcal{P}$.*

Proof. Since $W \in \mathcal{P}$, we can write W in the following form:

$$a^{k_1}b^{l_1}a^{k_2}b^{l_2} \cdots a^{k_m}\zeta a^{k_m} \cdots b^{l_2}a^{k_2}b^{l_1}a^{k_1},$$

where $\zeta \in \{a, b, \varepsilon\}$, $k_j, l_j = 1$, if $2 \leq j \leq m-1$, and $k_1, k_m = 0$.
Thus we have

$$\begin{aligned} \sigma(W)a &= (ab)^{k_1}a^{l_1} \cdots (ab)^{k_m}\sigma(\zeta)(ab)^{k_m} \cdots a^{l_2}(ab)^{k_2}a^{l_1}(ab)^{k_1}a \\ &= (ab)^{k_1}a^{l_1} \cdots (ab)^{k_m}\sigma(\zeta)a(ba)^{k_m} \cdots a^{l_2}(ba)^{k_2}a^{l_1}(ba)^{k_1}. \end{aligned}$$

Since $\sigma(\zeta)a$ is equal to a, aba, aa respectively according to ζ being ε, a, b, $\sigma(W)a$ is a palindrome with center a, b, ε respectively by the formula above. ■

Corollary 9.4.5. *Let $\zeta \in \mathcal{A}_2$. Suppose that $\tau \in \mathcal{G}_\sigma$ with $\beta \triangleright \tau(\zeta)$, then $\alpha\tau(\zeta)\beta^{-1} \in \mathcal{P}$.*

In particular, if $|\tau(\zeta)| \geq 3$, and $\alpha\beta \triangleright \tau(\zeta)$, then $\tau(\zeta)\beta^{-1}\alpha^{-1} \in \mathcal{P}$.

Proof. Let $\tau = \tau_n\tau_{n-1}\cdots\tau_1$.

We prove this corollary by induction as in Lemma 9.4.3. We only prove the case $\zeta = a$, the case of $\zeta = b$ can be proved in a similar way.

The case of $n = 1$ is evident.

Now suppose that $\beta \triangleright \tau_n\tau_{n-1}\cdots\tau_1(a)$ and $\alpha\tau_n\tau_{n-1}\cdots\tau_1(a)\beta^{-1} \in \mathcal{P}$.

If $\tau_{n+1} = \pi$, notice that the word $\pi(\tau_n\tau_{n-1}\cdots\tau_1(a))$ is obtained by exchanging the letters a and b in the word $\tau_n\tau_{n-1}\cdots\tau_1(a)$. So by the induction hypothesis, we get $\beta\pi(\tau_n\tau_{n-1}\cdots\tau_1(a))\alpha^{-1} \in \mathcal{P}$.

Now suppose that $\tau_{n+1} = \sigma$. Notice that $\alpha \triangleright \sigma\tau_n\tau_{n-1}\cdots\tau_1(a)$. Thus

$$\begin{aligned}\beta\sigma\tau_n\tau_{n-1}\cdots\tau_1(a)\alpha^{-1} &= \beta\sigma(\alpha^{-1}\alpha\tau_n\tau_{n-1}\cdots\tau_1(a)\beta^{-1}\beta)\alpha^{-1}\\ &= \beta\sigma(\alpha^{-1})\sigma(\alpha\tau_n\tau_{n-1}\cdots\tau_1(a)\beta^{-1})\sigma(\beta)\alpha^{-1}.\end{aligned}$$

By the induction hypothesis, $\alpha\tau_n\tau_{n-1}\cdots\tau_1(a)\beta^{-1} \in \mathcal{P}$. On the other hand, by a simple calculation, we have either $\beta\sigma(\alpha^{-1}) = a^{-1}$, $\sigma(\beta)\alpha^{-1} = \varepsilon$, or $\beta\sigma(\alpha^{-1}) = \varepsilon$, $\sigma(\beta)\alpha^{-1} = a$. Hence by Lemma 9.4.4, we get

$$\beta\sigma\tau_n\tau_{n-1}\cdots\tau_1(a)\alpha^{-1} \in \mathcal{P}.$$

■

Let $\tau(a) = \tau(b)U$ be the factorization of Lemma 9.4.3. Let $\tau = \sigma^{n_k}\pi\cdots\sigma^{n_2}\pi\sigma^{n_1}$, then $U = \sigma^{n_k}\pi\cdots\sigma^{n_2}\pi\sigma^{n_1-1}(b)$. Thus by Lemma 9.4.3 and Corollary 9.4.5, we get:

Corollary 9.4.6. *Let $\tau \in \mathcal{G}_\sigma$ and let $\alpha\beta \triangleright \tau(a)$.*

1. *If $|\tau(b)| = 1$, then $\tau(a) = a^n b$ for some n, i.e., $\tau(a)$ is the product of palindromes a^n and b;*
2. *If $|\tau(b)| = 2$, then $\tau(a)$ is a palindrome;*
3. *If $|\tau(b)| > 2$, then $\tau(a)$ is the product of palindromes $\tau(b)\alpha^{-1}\beta^{-1}$ and $\beta\alpha u$.*

Lemma 9.4.7. *Suppose that $W \in \mathcal{A}_2^*$ is a primitive word and suppose that $W = U_1U_2$ is a product of two palindromes U_1 and U_2.*

1. *If $|U_1|, |U_2| \in 2\mathbb{N}+1$, then for any k, $C_k(W) \notin \mathcal{P}$.*
2. *If $|U_1|, U_2| \in 2\mathbb{N}$, then $C_{|U_1|/2}(W) \in \mathcal{P}$, $C_{|U_1|+|U_2|/2}(W) \in \mathcal{P}$. For other k, $C_k(W) \notin \mathcal{P}$;*
3. *If $|U_1| \in 2\mathbb{N}$, $|U_2| \in 2\mathbb{N}+1$ (or $|U_1| \in 2\mathbb{N}+1$, $|U_2| \in 2\mathbb{N}$), then $C_{|U_1|/2}(W) \in \mathcal{P}$ (or $C_{|U_1|+|U_2|/2}(W) \in \mathcal{P}$). For other k, $C_k(W) \notin \mathcal{P}$.*

Proof. We only prove statement 1., the other cases can be discussed in the same way.

Notice that at least one of $|U_1|$, $|U_2|$ is larger than 2 (otherwise U_1, U_2 will be a^2 or b^2). Suppose that without loosing generality $|U_1| = 3$. Then we can write $U_1 = xU_1'x$, where $x \in \mathcal{A}_2$, $U_1' \in \mathcal{P}$. Thus $C_1(W) = C_1(U_1U_2) = (U_1')(xU_2x)$ is a product of two palindromes, and $C_1(U_1U_2) \notin \mathcal{P}$. Since $|U_1'|, |xU_2x| \in 2\mathbb{N}+1$ and $U_1', xU_2x \in \mathcal{P}$, we can repeat the discussion above which follows the proof. ■

Lemma 9.4.8. *Let $\tau \in \mathcal{G}_\sigma$. Suppose that $|\tau(a)| \in 2\mathbb{N}$. If $\tau(a) = U_1U_2$ is a product of two palindromes, then $|U_1|, |U_2| \in 2\mathbb{N}+1$.*

Proof. If $|U_1|, |U_2| \in 2\mathbb{N}$, then $|U_1|_a + |U_1|_b$, $|U_2|_a + |U_2|_b \in 2\mathbb{N}$. Thus both components of $\mathbf{l}(\tau(a))$ are even which follows that $|\det M_\tau| \in 2\mathbb{N}$. But we know that $\det M_\tau$ must be ± 1. ∎

From Corollary 9.4.6, Lemma 9.4.7, Lemma 9.4.8 and Propositions 9, 10, 11 of [131], we obtain

Proposition 9.4.9. *Let $\tau \in \mathcal{G}_\sigma$.*

1. *Any conjugate of $\tau(a)$ is primitive.*
2. *$|C(\tau(a))| = |\tau(a)|$. That is, all conjugates of $\tau(a)$ are distinct.*
3. *Any conjugation of $\tau(a)$ (containing $\tau(a)$ itself) is either a palindrome, or a product of two palindromes. In the later case, the factorization is unique.*
4. *$C(\tau(a)) = \overline{C(\tau(a))}$, where $\overline{C(\tau(a))} = \{\overline{W};\ W \in C(\tau(a))\}$.*
5. *If $|\tau(a)| \in 2\mathbb{N}$, there is no palindrome in $C(\tau(a))$; if $|\tau(a)| \in 2\mathbb{N}+1$, there is only one palindrome in $C(\tau(a))$.*

9.4.2 Decomposition into singular words and its application

Similarly as in the case of the Fibonacci infinite word, we will introduce singular words for the invertible substitutions in $\mathcal{G}_\sigma$ and study their properties.

Let $\tau \in \mathcal{G}_\sigma$ and let $u_\tau = \tau(u_\tau) = w_1w_2 \cdots w_k \cdots$ be the fixed point of τ. Then for any $n \in \mathbb{N}$, we have

$$u_\tau = \tau^n(u_\tau) = \tau^n(w_1)\tau^n(w_2)\cdots\tau^n(w_k)\ldots \tag{9.3}$$

We now discuss the properties of the factors of the infinite word u_τ.

Definition 9.4.10. *We denote $\tau^n(a)$ by A_n, and $\tau^n(b)$ by B_n.*

Notice that if $\tau \in \mathcal{G}_\sigma$, then for any $n \geq 2$, $\tau^n \in \mathcal{G}_\sigma$. Therefore the conclusions about τ which we have obtained above hold also for τ^n. In particular, A_n and B_n are primitive. We also remark that A_n and B_n always have a different final letter.

Lemma 9.4.11. *Any factor of length $|A_n|$ of u_τ is contained either in A_nA_n or B_nA_n.*

Proof. Let W be a factor of u_τ of length $|A_n|$. Since the decomposition of τ in product of σ, π begins with σ (from the definition of $\mathcal{G}_\sigma$, we have $n_k > 0$) it follows that the fixed point contains only isolated occurrences of b, hence it has a canonical decomposition in A_n and B_n where no two consecutive B_n occur. Hence W will be contained in one of the following four words: A_nA_n, A_nB_n, B_nA_n, $A_nB_nA_n$. We have $B_n \triangleleft A_n$, so $A_nB_n \prec A_nA_n$.

Let $W \prec A_n B_n A_n$, write $W = W_1 B_n W_2$. Then $W_1 \rhd A_n, W_2 \lhd A_n$. Let $A_n = B_n U_n$ be the factorization as in Lemma 9.4.3. Then $U_n \lhd A_n$ by Lemma 9.4.3.3. Since $|W| = |A_n| = |B_n| + |U_n|$, $|W_2| < |U_n|$. Consequently $W_2 \lhd U_n$, and hence $W = W_1 B_n W_2 \prec A_n B_n U_n = A_n A_n$. ∎

We are going to study the two cases.

Lemma 9.4.12. *Let $W \prec A_n A_n$ with $|W| = |A_n|$, then $W \in C(A_n)$.*

Proof. Since $W \prec A_n A_n$, and $|W| = |A_n|$, we can write $W = UV$ with $U \rhd A_n, V \lhd A_n$, and $|U| + |V| = |A_n|$, which follows that $A_n = VU$. That is, $W = C_{|V|}(A_n)$. ∎

Since all conjugates of A_n are distinct by Primitivity of A_n, we get

Corollary 9.4.13. *The set of the factors of length $|A_n|$ of A_n^k, $k = 2$ is exactly $C(A_n)$.*

Now we study the factors of the word $B_n A_n$. For this aim, we introduce *singular words* of u_τ as follows:

Definition 9.4.14. *The n-th singular words of u_τ with respect to a or b are defined respectively as:*

$$W_{n,a} = \beta A_n \alpha^{-1}, \quad W_{n,b} = \alpha B_n \beta^{-1},$$

where α (respectively β) is the last letter of A_n (respectively B_n).

From the definition of the singular words, we get immediately:

Lemma 9.4.15. *With the notation above, we have*

$$\begin{pmatrix} \mathbf{l}(W_{n,a}) \\ \mathbf{l}(W_{n,b}) \end{pmatrix} = \begin{cases} \begin{pmatrix} |A_n|_a - 1 & |A_n|_b + 1 \\ |B_n|_a + 1 & |B_n|_b - 1 \end{pmatrix} & \text{if } \alpha = a; \\ \begin{pmatrix} |A_n|_a + 1 & |A_n|_b - 1 \\ |B_n|_a - 1 & |B_n|_b + 1 \end{pmatrix} & \text{if } \alpha = b. \end{cases}$$

Hence the abelianizations of $W_{n,a}$ and A_n differ, and we get:

Corollary 9.4.16. $\forall n \in \mathbb{N}$, $W_{n,a} \notin C(A_n)$, $W_{n,b} \notin C(B_n)$.

Let $\alpha\beta \rhd A_n$ (so $\beta\alpha \rhd B_n$). By Lemma 9.4.3,

$$B_n A_n = B_n u_n B_n \alpha^{-1} \beta^{-1} \alpha\beta = A_n B_n \alpha^{-1} \beta^{-1} \alpha\beta.$$

Since $A_n B_n \alpha^{-1} \beta^{-1} \prec A_n B_n \prec A_n A_n$, we see that the first $|B_n| - 2$ factors of length $|A_n|$ of $B_n A_n$ are those of $A_n A_n$ which are distinct from each other by Corollary 9.4.13, and the $(|B_n| - 1)$-th factor is exactly $W_{n,a}$ which is not in $C(A_n)$ by Corollary 9.4.16. We get from the analysis above

Lemma 9.4.17. *Let $W \prec B_nA_n$ with $|W| = |A_n|$. Then W is either in $C(A_n)$ or equal to $W_{n,a}$. In particular, as a factor, $W_{n,a}$ appears only once in B_nA_n.*

Since we know that the fixed point is Sturmian, we deduce that $|\mathcal{L}_{|A_n|}| = |A_n| + 1$, and from the previous lemma we obtain:

Proposition 9.4.18. *Let $\tau \in \mathcal{G}$, $n \in \mathbb{N}$. Then $\mathcal{L}_{|A_n|} = C(A_n(a)) \bigcup \{W_{n,a}\}$, $\mathcal{L}_{|B_n|} = C(B_n(b)) \bigcup \{W_{n,b}\}$.*

We now discuss the properties of the singular words. The above proposition can be rephrased: since the fixed word is Sturmian, it is balanced. Hence, words of the same length as $\tau(a)$ can only have the same number of a as $\tau(a)$, or one more or less a. We have shown that all words of same length as $\tau(a)$, except one, the singular word, have same number of a as $\tau(a)$. We will see that this difference appears in a very conspicuous way: either $W_{n,a}$ has b as initial and final letter, or $a^{p(\tau)+1}$ as initial and final prefix, where $p(\tau)$ is the minimum of the number of a's that separate two occurrences of b. ($p(\tau)$ can also be defined in the following way: let $(\sigma\pi)^k$ the highest power of $\sigma\pi$ that occurs as prefix in the decomposition of τ in the generators σ, π; then $p(\tau) = k + 1$.

Proposition 9.4.19. *$\forall n, m \in \mathbb{N}$, $W_{n,a}, W_{n,b}$ and $\beta A_n^m B_n \alpha^{-1} \in \mathcal{P}$.*

Proof. The fact that $W_{n,a}, W_{n,b} \in \mathcal{P}$ follows immediately from the definition of the singular words and Proposition 9.4.5.

Let $A_n = B_nU_n$ be the factorization as in Lemma 9.4.3, then for any $m \geq 1$,

$$\beta A_n^m B_n \alpha^{-1} = ((\beta B_n \alpha^{-1})(\alpha U_n \beta^{-1}))^m (\beta B_n \alpha^{-1}),$$

by Corollary 9.4.6, $\beta B_n \alpha^{-1}, \alpha u_n \beta^{-1} \in \mathcal{P}$. Thus $\beta A_n^m B_n \alpha^{-1} \in \mathcal{P}$. ■

Lemma 9.4.20. *$W_{n,a} \triangleright W_{n+2,a}$, $W_{n,b} \triangleright W_{n+2,b}$.*

Proof. Let $\alpha\beta \triangleright \tau^n(a)$, then $\alpha\beta \triangleright \tau^{n+2}(a)$, thus

$$W_{n+2,a} = \alpha\tau^{n+2}(a)\beta^{-1} = \alpha\tau^n(\tau^2(a))\beta^{-1}.$$

We have $a \triangleleft \tau^2(a)$, so $\tau^2(a) = ua$ for some $u \in \mathcal{A}_2$. Thus $W_{n+2,a} = \alpha\tau^n(u)\tau^n(a)\beta^{-1}$ which yields the conclusion of the lemma. ■

Lemma 9.4.21. *Either $a^{p(\tau)+1} \triangleright W_{n,a}$, $a^{p(\tau)+1} \triangleleft W_{n,a}$, or $b \triangleright W_{n,a}$, $b \triangleleft W_{n,a}$.*

Proof. This follows from Proposition 9.4.18 and the definition of $W_{n,a}$. ■

Proposition 9.4.22. *$\forall n \in \mathbb{N}$, if $W_{n,a}$ is not a power of a, then $W_{n,a}$ is primitive.*

Proof. Suppose that $W_{n,a}$ is not a power of a. If $W_{n,a} = w^p$ for some $w \in \mathcal{A}_2^*$ and $p \geq 2$, then $W_{n,a}$ will be equal to one of its conjugates. But we will then have either $b^2 \prec u_\tau$ or $a^{2p(\tau)+2} \prec u_\tau$. This is impossible. ∎

Let $u_\infty = w_1 \cdots w_n \cdots$ be an infinite word over $\mathcal{A}_2$. Let $W \prec u_\infty$ be a word which appears infinitely many times in u_∞. If any two adjacent $W's$ (i.e., two successive occurrences) appearing in u_∞ are separated by a factor of u_∞ (this assertion is equivalent to $\nexists U \prec u_\infty$ such that $U = XYZ$ with $W = XY = YZ$), we say that the word W possesses the *positive separation property*, and the factor is called a *separate factor* (with respect to W). If any separate factor is not equal to ε, we say that W is *strongly separated* (otherwise, we say that W is *weakly separated*).

Definition 9.4.23. *A word $W \in \mathcal{A}_2^*$ of the form $W = (UV)^k U$, where $k > 0$, UV is a primitive word, is called a* sesquipower. *The positive integer k is said to be the* order *of the sesquipower. A sesquipower of order larger than 1 is called a* strong sesquipower.

From Lemma 9.4.12, Lemma 9.4.17, and the definition of $W_{n,a}$, we obtain the following

Theorem 9.4.24. *Let $\tau \in \mathcal{G}_\sigma$ and let $\alpha\beta \triangleright A_n$. For $n \geq 1$, we have*

$$u_\tau = W_0 W_{n,a} z_1^{(n)} W_{n,a} z_2^{(n)} \cdots z_k^{(n)} W_{n,a} z_{k+1}^{(n)} \cdots,$$

where $W_0 = A_n^{p(\tau)} B_n \alpha^{-1}$, $\forall i$, $z_i^{(n)} \in \{\beta A_n^{p(\tau)-1} B_n \alpha^{-1}, \beta A_n^{p(\tau)} B_n \alpha^{-1}\}$. We call the above decomposition of u_τ the $n-$decomposition of u_τ,

Denote by $u_\tau(z^{(n)})$ the infinite word $z_1^{(n)} z_2^{(n)} \ldots z_k^{(n)} \ldots$.

From the discussions above and Proposition 9.4.19, we obtain

Theorem 9.4.25. *Let $\tau \in \mathcal{G}_\sigma$, then for any n,*

1. *$W_{n,a}$ is strongly separated.*
2. *The separate factor is either $\beta A_n^{p(\tau)-1} B_n \alpha^{-1}$, or $\beta A_n^{p(\tau)} B_n \alpha^{-1}$.*
3. *The separate factors are sesquipower palindromes of order $p(\tau)$ and $p(\tau)-1$ respectively.*

Example 9.4.26. Let $\tau = (\sigma\pi)^{n-1}\sigma$, then

$$\tau = (a^n b, a), \quad p(\tau) = n.$$

Consider $1-$decomposition of u_τ, we have

$$ab \triangleright A_1^n = (a^n b)^n, \quad W_0 = (A_1)^n B_1 a^{-1} = (a^n b)^n, \quad W_{1,a} = a(a^n b) b^{-1} = a^{n+1}.$$

Put

$$A = b A_1^n B_1 a^{-1} = b(a^n b)^n a a^{-1} = b(a^n b)^{n-1}, \quad B = b(a^n b)^n.$$

When $n = 1$, $\tau = \sigma$, then $\forall m \in \mathbb{N}$, $u_\sigma(z^{(m)}) = u_\sigma$ over $\{A, B\}$;
When $n = 2$, $\tau = \sigma\pi\sigma$, then

$$u_{\sigma\pi\sigma}(z^{(1)}) = ABABAABABAABABABAABABAABABABAABA\ldots$$

We see that $u_{\sigma\pi\sigma}(z) \neq u_{\sigma\pi\sigma}$ over $\{A, B\}$. A calculation on computer shows that

$$u_{\sigma\pi\sigma}(z^{(1)}) = u_\tau = u_\tau(z^{(1)})$$

where $\tau = (ab, aba) = \sigma\sigma\pi$. ■

As said in the introduction, the motivation of this section is to generalize the properties of the factors of the Fibonacci word to the case of all invertible substitutions. By comparing with the results of Sec. 9.3, we see that one main difference is the structure of the singular words and the singular decomposition of the infinite word according to the singular words. In fact, the structure of the singular words of a general invertible substitution is much more complicated than that of the Fibonacci substitution: for example, all singular words and separate words of the Fibonacci word are sesquipowers of order 1, i.e, weak sesquipowers; on the other hand, those of a general invertible substitution are strong sesquipowers. But we have seen that the singular words still play an important role in the studies of the factors, such as power of factors, overlap of factors and local isomorphism. On the other hand, singular words and their applications can be generalized to the case of Sturmian words [104].

Remark. By introducing *patterns* in high dimensional space (see for example [24, 327]), we can generalize the definition of local isomorphism to the colored lattice, that are applicable in the studies of quasicrystals [459]. But it is a difficult problem to characterize local isomorphism for the general case. In fact, in Theorem 9.2.4, we only deal with the invertible substitutions over the alphabet of two letters. We do not know any results for the general substitutions (which are non-invertible) over $\mathcal{A}_2$. For the alphabet over more than two letters, the question is still open even for invertible substitutions.