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DIZERTAČNÍ PRÁCE

Beta-celá čísla a kvazikrystaly
(Beta-integers and Quasicrystals)

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Beta-integers and Quasicrystals

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Preface

This thesis has been prepared within the scope of a joint research program "Co-tutelle Internationale de Thèse" between two universities: Czech Technical University in Prague and University Paris Diderot - Paris 7. In order to acquit a claim of "Co-tutelle" Agreement, the abstract is written in English and in French.

Abstract

The set of β-integers $\mathbb{Z}_\beta$ is a generalization of the set $\mathbb{Z}$ of ordinary integers. $\mathbb{Z}_\beta$ consists of real numbers which are polynomial in β when expanded in the base β using the well-known greedy algorithm. As every suitable generalization, β-integers coincide with integers for β being an integer base. Nevertheless, the situation changes significantly if $\beta \notin \mathbb{Z}$. In this case, the set $\mathbb{Z}_\beta$ is not periodic any more and it conserves only partially properties of integers: $\mathbb{Z}_\beta$ has no accumulation points, the distances between consecutive elements of $\mathbb{Z}_\beta$ are bounded by 1, $\mathbb{Z}_\beta$ is self-similar with self-similarity factor β, and is not invariant under translation.

There are several fields of application of this interesting alternative of ordinary integers: modeling of quasicrystals, random number generators, non-standard wavelet analysis, or theory of discrete Schrödinger operators with aperiodic potentials.

The content of this work may be divided into three essential parts:

1. Combinatorics on words with emphasis on infinite words coding β-integers
2. Arithmetics of β-integers
3. Application of β-integers in physics

Let us point out several contributions based on results of this thesis that have been published or submitted to referred journals during the last three years:

(I) Ľ. B., *Complexity for infinite words associated with quadratic non-simple Parry numbers*, Journal of Geometry and Symmetry in Physics **7** (2006), 1–11

(II) Ľ. B., Z. Masáková, *Palindromic complexity of infinite words associated with non-simple Parry numbers*, to appear in RAIRO - Theor. Inform. Appl. (2008)

(III) Ľ. B., E. Pelantová, W. Steiner, *Sequences with constant number of return words*, to appear in Monatshefte für Mathematik (2007)

(IV) Ľ. B., *Return words and recurrence function of a class of infinite words*, Acta Polytechnica **47** (2007), 15–19

(V) Ľ. B., E. Pelantová, *A note on symmetries in the Rauzy graph and factor frequencies*, submitted to Theoret. Comput. Sci. (2007)

(VI) Ľ. B., E. Pelantová, O. Turek, *Combinatorial and arithmetical properties of infinite words associated with quadratic non-simple Parry numbers*, RAIRO - Theor. Inform. Appl. **41** (2007), 123–136

(VII) Ľ. B., J.-P. Gazeau, E. Pelantová, *Asymptotic behavior of beta-integers*, submitted to Letters in Mathematical Physics (2008)

In the sequel, we give some primary ideas of the content and the structure of the thesis and underline the most important results. If the results have been published, we refer to the corresponding paper in the above list.

A brief history of quasicrystals and their most common mathematical models are described in the introductory chapter 1. We introduce ibidem numeration systems with non-integer bases together with a few words on positional numeration systems in general. Finally, the role of β-integers as one-dimensional models of quasicrystals and as coordinate labels of β-lattices (more dimensional models of quasicrystals) is highlighted.

Chapter 2 is preliminary and includes all underlying definitions from the field of β-numeration and from combinatorics on words. Particularly important is the coding of non-negative β-integers, realizing only a finite number of distances between consecutive elements, with letters. Such numbers β are called Parry numbers and the associated infinite word is denoted u_β. Results concerning combinatorics on words u_β may be then reformulated in terms of β-integers: the number of local configurations of $\mathbb{Z}_\beta$ is described by means of the factor complexity of u_β, the number of mirror symmetrical local configurations is linked with the palindromic complexity of u_β, the densities of local configurations in the whole one-dimensional space are related to the factor frequencies of u_β, etc.

Chapter 3 deals with factor complexity which indicates how many different factors of a fixed length an infinite word contains. We provide a summary of known results on the complexity of some selected infinite words and classes of words – Thue-Morse word, period doubling word, Rote word, a palindromeless reversal closed word, infinite words associated with simple and non-simple Parry numbers – with an eye illustrating the characteristics and methods studied in the sequel on this "sample". **As a new result, we describe the factor complexity of u_β associated with a quadratic non-simple Parry number (I).**

In Chapter 4, we deal with another type of complexity – palindromic complexity – which describes how rich an infinite word is in palindromes of a fixed length. We recall the palindromic complexity of words in our illustrative sample. **Newly, we deduce an exact formula for the palindromic complexity of u_β associated with a quadratic non-simple Parry number (II).**

In Chapter 5, we reopen the investigation of palindromes. An interesting task is to compare two measures of the variety of palindromes in an infinite word: palindromic complexity – we call the words with maximal palindromic complexity *opulent in palindromes* – and the degree of saturation of the prefixes of an infinite word by palindromes – we say that an infinite word is *full* if all its prefixes contain the maximal possible number of palindromes. It is a recent result [25] that these two notions – opulent and full – coincide for uniformly recurrent infinite words. **We derive a new elegant and short proof of a slightly stronger result – the equivalence of fullness and opulence for infinite words with language closed under reversal.**

In Chapter 6, we study return words in infinite words – a return word of a factor is any word we read between two consecutive occurrences of the factor in the corresponding infinite word.

The study of return words is initiated by **the description of some simple ideas facilitating the task**. As a practical application of these useful rules, **we determine the return words of factors of several infinite words** in our illustrative sample. Furthermore, **an insight into the characterization of infinite words with a constant number of return words for every factor is offered (III).** The last topic linked with return words is the study of recurrence function which to every n associates the minimal length $R(n)$, provided it exists, such that every segment of length $R(n)$ of the infinite word in question contains all factors of length n. **We derive the recurrence function of u_β associated with a quadratic non-simple Parry number (IV).**

Chapter 7 is devoted to the study of factor frequencies. It demonstrates the visualizing power of Rauzy graphs. With the help of Rauzy graphs, **we deduce for infinite words whose language is closed under reversal, or, eventually, under another symmetry, a suitable upper bound in terms of factor complexity on the number of factor frequencies (V)**. We manifest the accuracy of the obtained upper bound on several classes of infinite words. Furthermore, we suggest a method, based on a meticulous inspection of the evolution of Rauzy graphs, enabling to describe the set of factor frequencies for every fixed length. This method provides explicit descriptions while so far known methods lead only to recurrent formulae. As an illustration, **we derive the factor frequencies of u_β associated with a quadratic non-simple Parry number and of the palindromeless reversal closed word**.

In Chapter 8, an almost untutored topic of balances is inspected. An infinite word over the alphabet $\{a, b\}$ is called c-balanced if for any couple of its factors of the same length, the number of a's contained in these factors differs at most by c. **We find the optimal balance bound on u_β associated with a quadratic non-simple Parry number (VI).**

Chapter 9 is a smooth passage from combinatorics on words to arithmetics. The chapter pursues two goals. First, **we determine the maximal number $L_\oplus(\beta)$ of β-fractional positions, in case of β being a quadratic non-simple Parry number**, which may arise as a result of addition of two β-integers, provided the β-expansion of the sum is finite. Second, we point out to which extent arithmetics can serve combinatorics and vice versa. In particular, **we stress the closeness of the balance property and the upper and lower bounds on $L_\oplus(\beta)$ for u_β associated with a quadratic non-simple Parry number (VI)**.

Chapter 10 offers also a smooth transition, this time from mathematics to physics. In view of the quasiperiodic distribution of β-integers on the real line, it is natural to investigate how much the set $\mathbb{Z}_\beta = \{b_n \mid n \in \mathbb{Z}\}$ differs from the set $\mathbb{Z}$ of ordinary integers, according to the nature of β. Parry numbers give rise to β-integers which realize only a finite number of distances between consecutive elements and so appear as the most comparable to ordinary integers. **We find a simple formula for the constant c_β such that $b_n \sim c_\beta n$ in case of Parry numbers β. In addition, we prove for a class of Pisot numbers that the sequence $(b_n - c_\beta n)$ is bounded (VII).**

Chapter 11 is devoted to Schrödinger operators with aperiodic potentials. We sum up the needed notions from functional analysis in Appendix A. We recall an extensively studied concept – discrete Schrödinger operators with potentials modeled by infinite aperiodic words. Putting together several methods relying on combinatorial properties, we deduce for which Parry numbers β, the corresponding Schrödinger operator with potential generated by u_β has purely singular continuous spectrum. In such cases, the infinite word u_β is a suitable model of the potential in a quasicrystalline material.

In Chapter 12, we focus on diffraction on quasicrystals. We summarize the necessary mathematical background in Appendix B. We ask the following question: "For which β does the set $\mathbb{Z}_\beta$ serve as a suitable one-dimensional model for quasicrystals?" Combining results from divers papers, we answer this question partially and we indicate how the results from Chapter 10 concerning asymptotic behavior might be used in order to describe diffraction spectra of $\mathbb{Z}_\beta$.

Résumé

L'ensemble de β-entiers $\mathbb{Z}_\beta$ représente une généralisation de l'ensemble des entiers ordinaires. $\mathbb{Z}_\beta$ consiste des nombres réels dont le développement en base β, obtenu par l'algorithme glouton, est un polŷnome en β, autrement dit, la partie fractionnaire du développement en base β est nulle. Comme toute généralisation appropriée, les β-entiers coïncident avec les entiers pour une base β entière. Par contre, la situation change considérablement si $\beta \notin \mathbb{Z}$. Dans ce cas, l'ensemble $\mathbb{Z}_\beta$ n'est plus périodique et ne garde les propriétés des entiers que partiellement: $\mathbb{Z}_\beta$ ne contient pas de points d'accumulation, les distances entre les éléments consécutifs de $\mathbb{Z}_\beta$ sont bornées par 1, $\mathbb{Z}_\beta$ est autosimilaire – β étant un facteur d'autosimilarité – $\mathbb{Z}_\beta$ n'est pas invariant sous la translation.

Il y a plusieurs domaines d'application de cette alternative aux entiers ordinaires: modélisation mathématique des quasicristaux, générateurs de nombres aléatoires, analyse en ondelettes nonstandard ou théorie des opérateurs de Schrödinger discrets avec potentiels apériodiques.

Le contenu de ce travail peut être divisé en trois parties essentielles:

1. Combinatoire des mots infinis associés aux β-entiers
2. Arithmétique des β-entiers
3. Application des β-entiers en physique

Soulignons les contributions basées sur les résultats de cette thèse qui ont été publiées ou soumises aux journaux avec arbitrage durant les trois dernières années:

(I) Ľ. B., *Complexity for infinite words associated with quadratic non-simple Parry numbers*, Journal of Geometry and Symmetry in Physics **7** (2006), 1–11

(II) Ľ. B., Z. Masáková, *Palindromic complexity of infinite words associated with non-simple Parry numbers*, à paraître dans RAIRO Theor. Inform. Appl. (2008)

(III) Ľ. B., E. Pelantová, W. Steiner, *Sequences with constant number of return words*, à paraître dans Monatshefte für Mathematik (2007)

(IV) Ľ. B., *Return words and recurrence function of a class of infinite words*, Acta Polytechnica **47** (2007), 15–19

(V) Ľ. B., E. Pelantová, *A note on symmetries in the Rauzy graph and factor frequencies*, soumis à Theoret. Comput. Sci. (2007)

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(VII) Ľ. B., J.-P. Gazeau, E. Pelantová, *Asymptotic behavior of beta-integers*, soumis à Letters in Mathematical Physics (2008)

Dans ce qui suit, nous esquissons le contenu et la structure de la thèse et nous soulignons les résultats les plus importants. Dans le cas des résultats déjà publiés, le numéro de l'article correspondant dans la liste ci-dessus est rappelé.

L'histoire des quasicristaux en abrégé et leur modèles mathématiques les plus employés sont décrits dans le premier chapitre. Les systèmes de numération aux bases non-entières sont alors introduits. Finalement, le rôle des β-entiers comme modèles des quasicristaux unidimensionnels de même que comme coordonnées de modèles multidimensionnels – β-réseaux – est mis en évidence.

Le chapitre 2 est préliminaire et inclut toutes les définitions fondamentales concernant les domaines de β-numération et de combinatoire des mots infinis. D'une importance particulière est le codage par lettres des β-entiers non-négatifs qui ne possèdent qu'un nombre fini de distances entre leurs éléments consécutifs. Un tel nombre β est appelé nombre de Parry et les mots infinis associés aux nombres de Parry sont notés u_β. Les résultats concernant la combinatoire des mots u_β peuvent être reformulés en termes de β-entiers: le nombre de configurations locales de $\mathbb{Z}_\beta$ est décrit par l'intermédiare de la complexité de u_β, le nombre de configurations locales stables sous la symétrie miroir est lié à la complexité palindromique de u_β, les densités de configurations locales dans l'espace total sont en relation avec les fréquences des facteurs de u_β.

Le chapitre 3 concerne la complexité des facteurs d'un mot infini qui indique le nombre de facteurs de chaque longueur contenus dans le mot infini en question. Nous fournissons un sommaire de résultats sur la complexité de certains mots infinis et de certaines classes de mots infinis – le mot de Thue-Morse, le mot associé à la suite dite doublement de période, le mot de Rote, un mot pauvre en palindromes stable sous la symétrie miroir, les mots infinis associés aux nombres de Parry simples et non-simples. Cet échantillon nous servira dans les chapitres suivants d'illustration des propriétés étudiées. **Un nouveau résultat est la dérivation de la complexité du mot u_β associé aux nombres de Parry quadratiques non-simples (I).**

Dans le chapitre 4, nous traitons un autre type de complexité – la complexité palindromique – qui décrit combien un mot infini est riche en palindromes de chaque longueur. Nous rappelons la complexité palindromique des mots de notre échantillon illustratif. **Nous déduisons une nouvelle formule explicite de la complexité palindromique du mot u_β associé aux nombres de Parry quadratiques non-simples (II).**

Dans le chapitre 5, nous retournons à l'étude des palindromes. Une tâche intéressante est de comparer deux mesures de variété de palindromes dans un mot infini: la complexité palindromique – les mots dont la complexité palindromique est maximale sont appelés *opulents en palindromes* – et le degré de saturation de préfixes d'un mot infini en palindromes – un mot infini est dit *plein* si tous ses préfixes contiennent le nombre maximal de palindromes. Un résultat récent [25] établit que les deux notions – opulent en palindromes et plein – coïncident pour les mots infinis uniformément récurrents. **Nous présentons une nouvelle démonstration, courte et élégante, d'un résultat légèrement plus puissant – l'équivalence entre plénitude et opulence pour les mots infinis dont le langage est stable sous la symétrie miroir.**

Le chapitre 6 est consacré à l'étude des mots de retour dans les mots infinis – un mot de retour d'un facteur est chaque mot lu entre des occurrences consécutives de ce facteur dans le mot infini en question. L'étude des mots de retour est entamée par **une description de**

quelques idées simples qui facilitent la tâche. Comme application pratique de ces règles utiles, **nous déterminons les mots de retour de facteur de quelques mots infinis** dans notre échantillon illustratif. On donne ensuite **la caractérisation des mots infinis ayant un nombre constant de mots de retour de chaque facteur (III).** Le dernier sujet lié aux mots de retour est l'étude de la fonction de récurrence qui associe à chaque n la longueur minimale $R(n)$, à condition qu'elle existe, telle que chaque segment de longueur $R(n)$ du mot infini en question contient tous les facteurs de longueur n. **Nous dérivons la fonction de récurrence du mot u_β associé aux nombres de Parry quadratiques non-simples (IV).**

Le chapitre 7 se concentre sur les fréquences des facteurs d'un mot infini. Il illustre la puissance de visualisation offerte par les graphes de Rauzy. A l'aide des graphes de Rauzy, **nous obtenons pour les mots infinis dont le langage est stable sous la symétrie miroir, ou, eventuellement, sous une autre symétrie, une borne optimale pour le nombre de fréquences des facteurs en termes de la complexité des facteurs. (V)**. Nous montrons la précision de cette borne sur plusieurs classes de mots infinis. De plus, nous proposons une méthode basée sur un examen attentif de l'évolution des graphes de Rauzy qui permet de décrire l'ensemble des fréquences des facteurs pour chaque longueur. Cette méthode fournit une description explicite tandis que les méthodes précédentes ne donnent que des formules récurrentes. Comme illustration, **nous dérivons les fréquences des facteurs du mot u_β associé aux nombres de Parry quadratiques non-simples et du mot pauvre en palindromes stable sous la symétrie miroir**.

Dans le chapitre 8, nous examinons la notion presque inexplorée d'équilibre. Un mot infini sur l'alphabet $\{a, b\}$ est appelé c-équilibré si, pour chaque paire de ses facteurs de même longueur, le nombre de lettres a contenus dans ces facteurs diffère au plus de c. **Nous trouvons la borne optimale à c telle que le mot u_β associé aux nombres de Parry quadratiques non-simples (VI) est c-équilibré.**

Le chapitre 9 est un passage en douceur entre la combinatoire des mots infinis et l'arithmétique. Le chapitre poursuit deux buts. Premièrement, **nous déterminons le nombre maximal $L_\oplus(\beta)$ de positions β-fractionnaires, dans la cas où β est un nombre de Parry quadratique non-simple**, qui peut apparaître à la suite de l'addition de deux β-entiers, à condition que la β-expansion de la somme soit finie. Deuxièmement, nous soulignons comment l'arithmétique peut servir à la combinatoire et vice versa. Particulièrement, **nous mettons en évidence la proximité de l'équilibre et des bornes supérieure et inférieure de $L_\oplus(\beta)$ pour le mot u_β associé aux nombres de Parry quadratiques non-simples (VI)**.

Le chapitre 10 offre aussi une transition en douceur, cette fois entre les mathématiques et la physique. En vue de la distribution quasipériodique des β-entiers sur la droite réelle, il est naturel de chercher jusqu'à quel point les ensembles $\mathbb{Z}_\beta = \{b_n \mid n \in \mathbb{Z}\}$ et $\mathbb{Z}$ se ressemblent, par rapport à la nature de β. Les nombre de Parry produisent des β-entiers qui ne possèdent qu'un nombre fini de distances entre les éléments consecutifs et alors apparaîssent comme les plus comparables aux entiers. **Nous déduisons une formule simple pour la constante c_β telle que $b_n \sim c_\beta n$ dans le cas d'un nombre de Parry β. De plus, nous montrons pour une classe de nombres de Pisot que la séquence $(b_n - c_\beta n)$ est bornée (VII).**

Le chapitre 11 est dédié aux opérateurs de Schrödinger avec potentiels apériodiques. Les notions nécessaires de l'analyse fonctionnelle sont récapitulées dans l'appendice A. Nous rappelons un concept extensivement étudié – les opérateurs de Schrödinger discrets avec potentiels provenant des mots apériodiques. Combinant plusieurs méthodes fondées sur les propriétés combinatoires, nous caractérisons les nombres de Parry β pour lesquels l'opérateur de Schrödinger dont le potentiel est généré par u_β a un spectre purement singulier continu. Dans de tels cas, le mot infini u_β sert de modèle convenable pour le potentiel dans un matériau quasicristallin.

Dans le chapitre 12, nous étudions la diffraction sur les quasicristaux. La base mathématique est résumée dans l'appendice B. Nous posons la question suivante: "Pour quels β l'ensemble $\mathbb{Z}_\beta$, sert-il de modèle unidimensionnel convenable pour les quasicristaux?" Reliant les résultats de divers articles, nous répondons à cette question partiellement. Finalement, nous indiqueons comment les résultats du chapitre 10 concernant le comportement asymptotique peuvent aider à décrire le spectrum de diffraction de $\mathbb{Z}_\beta$.

Contents

Chapter 1

Introduction

1.1 Quasicrystals – a surprise for crystallographers

Crystals have been admired for their perfect geometrical forms for ages. The observed regular external form made the 19th century savants postulate a regular internal structure generated by a simple repetition of a single motive. Crystals, or ordered solids, were then understood as being periodic arrangements of atoms. In the language of mathematics, an *ideal crystal* is defined as a finite union of translated copies of the same lattice. Given an arbitrary basis $(x_1, x_2, ..., x_d)$ in $\mathbb{R}^d$, the set $L \subset \mathbb{R}^d$ of all integer combinations of the given system, i.e., defined by

$$L = \Big\{ \sum_{i=1}^{d} a_i x_i \;\Big|\; a_i \in \mathbb{Z} \;\; \text{for all} \;\; i \in \{1, 2, ..., d\} \Big\},$$

is called a *lattice* in $\mathbb{R}^d$ with *basis* $(x_1, x_2, ..., x_d)$. Besides translational symmetry, another observed remarkable property of crystals is their rotational symmetry. However, lattice theory implies that any periodic planar (2-dimensional) or space (3-dimensional) structure admits neither rotational symmetries of order greater than 6 nor 5-fold rotational symmetry.

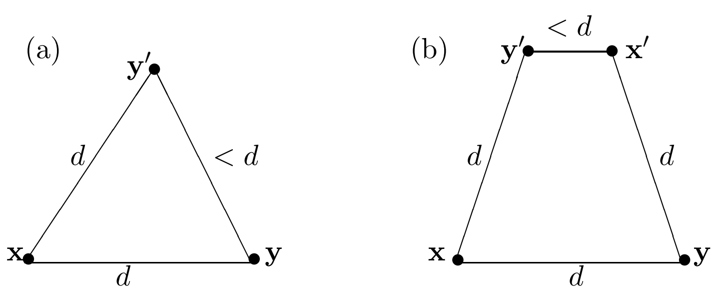


Fig. 1.1: (a) The rotation angle cannot be less than $\pi/3$. (b) The rotation angle cannot be $2\pi/5$.

Let us assume that there exists a planar set that is equal to a finite union of translated copies of the same lattice and that is invariant under N-fold rotation. There is obviously a minimal distance between its points – rotation centers. Let x and y be rotation centers such that their distance is minimal, say $d = |x - y|$. The counterclockwise rotation through $2\pi/N$ radians about x carries y to another rotation center y' so that $|y - y'| \geq d$. This is possible only if $N \leq 6$. (See Figure 1.1 (a).) If $N = 5$, then $|y - y'| > d$, but another problem arises. Since y is also a rotation center, the clockwise rotation about this point must carry x to another rotation center x'. But $|x' - y'| < d$. (See Figure 1.1 (b).) The same argument is valid in 3-dimensional space since every rotation is a rotation of a plane about an orthogonal axis.

As a by-product of the previous explication, we conclude that any uniformly discrete planar set cannot have more than one center of N-fold rotational symmetry with $N = 5$ or $N > 6$.

Systematic studies on crystalline materials started at the beginning of the 19th century and achieved classification of crystals into 32 symmetry classes with respect to external symmetries (Hessel, 1830), 14 fundamental space lattices (Bravais, 1850), and 230 space groups – symmetrical possibilities of point configurations in the space so that their neighborhoods are identical (Fedorov, Schoenflies, 1891). A new experimental tool – X-rays – provided by Röntgen in 1895, together with the discovery of diffraction of X-rays by crystals due to an experiment by von Laue in 1912, caused a breakthrough in the study of crystals and gave birth to solid state physics. Until the 80's, crystallographers believed that translational symmetry (periodic internal configuration) is a synonym of a diffraction image consisting of sharp bright spots, also called *Bragg peaks*.

In 1984, crystallographers were stunned by the discovery of "a metallic phase with long-range orientational order and no translational symmetry" announced by Shechtman *et al.* [102], where *long-range orientational order* is such an order of an atomic configuration that produces a diffraction image consisting of Bragg peaks. The material in question was an alloy of aluminium and manganese, produced from a melt by a rapid cooling technique. Its diffraction image was characterized by

- a diffraction pattern like a dense constellation of more-or-less bright Bragg peaks, which is an indication of long-range orientational order,
- a spatial organization of Bragg peaks obeying 5- or 10-fold rotational symmetries, at least locally, which indicates a sort of icosahedral organization in real space with an axis of 5-fold rotational symmetry (incompatible with periodicity!),
- a spatial organization of Bragg peaks obeying specific scale invariance, more precisely, self-similar with a factor equal to some power of the so-called *golden mean* or *golden ratio* τ which is the larger root of the equation $x^2 - x - 1 = 0$, i.e., $\tau = \frac{1+\sqrt{2}}{5}$, and is manifestly consistent with 5-fold and 10-fold rotational symmetry since $\tau = 2\cos\frac{2\pi}{10}$.

In other words, Shechtman's discovery shows that periodicity is not synonymous with long-range order. This phenomenon was soon reproduced in many laboratories and it became clear that aperiodic crystals are not rare, but, on the contrary, widespread.

Such materials were baptized *quasicrystals*. Since a meaningful definition of a crystal should comprise quasicrystals as a particular case, the definition based on periodicity was not any longer sufficient. The International Union of Crystallography adopted in 1992 the following definition of a crystal. A *crystal* is any structure possessing long-range order, i.e., whose atomic configuration produces a diffraction image consisting of Bragg peaks. Up to now, there is no generally accepted definition of a crystal, respectively a quasicrystal, which would satisfy a mathematician. For a nice review on the history of crystallography consult Senechal [101].

1.2 Mathematical models of quasicrystals

The only broadly acknowledged concept of a set modeling atomic positions in any matter is a *Delone set*. A set $\Lambda \subset \mathbb{R}^d$ is called *Delone* if it satisfies two conditions:

Uniform discreteness

There exists $r > 0$ such that $|x - y| > r$ for any $x, y \in \Lambda$, $x \neq y$. This condition assures that Λ has no accumulation points.

Relative density

There exists $R > 0$ such that any ball $B(x, R)$ of radius R centered at the point x fulfils $B(x, R) \cap \Lambda \neq \emptyset$ for any $x \in \mathbb{R}^d$. This condition means that Λ does not contain unbounded gaps.

Delone sets may serve as models for a broad range of structures, from highly amorphous to highly symmetrical. Consequently, additional conditions are imposed on the Delone sets intended for modeling crystals. Thanks to the simplicity of its definition and the richness of structures it provides, *Meyer set* introduced by Meyer in [87] is a natural concept of crystalline models. It imposes geometrical restrictions on interatomic positions. We say that a Delone set $\Lambda \subset \mathbb{R}^d$ is *Meyer* if there exists a finite set $F \subset \mathbb{R}^d$ such that

$$\Lambda - \Lambda \subset \Lambda + F.$$

Lagarias in [75] proved that a Meyer set Λ can be equivalently defined as a Delone set satisfying that the set of all relative positions of its points, i.e., $\Lambda - \Lambda$, is also a Delone set. It is readily seen that any lattice L in $\mathbb{R}^d$ is a Meyer set since $L - L \subset L$. An ideal crystal Λ is likewise a Meyer set since if $\Lambda = L + S$, where S is a finite set of translations, then $\Lambda - \Lambda \subset \Lambda - S$. In other words, a Meyer set is a generalization of an ideal crystal.

Let us mention other physically reasonable conditions usually required from a Delone set Λ modeling a crystal.

Finite local complexity

It follows from a minimum energy argument that the number of various neighborhoods of points (atoms) in a Delone set must be finite. This requirement is formalized in the notion of *finite local complexity*: For every fixed radius r, the number of configurations of points from Λ contained in any ball of radius r is finite, i.e., $\#(\Lambda - \Lambda) \cap B(0, r) < \infty$. Remark that as an immediate consequence of the definition, every Meyer set has finite local complexity.

Repetitivity

Another logic requirement on the model of a crystal is that every configuration of points repeats in the modeling set infinitely many times. It refers to *repetitivity*: Every finite configuration of points in Λ occurs in Λ infinitely many times, and, moreover, points of occurrences of this configuration form themselves a Delone set.

Self-similarity

A set Λ is *self-similar* if $\beta\Lambda \subset \Lambda$ for some scaling factor $\beta \in \mathbb{R}$. Lattices are self-similar for every integer scaling factor. All up to now observed quasicrystals have been self-similar for an irrational scaling factor. More precisely, the involved irrationals related to the so-far observed crystallographically forbidden rotational symmetries are the following cyclotomic algebraic integers:

- $\tau = \frac{1+\sqrt{5}}{2} = 2\cos\frac{2\pi}{10}$, $\tau^2 = \frac{3+\sqrt{5}}{2} = 1 + 2\cos\frac{2\pi}{10}$ (5- and 10-fold rotational symmetry),
- $1 + \sqrt{2} = 2\cos\frac{2\pi}{8}$ (8-fold rotational symmetry),

- $2 + \sqrt{3} = 2\cos\frac{2\pi}{12}$ (12-fold rotational symmetry).

All these self-similarity factors are unitary Pisot numbers, i.e., algebraic integers larger than 1 all of whose conjugates are in modulus less than 1.

If a Meyer set is self-similar, then every its self-similarity factor must be a Pisot or a Salem number [75] (an algebraic integer > 1 all of whose conjugates are in modulus ≤ 1 and at least one of them has modulus equal to 1).

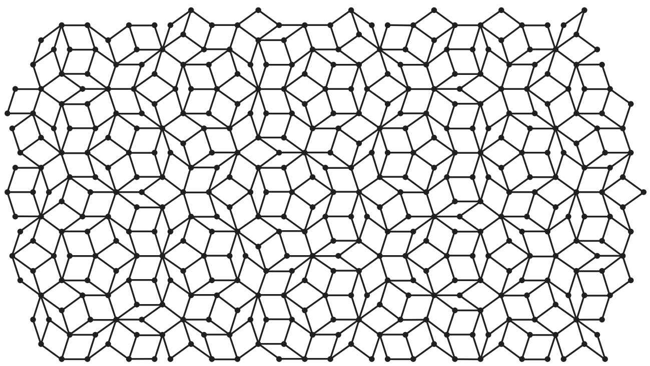


Fig. 1.2: Illustration of Penrose tiling.

The first model of quasicrystals – Penrose tiling – was known already a decade before the discovery of quasicrystals. It is an aperiodic tiling – filing without gaps and overlaps the whole plane – whose vertices form a repetitive Meyer set with patterns of any size obeying 10-fold rotational symmetry and whose diffraction image is made of Bragg peaks and exhibits global 10-fold rotational symmetry. In its simplest form, as illustrated in Figure 1.2, it consists of 36- and 72-degree rhombi, say A and B, with "matching rules" forcing the rhombi to line up against each other only in certain patterns. Penrose tiling is closely related to the golden mean τ. Not only τ^2 is its self-similarity factor, but τ also equals to the ratio of the area of B to the area of A and to the ratio of their frequencies of occurrences.

1.3 Cut-and-project sets

A rich class of Meyer sets can be obtained by the so-called *cut-and-project method*. Roughly speaking, one projects points of a higher dimensional lattice to a lower dimensional subspace and then chooses projections which have their projection to the complementary subspace in a given bounded region. The obtained set is called *cut-and-project set*; it was originally introduced by Meyer [88] under the name *model set*.

Before providing a general definition, let us mention a one-dimensional example of a cut-and-project set which is usually presented as a toy geometrical model of quasicrystals, introduced by Levine and Steinhardt in [82]. Consider a semi-open stripe $\mathcal{B}$ obtained by translating the unit square through the square lattice $\mathbb{Z}^2$ along the straight line V_1 of slope $\frac{1}{\tau}$. V_1 is referred to as the *physical* space. Then project on V_1, along a straight line V_2 perpendicular to V_1, the lattice points lying in $\mathcal{B}$. Note that the latter points belong to a unique path made of horizontal segments (their projection is denoted by A and its length is $\frac{\tau}{\sqrt{\tau^2+1}}$) and vertical segments (their projection is denoted by B and its length is $\frac{1}{\sqrt{\tau^2+1}}$). The resulting both-sided sequence of points lying in V_1 form a *Fibonacci cut-and-project set*, which is made of the projected paths and reads:

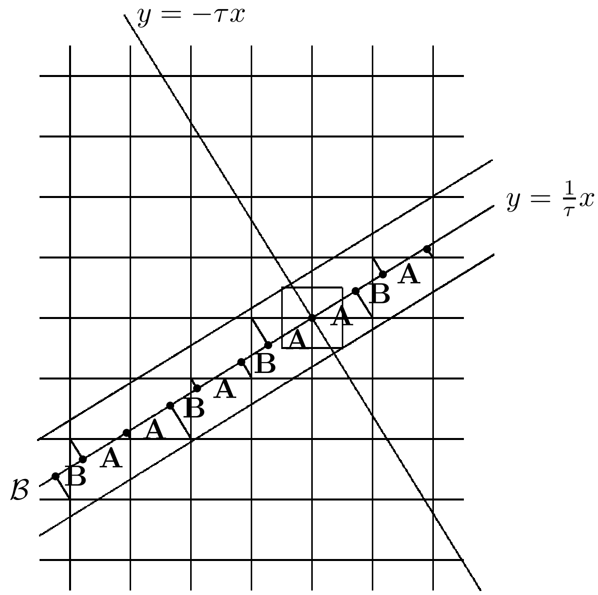


Fig. 1.3: Construction of a Fibonacci C&P set.

$\dots BAABABAABA\dots$. Note that a short link B is never adjacent to another B whereas two adjacent long links A can occur. V_2 is called the *internal* space, and $\mathcal{B} \cap V_2$ is the *acceptance window* or the *atomic surface*. The construction is illustrated in Figure 1.3.

The same Fibonacci cut-and-project set may be obtained through a purely algebraic procedure. Let us first consider the so-called extension ring of the algebraic integer τ

$$\mathbb{Z}[\tau] = \{m + n\tau \mid m, n \in \mathbb{Z}\} = \mathbb{Z} + \mathbb{Z}\tau.$$

$\mathbb{Z}[\tau]$ can be obtained as the projection onto V_1 along V_2 of the whole square lattice $\mathbb{Z}^2$, provided the set of projected points is multiplied by the scaling factor $\sqrt{\tau^2+1}$. There exists in this type of a ring an algebraic conjugation, called *Galois automorphism*, and defined by

$$x = m + n\tau \to x' = m + n\tau',$$

where $\tau' = \frac{-1}{\tau} = \frac{1-\sqrt{5}}{2}$ is the other root of the golden mean equation $x^2 - x - 1 = 0$. Then define the point set $\Sigma(\Omega)$ using an internal sieving rule in the ring $\mathbb{Z}[\tau]$ itself

$$\Sigma(\Omega) = \{m + n\tau \in \mathbb{Z}[\tau] \mid x' = m - n\tfrac{1}{\tau} \in \Omega\}.$$

The Fibonacci cut-and-project set constructed previously is precisely the set $\Sigma(\Omega)$ with $\Omega = [-\tau, 0)$ rescaled by $\frac{1}{\sqrt{1+\tau^2}}$.

Let us provide the promised more general definition of a *cut-and-project set*. Let V_1, V_2 be proper subspaces of $\mathbb{R}^d$ such that $V_1 \oplus V_2 = \mathbb{R}^d$. Let $\pi_1 : \mathbb{R}^d \to V_1$ be the projector onto V_1 along V_2 and $\pi_2 : \mathbb{R}^d \to V_2$ the projector onto V_2 along V_1. Keeping this notation, we have the following definitions.

A *cut-and-project scheme* is a triplet (V_1, V_2, L), where L is a lattice in $\mathbb{R}^d$ and L is required to be in a general position; that is, the restriction π_1 to L is an injection and $\pi_2(L)$ is dense in V_2. The situation is depicted below.

$$\begin{tikzcd} V_1 & \mathbb{R}^d \arrow[l, "\pi_1"'] \arrow[r, "\pi_2"] & V_2 \\ & \cup & \\ & L & \end{tikzcd}$$

Let (V_1, V_2, L) be a cut-and-project scheme and let $\Omega \subset V_2$ such that Ω is bounded, $\Omega^\circ \neq \emptyset$, and $\overline{\Omega^\circ} = \overline{\Omega}$. Then the set

$$\Sigma(\Omega) := \{\pi_1(x) \mid x \in L,\ \pi_2(x) \in \Omega\}$$

is called a *cut-and-project set* (in the sequel referred to as C&P set) with the *acceptance window* Ω. The space V_1 is usually called the *physical space* and V_2 the *internal space*.

Cut-and-project sets are aperiodic Meyer sets, and, under an additional condition that the boundary of the acceptance window has an empty intersection with $\pi_2(L)$, the set $\Sigma(\Omega)$ is repetitive. In addition, if Λ is a Meyer set, then there exist a C&P set $\Sigma(\Omega)$ and a finite set F such that $\Lambda \subset \Sigma(\Omega) + F$ (proved by Lagarias in [76]).

A nice example of a C&P scheme providing a rich class of C&P sets with 5-fold rotational symmetry has been introduced by Moody and Patera in [89]. The lattice L, known under the notation A_4, is a subset of $\mathbb{R}^4$ (it is known that 4 is the minimal dimension of a space containing a lattice with 5-fold rotational symmetry). The orientation of the basis lattice vectors is characterized by the so-called *coxeter graph*, plotted below.

$$A_4 \equiv \quad \begin{tikzcd} \alpha_1 \arrow[r, dash] & \alpha_2 \arrow[r, dash] & \alpha_3 \arrow[r, dash] & \alpha_4 \end{tikzcd}$$

If the vertices α_i and α_j are connected with an edge, then the 4-dimensional vectors α_i and α_j form an angle of $\pi/3$, otherwise, they are orthogonal. Both the physical space V_1 and the internal space V_2 are 2-dimensional and they are chosen so that the C&P set has 10-fold rotational symmetry if and only if the acceptance window Ω exhibits 10-fold rotational symmetry. In Figure 1.4, the corresponding C&P set for a circular window Ω is illustrated.

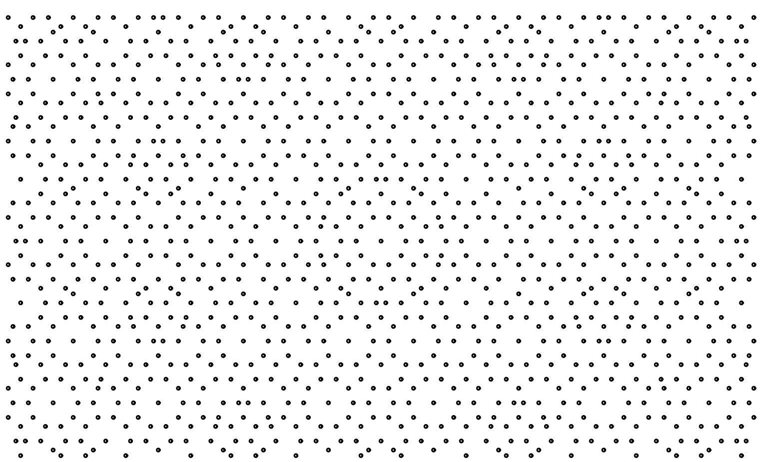


Fig. 1.4: A planar C&P set with 10-fold rotational symmetry.

De Bruijn proved that Penrose tilings may be obtained as two-dimensional projections from a five-dimensional cubic lattice.

Hereafter, we restrict ourselves to one-dimensional models of quasicrystals. It is evidently pointless to speak about rotational symmetries - that led to the discovery of quasicrystals - on one-dimensional structures. Nevertheless, every C&P set is a union of one-dimensional C&P sets. In fact, every straight line containing at least two points of a higher-dimensional C&P set contains infinitely many of them, and they form a one-dimensional C&P set. This fact justifies the importance of one-dimensional models.

Self-similarity is well understood for one-dimensional C&P sets. A one-dimensional C&P sequence $\Sigma_{\epsilon,\eta}(\Omega) = \{m + n\eta \in \mathbb{Z}[\eta] \mid x' = m + n\epsilon \in \Omega\}$ is self-similar if and only if ϵ is a quadratic algebraic number, η is its conjugate, and the closure $\overline{\Omega}$ of Ω contains the origin; moreover, if β is a self-similar factor of $\Sigma_{\epsilon,\epsilon'}(\Omega)$, then β is a quadratic Pisot number in $\mathbb{Q}[\epsilon]$, as shown by Gazeau, Masáková, and Pelantová in [61].

Moreover, one-dimensional C&P sets have only two or three distinct distances between neighboring points. Thus, if we associate with different distances different letters, we obtain an aperiodic both-sided infinite word over a 2- or 3-letter alphabet. The infinite word matching with the Fibonacci C&P sequence is illustrated in Figure 1.3, provided the letter A is identified with the distance $A = \frac{\tau}{\sqrt{1+\tau^2}}$ and the letter B with the distance $B = \frac{1}{\sqrt{1+\tau^2}}$.

A great number of properties of one-dimensional C&P sets depend only on the associated infinite word, say u, and not on the distances between neighbors – the number of local configurations of atoms is described by the factor complexity of u, the number of mirror symmetrical local configurations is linked with the palindromic complexity of u, the repetitions of local configurations are in relation with the return words of factors of u, an equable distribution of atoms is pertinent to the balance property of u, or the densities of local configurations in the whole one-dimensional space are related to the factor frequencies in u. In addition, under some very general condition [61], an infinite both-sided word corresponding to a self-similar C&P set may be easily generated, namely it is a fixed point of a nontrivial morphism, or it is a letter-to-letter image of such a fixed point. Hence, combinatorics on words deepens the insight into one-dimensional aperiodic structures.

1.4 Beta-integers and beta-lattices

In this thesis, as the title prompts, the main focus is consecrated to β-integers, another one-dimensional structure modeling, under certain additional conditions, quasicrystals. Let us briefly explain where this interesting structure comes from.

The need of an efficient manipulation of real numbers in computers has incited an extensive study of various numeration systems. Roughly speaking, *numeration systems* are algorithmic ways of coding numbers, usually with a finite number of symbols. In the particular case of *positional numeration systems*, numbers are represented by means of an ordered set of symbols where the value of a symbol depends on its position.

Preponderant positional numeration systems are those ones with an integer base $q > 1$. Provided no representation ends in $(q-1)^\omega$, every non-negative real number x can be uniquely expressed in such a system as

$$x = \sum_{i=-\infty}^{k} a_i q^i \quad \text{with } a_i \in \{0, 1, \ldots, q-1\}.$$

The principle role in our every-day life plays the decimal numeration system (base 10), the historical reason being obvious – we have 10 fingers. Computers are based on the binary numeration system (base 2), and the way we measure time and angles is probably a reminder of the Babylonian sexagesimal system (base 60).

In order to describe β-integers, we need to generalize the positional numeration system with an integer base – we allow any real number $\beta > 1$ to be the base of the numeration system in question. Such a generalized numeration system was introduced and studied by Rényi [98] who showed that any real non-negative number may be represented in the base β with integer coefficients belonging to the interval $[0, \beta)$. A particular representation – the β-*expansion* – is obtained using the so-called *greedy algorithm*. As every suitable generalization, such a numeration system coincides with an integer base numeration system for β being an integer. Nevertheless, for a non-integer base β, the numeration system changes dramatically and new phenomena appear.

The first remarkable difference is that there might exist several representations of a number over the same set of coefficients. As indicated already by the adjective *greedy* describing the algorithm, the β-expansion is the greatest one among all representations of the same number in the base β with respect to the radix order.

Natural questions to ask are:
"Do we get, adding two numbers with a finite β-expansion, again a number with a finite β-expansion?" "If yes, how long may be the β-fractional part of the sum?"

If, for a fixed β, the response to the first question is affirmative, we say that the base β satisfies the *finiteness property*. An algebraic description of numbers fulfilling the finiteness property is an unsolved problem. It is however known, thanks to Frougny and Solomyak [56], that β satisfying this property is necessarily a Pisot number, which points out again the importance of this class of algebraic numbers.

An analogous role in numeration systems with irrational bases as integers play in numeration systems with integer bases is played by the set $\mathbb{Z}_\beta$ of real numbers which are polynomial in β when expanded in the base β, baptized *β-integers*. Of course, they coincide with integers, $\mathbb{Z}_\beta = \mathbb{Z}$, for $\beta \in \mathbb{N}$. The situation changes significantly if $\beta \notin \mathbb{N}$. In this case, the set $\mathbb{Z}_\beta$ is not equidistant any more and it conserves only partially properties of integers: $\mathbb{Z}_\beta$ has no accumulation points, the distances between consecutive elements of $\mathbb{Z}_\beta$ are bounded, $\mathbb{Z}_\beta$ is self-similar with self-similarity factor β, and not invariant under translation. For β being a Pisot number, $\mathbb{Z}_\beta$ forms a Meyer set (proved by Burdík *et al.* in [26]).

It is possible to define more dimensional structures based on $\mathbb{Z}_\beta$. A *beta-lattice* $\Lambda_\beta \subset \mathbb{R}^d$ based on $\mathbb{Z}_\beta$ is defined in the following way

$$\Lambda_\beta = \big\{\sum_{i=1}^{d} a_i x_i \mid a_i \in \mathbb{Z}_\beta \text{ for all } i \in \{1, 2, \ldots, d\}\big\},$$

where $(x_1, x_2, \ldots, x_d)$ is a basis of $\mathbb{R}^d$. An illustration of a two-dimensional τ-lattice is provided in Figure 1.5. Beta-lattices form a subset of a more general frame of *quasilattices*

$$\Lambda_\beta \subset \big\{\sum_{i=1}^{d} a_i x_i \mid a_i \in \mathbb{Z}[\beta] \text{ for all } i \in \{1, 2, \ldots, d\}\big\}.$$

Pisot cyclotomic quasilattices, i.e., based on a Pisot number β lying in the ring $\mathbb{Z}[\rho]$ generated by a cyclotomic number $\rho = 2\cos\frac{2\pi}{n}$, are particularly convenient to work with because they inherit the corresponding rotational symmetries. If β is a Pisot number, then not only $\mathbb{Z}_\beta$ is a Meyer set, but also the associated β-lattice Λ_β forms a Meyer set.

β-lattices Λ_β are self-similar sets with self-similarity factor β and $\mathbb{Z}_\beta$ is exactly the counting system with origin, i.e., the numerical frame in which we should think about structural properties of Λ_β, the same as the first crystallographers did with lattices and ordinary integers. As a matter of fact, the sets $\mathbb{Z}_\beta$ are natural candidates for labeling quasicrystalline nodes in 1, 2, and 3 dimensions, and also the Bragg peaks in related diffraction patterns (see Figure 1.5).

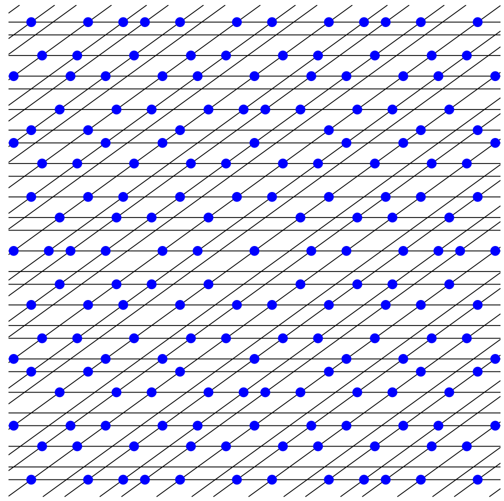


Fig. 1.5: Illustration of a τ-lattice in $\mathbb{R}^2$ with base $\big((1,0),(\cos\frac{\pi}{5},\sin\frac{\pi}{5})\big)$, labeling a two-dimensional quasicrystal.

Besides the above presented application of β-integers in the theory of quasicrystals, the necessity, or, at least, the opportunity to use this interesting alternative of ordinary integers appears in several other fields.

Aperiodicity of $\mathbb{Z}_\beta$ may be for instance used for improving the properties of random number generators, studied by Guimond *et al.* in [64]. The usual numerical generation raises the standard problems of finite computer precision. The possibility to generate β-integers, for a particular class of β, using substitutions circumvents such difficulties; the set is then generated with absolute precision by a symbolic method.

Another domain of application is non-standard wavelet analysis making use of self-similarity of $\mathbb{Z}_\beta$ (developed by Anderle and El-Kharrat in [5]).

A large number of mathematical physicists are interested in discrete Schrödinger operators with aperiodic potentials. Such potentials may be modeled by infinite words coding $\mathbb{Z}_\beta$.

Chapter 2

Preliminaries

This chapter includes all underlying definitions from the field of β-numeration. The fundamental notion of β-integers is introduced, basic arithmetical and geometrical properties of the set $\mathbb{Z}_\beta$ of β-integers are summarized, and, with fundamentals from combinatorics on words at hand, $\mathbb{Z}_\beta$ having only a finite number of distances between neighboring points (in this case, β is called a *Parry number*) is coded by infinite words u_β and elementary combinatorial properties of these words are resumed. In the background of combinatorics on words, we provide definitions of all characteristics we intend to study in the sequel. Last but not least, the preliminary chapter describes Sturmian words. These words deserve attention since it was the Fibonacci word, a notorious word belonging to this class, that served as a first and so far most studied one-dimensional model of quasicrystals. In addition, thanks to their minimal complexity among aperiodic words, Sturmian words are "uncrowned kings of the realm of combinatorics on words" – every phenomenon is usually first studied for them. We keep in the following chapters this tradition; we sum up first what is known in the case of Sturmian words for every investigated combinatorial characteristics.

We denote in what follows the set of complex numbers by $\mathbb{C}$, of real numbers by $\mathbb{R}$, of rational numbers by $\mathbb{Q}$, of integers by $\mathbb{Z}$, of positive integers by $\mathbb{N}$, and of non-negative integers by $\mathbb{N}_0$.

2.1 Beta-numeration and beta-integers

We present elementary notions related to β-numeration. For more details consult Chapter 7 in the Lothaire book [84] as well as references therein.

2.1.1 Beta-representation

Let $\beta > 1$ and $x \geq 0$ be real numbers. Any convergent series of the form

$$x = \sum_{i=-\infty}^{k} x_i \beta^i,$$

where $x_i \in \mathbb{N}_0$ and $x_k \neq 0$, is called a *β-representation* of x. Just as it is usual for the decimal numeration system, we denote the β-representation of x by

$$x_k x_{k-1} \cdots x_0 \bullet x_{-1} \cdots \qquad \text{if } \ k \geq 0,$$

and

$$0 \bullet \underbrace{0 \cdots 0}_{(-1-k) \text{ times}} x_k x_{k-1} \cdots \qquad \text{otherwise.}$$

If a β-representation ends in infinitely many zeroes, it is said to be *finite* and the ending zeroes are omitted. The most usual base β for representations of real numbers is the integer base. It is well-known that, in this case, every $x \geq 0$ has a β-representation. If we admit only $\{0, 1, \ldots, \beta - 1\}$ as the set of coefficients and if we avoid the suffix $(\beta - 1)^\omega$, where ω signifies an infinite repetition, then there exists a unique β-representation of every x; it is called the *standard* β-representation. For $\beta = 10$, it is the usual *decimal* representation, and, for $\beta = 2$, the *binary* representation. Even if β is not an integer, every positive number x has at least one β-representation. This representation can be obtained by the following *greedy algorithm:*

1. Find $k \in \mathbb{Z}$ such that $\beta^k \leq x < \beta^{k+1}$ and put $x_k := \lfloor \frac{x}{\beta^k} \rfloor$ and $r_k := \{\frac{x}{\beta^k}\}$, where $\lfloor x \rfloor$ denotes the lower integer part and $\{x\} = x - \lfloor x \rfloor$ denotes the fractional part of x.

2. For $i < k$, put $x_i := \lfloor \beta r_{i+1} \rfloor$ and $r_i := \{\beta r_{i+1}\}$.

2.1.2 Beta-expansion

The representation of a positive number x in a base β obtained by the greedy algorithm is called the *β-expansion* of x and the coefficients of the β-expansion clearly satisfy: $x_k \neq 0$ and $x_i \in \mathbb{N}_0 \cap [0, \beta)$ for all $i \leq k$. We use the notation $\langle x \rangle_\beta$ for the β-expansion of x. For β being an integer, the β-expansion coincides with the standard β-representation. In order to explain what makes the β-expansion special among many β-representations of every positive real number, it is necessary to introduce the *radix order* on the set of β-representations. A β-representation $x_k \cdots x_0 \bullet x_{-1} \cdots$ is greater with respect to the radix order than a β-representation $y_l \cdots y_0 \bullet y_{-1} \cdots$ if

1. either $k > l$,
2. or $k = l$ and $x_j > y_j$ for $j = \max\{i \leq k \mid x_i \neq y_i\}$, in other words, $x_k \cdots x_0 x_{-1} \cdots$ is *lexicographically* greater than $y_k \cdots y_0 y_{-1} \cdots$.

The greedy algorithm implies that, among β-representations, the β-expansion is the largest according to the radix order. Let us append that the radix order corresponds to the ordering of real numbers: For all $x, y \in [0, +\infty)$, the inequality $x < y$ holds if and only if $\langle x \rangle_\beta$ is smaller than $\langle y \rangle_\beta$ according to the radix order.

Example 2.1.1. *Let β be equal to the golden mean $\tau = \frac{1+\sqrt{5}}{2}$, which has been brought to the attention of the reader already in the introduction. We recall that τ is the larger root of the polynomial $x^2 - x - 1$. Applying the greedy algorithm, we get for instance the following τ-expansions: $\langle \frac{\sqrt{5}-1}{2} \rangle_\tau = 0 \bullet 1$, $\langle \frac{3+\sqrt{5}}{2} \rangle_\tau = 100\bullet$, $\langle \frac{5+3\sqrt{5}}{10} \rangle_\tau = 1 \bullet (0001)^\omega \cdots$. Other τ-representations of $\frac{5+3\sqrt{5}}{10}$ are for example $1 \bullet 00(0011)^\omega$ or $0 \bullet (1100)^\omega$.*

An immediate consequence of the definition of the β-expansion is the following equivalence:

$$\langle x \rangle_\beta = x_k \cdots x_1 x_0 \bullet x_{-1} \cdots \quad \Leftrightarrow \quad \langle \tfrac{x}{\beta} \rangle_\beta = x_k \cdots x_1 \bullet x_0 x_{-1} \cdots$$

Accordingly, it suffices to restrict the considerations to the interval $[0, 1)$ in order to determine the β-expansions of all real non-negative numbers.

2.1.3 Rényi expansion of unity

The β-expansion of numbers from the interval $[0,1)$ can be obtained by means of an extensively studied transformation $T_\beta : [0,1] \to [0,1)$ defined by

$$T_\beta(x) = \{\beta x\}. \tag{2.1}$$

It is easy to verify that for every $x \in [0,1)$, it holds $\langle x \rangle_\beta = 0 \bullet x_{-1}x_{-2}\cdots$ if and only if

$$x_{-i} = \lfloor \beta T_\beta^{i-1}(x) \rfloor. \tag{2.2}$$

For $x = 1$, the formula from (2.2) does not provide the β-expansion of 1 for the simple fact that $\langle 1 \rangle_\beta = 1\bullet$, however, it defines a powerful tool – the *Rényi expansion of unity* (introduced by Rényi in [98]). Let us slightly modify the notation of coefficients: we write t_i instead of x_{-i}. The *Rényi expansion of unity* in a base $\beta > 1$ is then defined as

$$d_\beta(1) = t_1t_2t_3\cdots, \quad \text{where} \quad t_i := \lfloor \beta T_\beta^{i-1}(1) \rfloor. \tag{2.3}$$

Every number $\beta > 1$ is characterized by its Rényi expansion of unity. Note that $t_1 = \lfloor \beta \rfloor \geq 1$. Contrariwise, not every sequence of non-negative integers is equal to $d_\beta(1)$ for some β. Parry resolved this problem in his paper [92]: A sequence $(t_i)_{i\geq 1}$, $t_i \in \mathbb{N}_0$, is the Rényi expansion of unity for some number $\beta > 1$ if and only if it satisfies

$$t_jt_{j+1}t_{j+2}\cdots \prec t_1t_2t_3\cdots \quad \text{for every } j > 1, \tag{2.4}$$

where $\prec$ stands for 'strictly lexicographically smaller'. It follows, in particular, that the Rényi expansion of unity is never purely periodic, i.e., $d_\beta(1)$ is never of the form $(t_1t_2\cdots t_m)^\omega$. Parry has moreover shown that the Rényi expansion of unity enables us to decide whether a given β-representation of x is its β-expansion or not. For this purpose, we define the *infinite Rényi expansion of unity* (it is the largest infinite β-representation of 1 with respect to the radix order) by

$$d_\beta^*(1) = \begin{cases} d_\beta(1) & \text{if} \quad d_\beta(1) \quad \text{is infinite}, \\ (t_1t_2\cdots t_{m-1}(t_m-1))^\omega & \text{if} \quad d_\beta(1) = t_1\cdots t_m \quad \text{with} \quad t_m \neq 0. \end{cases} \tag{2.5}$$

Proposition 2.1.2 (Parry condition)**.** *Let $d_\beta^*(1)$ be the infinite Rényi expansion of unity in a base $\beta > 1$. Let $\sum_{i=-\infty}^{k} x_i\beta^i$ be a β-representation of a non-negative number x. Then $\sum_{i=-\infty}^{k} x_i\beta^i$ is the β-expansion of x if and only if*

$$x_ix_{i-1}\cdots \prec d_\beta^*(1) \quad \textit{for all} \quad i \leq k. \tag{2.6}$$

Example 2.1.3. *For $\beta = \tau = \frac{1+\sqrt{5}}{2}$, the Rényi expansion of unity is $d_\tau(1) = 11$. Then, $d_\tau^*(1) = (10)^\omega$, and, according to the Parry condition, any sequence of coefficients in $\{0,1\}$, which does not end in $(10)^\omega$ and which does not contain the block 11, is the τ-expansion of a non-negative real number.*

2.1.4 Algebraic numbers: Pisot, Perron, Parry numbers

An *algebraic number* β is a root of a monic polynomial with rational coefficients. An *algebraic integer* β is a root of a monic polynomial with integer coefficients. Among such polynomials, the polynomial with the smallest degree n is called the *minimal polynomial* of β; the algebraic number β is then said to be of *order* n. The other roots $\beta^{(2)}, \ldots, \beta^{(n)}$ of the minimal polynomial are mutually distinct and are called *conjugates* of β. The minimal subfield of $\mathbb{C}$ containing β and $\mathbb{Q}$ is

$$\mathbb{Q}(\beta) = \{a_0 + a_1\beta + \cdots + a_{n-1}\beta^{n-1} \mid a_i \in \mathbb{Q}\}.$$

For any $j \in \{2, \ldots, n\}$, the map $\sigma_j : \mathbb{Q}(\beta) \to \mathbb{Q}(\beta^{(j)})$, defined for any polynomial g with rational coefficients by

$$\sigma_j(g(\beta)) = g(\beta^{(j)}),$$

is an isomorphism. In the case of a quadratic algebraic number β, the conjugate of β is denoted β', and, instead of $\sigma_2(x)$, we write x' for any $x \in \mathbb{Q}(\beta)$.

In the field of numeration, several classes of algebraic numbers are intensively studied. Let us introduce them and reveal the relation among them.

According to the properties of its conjugates, an algebraic integer $\beta > 1$ is called:

- a *Pisot number* if all its conjugates have modulus less than one,
- a *Perron number* if all its conjugates have modulus less than β.

In the sequel, particular attention is paid to real numbers $\beta > 1$ having an eventually periodic Rényi expansion of unity, i.e., $d_\beta(1) = t_1 \ldots t_m (t_{m+1} \ldots t_{m+r})^\omega$ for some $m, r \in \mathbb{N}_0$, called *Parry numbers*. For every Parry number β, it is easy to recover, from the eventual periodicity of $d_\beta(1)$, a monic polynomial with integer coefficients having β as a root, i.e., β is an algebraic integer. Let us point out that this so-called *Parry polynomial* is not necessarily the minimal polynomial of β. Notice that if β is a Parry number and $\beta \notin \mathbb{N}$, then β is necessarily irrational. (Rational numbers are not algebraic integers.)

It is difficult to characterize Parry numbers in the language of algebraic number theory. Only some partial results concerning algebraic characterization of Parry numbers are known, in particular,

$$\text{Pisot numbers} \quad \subset \quad \text{Parry numbers} \quad \subset \quad \text{Perron numbers},$$

where the first inclusion is proved in [18] and the second one in [84].

2.1.5 Definition of beta-integers

If $x = \sum_{i=-\infty}^{k} x_i\beta^i$ is the β-expansion of a non-negative number x, then $\sum_{i=-\infty}^{-1} x_i\beta^i$ is called the *β-fractional part* of x. Let us list some important notions adherent to β-expansions:

- Non-negative numbers x with vanishing β-fractional part are called *non-negative β-integers*, formally,
$$\mathbb{Z}_\beta^+ := \{x \geq 0 \bigm| \langle x \rangle_\beta = x_k x_{k-1} \cdots x_0 \bullet\}.$$
- The set of *β-integers* is then defined by
$$\mathbb{Z}_\beta := \left(-\mathbb{Z}_\beta^+\right) \cup \mathbb{Z}_\beta^+.$$
- All real numbers x such that the β-expansion of $|x|$ is finite form the set $Fin(\beta)$. Formally,
$$Fin(\beta) := \bigcup_{n \in \mathbb{N}_0} \frac{1}{\beta^n}\mathbb{Z}_\beta.$$
- For any $x \in Fin(\beta)$, we denote by $fp_\beta(x)$ the length of its fractional part, i.e.,
$$fp_\beta(x) = \min\{l \in \mathbb{N}_0 \bigm| \beta^l x \in \mathbb{Z}_\beta\}.$$

As already mentioned, the radix order on the set of β-representations corresponds to the natural order on the set of non-negative real numbers. Consequently, there exists a strictly increasing sequence $(b_n)_{n=0}^{\infty}$ such that

$$b_0 = 0 \quad \text{and} \quad \{b_n \mid n \in \mathbb{N}_0\} = \mathbb{Z}_\beta^+. \tag{2.7}$$

2.1.6 Arithmetical properties of beta-integers

If β is an integer, then, clearly, $\mathbb{Z}_\beta = \mathbb{Z}$, and, moreover, $\mathbb{Z}_\beta$ and $Fin(\beta)$ are closed under addition and multiplication. If $\beta \notin \mathbb{N}$, then the sets $\mathbb{Z}$ and $\mathbb{Z}_\beta$ do not coincide any more and are very different from the arithmetical point of view; in particular, $\mathbb{Z}_\beta$ is not closed under addition and multiplication for any $\beta \notin \mathbb{N}$.

Example 2.1.4. *For every $\beta > 1$, $\lfloor \beta \rfloor$ is a β-integer. However, if $\beta \notin \mathbb{N}$, let us show that $\lfloor \beta \rfloor + 1$ is not a β-integer. Clearly, there exists $k \in \mathbb{N}$ such that $\beta^k < \lfloor \beta \rfloor + 1 < \beta^{k+1}$. Since $1 > \lfloor \beta \rfloor + 1 - \beta^k > 0$, we find $i \in \mathbb{N}$ satisfying $\langle \lfloor \beta \rfloor + 1 \rangle_\beta = x_k \dots x_0 \bullet x_{-1} x_{-2} \dots = 10 \dots 0 \bullet 0 \dots 0 x_{-i} \dots$, where $x_{-i} \neq 0$.*

Even worse, for $\beta \notin \mathbb{N}$, the set $Fin(\beta)$ need not be closed under addition and multiplication, neither. The characterization of those β for which this pathological situation does not appear is so far an unsolved and probably very hard problem. Mathematically, one wants to describe β for which the set $Fin(\beta)$ is a subring of $\mathbb{R}$. Frougny and Solomyak have shown in [56] that a necessary condition for this so-called *finiteness property* is that β is a Pisot number. Some sufficient conditions can be found in [2, 56, 68].

If the sum or the product of two β-integers has a finite β-expansion, one can naturally ask how long the β-fractional part of the result is. The following notion is meaningful even for a base β such that the sum of two β-integers does not have always a finite β-expansion.

- $L_\oplus(\beta) := \min\{L \in \mathbb{N}_0 \mid x, y \in \mathbb{Z}_\beta, x + y \in Fin(\beta) \Longrightarrow fp_\beta(x+y) \leq L\}$.
- $L_\otimes(\beta) := \min\{L \in \mathbb{N}_0 \mid x, y \in \mathbb{Z}_\beta, xy \in Fin(\beta) \Longrightarrow fp_\beta(xy) \leq L\}$.

If the argument of the minimum is an empty set, we set $L_\oplus(\beta) := \infty$ or $L_\otimes(\beta) := \infty$. The task to determine the set of numbers β for which $L_\oplus(\beta)$ and $L_\otimes(\beta)$ are finite is still not fully solved. Some important steps in this direction are the results (proved in [56], [65], respectively) stating that $L_\oplus(\beta)$ and $L_\otimes(\beta)$ are finite for Pisot numbers β. More recently, Bernat in [13] improved the previous results by showing that the sets $L_\oplus(\beta)$ and $L_\otimes(\beta)$ are finite for Perron numbers β.

2.1.7 Geometrical properties of beta-integers

Since $\mathbb{Z}_\beta = \mathbb{Z}$ for $\beta \in \mathbb{N}$, the distance between the neighboring elements of $\mathbb{Z}_\beta$ is always 1. The situation changes dramatically if $\beta \notin \mathbb{N}$. In this case, the number of different distances between neighboring elements of $\mathbb{Z}_\beta$ is at least 2 and the set $\mathbb{Z}_\beta$ keeps only partially the resemblance to $\mathbb{Z}$:

1. $\mathbb{Z}_\beta$ has no accumulation points.
2. $\mathbb{Z}_\beta$ is relatively dense ; the distances between consecutive β-integers are bounded by 1.
3. $\mathbb{Z}_\beta$ is self-similar, by virtue of the inclusion $\beta\mathbb{Z}_\beta \subset \mathbb{Z}_\beta$.
4. $\mathbb{Z}_\beta$ is not invariant under translation; in other words, $\mathbb{Z}_\beta$ is aperiodic.

5. $\mathbb{Z}_\beta$ forms a Meyer set if β is a Pisot number, i.e., $\mathbb{Z}_\beta - \mathbb{Z}_\beta \subset \mathbb{Z}_\beta + F$ for a finite set $F \subset \mathbb{R}$ (proved by Burdík *et al.* in [26]).

Thurston [105] has shown that distances between neighbors of $\mathbb{Z}_\beta$ form the set $\{\Delta_k \mid k \in \mathbb{N}_0\}$, where

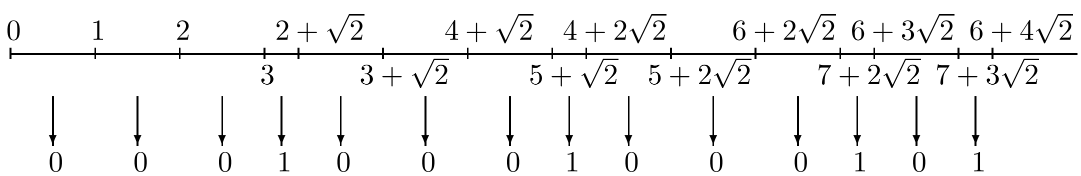
$$\Delta_k := \sum_{i=1}^{\infty} \frac{t_{i+k}}{\beta^i}. \tag{2.8}$$

It is evident that the set $\{\Delta_k \mid k \in \mathbb{N}_0\}$ is finite if and only if $d_\beta(1)$ is eventually periodic. If the number of distances of neighbors in $\mathbb{Z}_\beta$ is finite, we can associate with every distance a letter. Thus, we obtain an infinite word u_β coding $\mathbb{Z}_\beta^+$, as indicated in Example 2.1.5, and the study of combinatorial properties of this word can be then interpreted in the framework of $\mathbb{Z}_\beta$.

Example 2.1.5. *Let $d_\beta(1) = 31^\omega$. It is a well defined Rényi expansion of unity. From the equality $1 = \frac{3}{\beta} + \sum_{i \geq 2} \frac{1}{\beta^i}$, we deduce that $\beta = 2 + \sqrt{2}$. According to the formula (2.8), we learn that the distances between neighboring β-integers take two values: $\Delta_0 = 1$ and $\Delta_1 = \frac{1}{\beta - 1} = \sqrt{2} - 1$. Applying the Parry condition (2.6), we learn that the first fifteen smallest non-negative β-integers and their β-expansions are the following:*

$$\begin{array}{rrr}
\langle 0 \rangle_\beta = 0\bullet & \langle 1 \rangle_\beta = 1\bullet & \langle 2 \rangle_\beta = 2\bullet \\
\langle 3 \rangle_\beta = 3\bullet & \langle 2+\sqrt{2} \rangle_\beta = 10\bullet & \langle 3+\sqrt{2} \rangle_\beta = 11\bullet \\
\langle 4+\sqrt{2} \rangle_\beta = 12\bullet & \langle 5+\sqrt{2} \rangle_\beta = 13\bullet & \langle 4+2\sqrt{2} \rangle_\beta = 20\bullet \\
\langle 5+2\sqrt{2} \rangle_\beta = 21\bullet & \langle 6+2\sqrt{2} \rangle_\beta = 22\bullet & \langle 7+2\sqrt{2} \rangle_\beta = 23\bullet \\
\langle 6+3\sqrt{2} \rangle_\beta = 30\bullet & \langle 7+3\sqrt{2} \rangle_\beta = 31\bullet & \langle 6+4\sqrt{2} \rangle_\beta = 100\bullet
\end{array}$$

Associating $\Delta_0 \to 0$ and $\Delta_1 \to 1$, we get an infinite word u_β illustrated in Figure 2.1.



$u_\beta = \mathbf{00010001000101}000100010001010001000100010100010 1\ldots$

Fig. 2.1: Illustration of the coding of distances in $\mathbb{Z}_\beta$ resulting in an infinite word u_β.

2.2 Combinatorics on words

We introduce here basic terms and all combinatorial characteristics we intend to study in the following chapters. A comprehensive survey from various points of view – general, algebraic, applied combinatorics on words – is provided in the Lothaire books [83], [84], [85].

2.2.1 Finite words

An *alphabet* $\mathcal{A}$ is a finite set of symbols, called *letters*. A finite sequence of letters forms a *word*. Let us equip the set of all words $\mathcal{A}^*$ over the alphabet $\mathcal{A}$ with a binary operation - *concatenation*

– defined, for any two words, as

$$(w_1, w_2, \ldots, w_n)(v_1, v_2, \ldots, v_m) = (w_1, w_2, \ldots, w_n, v_1, v_2, \ldots, v_m).$$

Obviously, concatenation is an associative operation, we may thus use the notation $w_1 w_2 \ldots w_n$ instead of $(w_1, w_2, \ldots, w_n)$ for finite words. The empty sequence of letters, called the *empty word* ε, plays the role of a neutral element in $\mathcal{A}^*$. Consequently, $\mathcal{A}^*$ equipped with the operation of concatenation turns out to be a monoid. The *length* of a word w is the number of letters contained in w and is denoted by $|w|$, while $|w|_a$ denotes the number of occurrences of a letter $a \in \mathcal{A}$ in the word w. Therefore, $|w| = \sum_{a \in \mathcal{A}} |w|_a$. The length of the empty word is zero.

2.2.2 Infinite words

Analogously as in the case of finite words, we denote by $\mathcal{A}^{\mathbb{N}_0}$ the set of right-sided infinite words over the alphabet $\mathcal{A}$, i.e., sequences of letters of $\mathcal{A}$ indexed by non-negative integers, and by $\mathcal{A}^{\mathbb{Z}}$ the set of both-sided infinite words over $\mathcal{A}$, i.e., sequences of letters of $\mathcal{A}$ indexed by integers. Concatenation is well defined also for wu, where $w \in \mathcal{A}^*$ and $u \in \mathcal{A}^{\mathbb{N}_0}$. The concatenation of k words $w \in \mathcal{A}^*$ is denoted by w^k, the concatenation of infinitely many words w by w^ω. In the sequel, we focus on right-sided infinite words $u = u_0 u_1 u_2 \ldots$. We call them *infinite words* for short, while both-sided infinite words are called *biinfinite*.

An essential notion in the context of infinite words is periodicity. An infinite word u is said to be *eventually periodic* if there exist finite words v, w such that $u = vw^\omega$. We call u *purely periodic* if $v = \varepsilon$. An infinite word which is not eventually periodic is called *aperiodic*.

Let us introduce usual topology induced by the following metric on $\mathcal{A}^* \cup \mathcal{A}^{\mathbb{N}_0}$. Let u, u' be two words (finite or infinite) in $\mathcal{A}^* \cup \mathcal{A}^{\mathbb{N}_0}$, $u \neq u'$. If one of them is finite, take any symbol, say $\triangle$, which is not contained in the alphabet $\mathcal{A}$, and extend the word by $\triangle^\omega$ to the right. If both of the words u, u' are finite, take two distinct symbols out of the alphabet $\mathcal{A}$ for their extension to the right. Then the distance of $u = u_0 u_1 \ldots$ and $u' = u'_0 u'_1 \ldots$ is defined by

$$d(u, u') = (1 + \inf\{k \geq 0 \mid u_k \neq u'_k\})^{-1}. \tag{2.9}$$

We put $d(u, u) = 0$. Briefly speaking, two words are close to each other if they share a long "prefix" (defined in the next section).

Example: *For words* $u = (01)^\omega,\ u' = 01010,\ u'' = 01011$, *the distances are as follows*

$$d(u, u') = \frac{1}{6},\ d(u, u'') = \frac{1}{5},\ d(u', u'') = \frac{1}{5}.$$

The space $\mathcal{A}^* \cup \mathcal{A}^{\mathbb{N}_0}$ equipped with the metric d is known to be a complete and compact metric space (see [84]).

2.2.3 Language

From now on, if an infinite word u is defined over an alphabet $\mathcal{A}$, then take it that every letter from $\mathcal{A}$ occurs in u.

We are given a word u over an alphabet $\mathcal{A}$. A finite word w is called a *factor* (or a *subword*) of a word u (finite or infinite) if there exist a finite word $w^{(1)}$ and a word $w^{(2)}$ (finite or infinite) such that $u = w^{(1)} w w^{(2)}$. The factor $w^{(1)}$ is a *prefix* of u (a *proper prefix* if $u \neq w^{(1)}$) and $w^{(2)}$ is a suffix of u (a *proper suffix* if $u \neq w^{(2)}$).

In general, a *language* is any subset of $\mathcal{A}^*$. The *language* $\mathcal{L}(u)$ (often denoted also $F(u)$ in the literature) of a word u (finite or infinite) over $\mathcal{A}$ is the set of all factors of u. Such languages are *factorial*, i.e., $\mathcal{L}(u)$ contains with every element w also all factors of w. A remarkable property of the languages of infinite words is that every factor is extendable to the right. In other words, for every factor w, one can find at least one letter $a \in \mathcal{A}$ such that wa belongs to $\mathcal{L}(u)$. However, there exist infinite words with prefixes not extendable to the left.

2.2.4 Recurrence

Infinite words whose every factor is extendable to the left are called *recurrent*. Let us mention two other equivalent definitions of recurrence. An infinite word u is recurrent if each of its factors occurs at least twice, or, equivalently, if each of its factors occurs infinitely many times in u. An infinite word u is *uniformly recurrent* if for any $n \in \mathbb{N}$, there exists $R \in \mathbb{N}$ such that any subword of u of length R contains all factors of length n. Evidently, the number R depends on n; the minimal such value is denoted $R(n)$.

The language of a uniformly recurrent word u is minimal in a certain sense: If the language of an infinite word v satisfies $\mathcal{L}(v) \subset \mathcal{L}(u)$, then necessarily $\mathcal{L}(v) = \mathcal{L}(u)$. In the theory of dynamical systems, the uniform recurrence of an infinite word is equivalent with the minimality of the associated dynamical system (consult Queffélec [95]).

A subclass of uniformly recurrent words is formed by linearly recurrent words. An infinite uniformly recurrent word u is said to be *linearly recurrent* if there exists a positive constant K such that $R(n) \leq Kn$ for every $n \in \mathbb{N}$; u is then often called *linearly recurrent with constant* K.

2.2.5 Return words

Roughly speaking, for a given factor w of an infinite word u, a return word of w is any segment between two successive occurrences of the factor w. A precise definition follows. Let w be a factor of an infinite word $u = u_0u_1u_2\ldots$. An integer j is called an *occurrence* of w in u if w is a prefix of $u_ju_{j+1}\ldots$. Let j, k, $j < k$, be two successive occurrences of w. Then $u_ju_{j+1}\ldots u_{k-1}$ is a *return word* of w. The set of all return words of w is denoted by $Ret(w)$,

$$Ret(w) = \{u_ju_{j+1}\ldots u_{k-1} \mid j, k \text{ being successive occurrences of } w \text{ in } u\}. \tag{2.10}$$

If v is a return word of w, then the word vw is called a *complete return word* of w.

Example: *For the infinite word $u = (010)^\omega$, the sets of return words of letters are $Ret(0) = \{0, 01\}$, $Ret(1) = \{100\}$, and any factor of length greater than 1 has only one return word. A return word of a factor may be shorter than the factor itself, e.g., $Ret(010010) = 010$.*

It is not difficult to see that an infinite recurrent word is uniformly recurrent if and only if the set of return words of any of its factors is finite. If the infinite word u is moreover linearly recurrent with constant K (defined in Section 2.2.4), then, for every factor w of u, the number of return words of w fulfills $\#Ret(w) \leq (K-1)K^2$ (consult Durand [45]).

It is readily seen that infinite recurrent words are either purely periodic or aperiodic. The number of return words of factors of a recurrent purely periodic word u can be easily determined. If we denote its minimal period v, i.e., $u = v^\omega$, then $\#Ret(w) = 1$ for every $w \in \mathcal{L}(u)$ with $|w| \geq |v|$. Return words in aperiodic recurrent words is the object of our further study.

2.2.6 Factor frequency

A natural question to ask is how often a factor w occurs in a given infinite word u. We say that a number $\rho(w)$ is the *(factor) frequency* of w (in u) if for every $k \in \mathbb{N}_0$, it holds

$$\lim_{n\to\infty} \frac{\#\{\text{occurrences of } w \text{ in } u_k \dots u_{k+n-1}\}}{n} = \rho(w). \tag{2.11}$$

Quite usual, however weaker, is the definition of factor frequency $\rho(w)$ considering occurrences of w exclusively in the prefixes of u. Durand in [46] has proved that factor frequencies of linearly recurrent words exist.

It is easy to determine factor frequencies in purely periodic words. Let $u = v^\omega$, where v is chosen to be minimal. Then, clearly, for every $n \geq |v|$, the set of frequencies of factors of length n has only one element $\frac{1}{|v|}$.

2.2.7 Balance property

To express the degree of variability in an infinite word u, the balance property serves as a suitable tool; in particular, to measure the distribution of letters. We say that an infinite word u over $\mathcal{A}$ is *c-balanced*, if for every $a \in \mathcal{A}$ and for every pair of factors w, $\hat{w}$ of u of the same length $|w| = |\hat{w}|$, we have $||w|_a - |\hat{w}|_a| \leq c$. Note that in the case of a binary alphabet, say $\mathcal{A} = \{0,1\}$, this condition may be rewritten in a simpler way: an infinite word u is *c-balanced*, if for every pair of factors w, $\hat{w}$ of u with $|w| = |\hat{w}|$, we have $||w|_0 - |\hat{w}|_0| \leq c$. We call 1-balanced words simply *balanced*.

2.2.8 Factor complexity

Another measure of variability of local configurations in an infinite word u is provided by its factor complexity. Let us denote by $\mathcal{L}_n(u)$ the set of factors of length n of the infinite word u. Then, the *factor complexity* (or *complexity*) of u is a function $\mathcal{C}_u : \mathbb{N}_0 \to \mathbb{N}$ which associates to every n the number of different factors of length n of the infinite word u, i.e.,

$$\mathcal{C}_u(n) = \#\mathcal{L}_n(u). \tag{2.12}$$

We often omit the index u and write $\mathcal{C}$ instead of $\mathcal{C}_u$, provided no confusion is likely.

Let us stress a close link between periodicity and complexity. The complexity of eventually periodic words is bounded (as shown by Hedlund and Morse [66]). On the other hand, if there exists $n \in \mathbb{N}$ such that $\mathcal{C}_u(n) \leq n$, then the complexity is bounded and the infinite word u is eventually periodic. In consequence, the complexity of aperiodic words satisfies $\mathcal{C}(n) \geq n+1$ for all $n \in \mathbb{N}_0$. The aperiodic words with the lowest possible complexity ($\mathcal{C}(n) = n+1$ for all $n \in \mathbb{N}_0$) are called *Sturmian*. These words are binary since $\mathcal{C}(1) = 2$. Sturmian words are important for many reasons. We devote them entirely Section 2.4.

2.2.9 Special factors

Let w be a factor of an infinite word u over $\mathcal{A}$. We say that $a \in \mathcal{A}$ is a *right extension* of w in u if wa belongs to $\mathcal{L}(u)$. We denote by $Rext(w)$ the set of all right extensions of w in u, i.e.,

$$Rext(w) = \{a \in \mathcal{A} \mid wa \in \mathcal{L}(u)\}. \tag{2.13}$$

If $\#Rext(w) \geq 2$, then the factor w is called *right special* (RS for short). Analogously, we define *left extensions, $Lext(w)$, left special factors* (LS factors). Moreover, we say that a factor w is *bispecial* (BS) if w is LS and RS. Sometimes, we also call a factor *special* if it is LS or RS. Using this notation, it is possible to express $\mathcal{L}_{n+1}(u)$ by means of factors of length n

$$\mathcal{L}_{n+1}(u) = \bigcup_{w\in\mathcal{L}_n(u)} \{wa \mid a \in \mathit{Rext}(w)\} = \bigcup_{w\in\mathcal{L}_n(u)} \{aw \mid a \in \mathit{Lext}(w)\}. \tag{2.14}$$

The following proposition presents a well-known formula due to Cassaigne [27] for *the first difference of complexity* $\Delta\mathcal{C}(n) = \mathcal{C}(n+1) - \mathcal{C}(n)$ of an infinite word u, based on the description of RS, respectively LS factors of length n. It is a direct consequence of Equation (2.14).

Proposition 2.2.1. *Let u be an infinite recurrent word, then, for all $n \in \mathbb{N}_0$, the first difference of complexity has the following form*

$$\Delta\mathcal{C}(n) = \sum_{w\in\mathcal{L}_n(u)\ RS} \big(\#\mathit{Rext}(w) - 1\big) = \sum_{w\in\mathcal{L}_n(u)\ LS} \big(\#\mathit{Lext}(w) - 1\big). \tag{2.15}$$

Remark 2.2.2. *If u is not a recurrent word, then there exists an integer $n \in \mathbb{N}$ such that every prefix of u of length $\geq n$ occurs only once in u; we say that the prefix is unioccurrent. Observing the extensibility of factors of u to the left, we see that each LS factor w contributes to the complexity growth by $\#\mathit{Lext}(w) - 1$, while the unioccurrent prefix decreases the complexity by 1. To sum up, the following formula is valid*

$$\Delta\mathcal{C}(n) = \sum_{w\in\mathcal{L}_n(u)\ LS} \big(\#\mathit{Lext}(w) - 1\big) - \#\{v \in \mathcal{L}_n(u) \mid v \textit{ is a unioccurrent prefix of } u\}.$$

2.2.10 Palindromes

The *mirror map* associates with every word $w = w_1w_2\dots w_n \in \mathcal{A}^*$ its reversal $\overline{w} = w_n\dots w_2w_1$. A *palindrome* is then a word which is invariant under this map. Evidently, not every word v is a palindrome, nevertheless, any v is a prefix of a palindrome. The shortest such palindrome is called the *right palindromic closure* of v and is denoted by $v^{(+)}$.

Example: $(010)^{(+)} = 010$, $(0100)^{(+)} = 010010$, $(11110)^{(+)} = 111101111$.

In resemblance to the set $\mathcal{L}_n(u)$ of factors of length n and the factor complexity $\mathcal{C}_u(n)$ of an infinite word u, let us denote by $\mathcal{P}al_n(u)$ the set of palindromes of length n contained in u and let us define the *palindromic complexity* of u as a function $\mathcal{P}_u : \mathbb{N}_0 \to \mathbb{N}_0$ associating to every n the number of different palindromes of length n contained in the infinite word u, i.e.,

$$\mathcal{P}_u(n) = \#\mathcal{P}al_n(u). \tag{2.16}$$

Similarly as for the factor complexity, we usually replace $\mathcal{P}_u$ by $\mathcal{P}$ for the palindromic complexity.

In case of uniformly recurrent words, only languages closed under reversal may have infinitely many distinct palindromes. Formally, a language $\mathcal{L}(u)$ is *closed under reversal*, if for every factor, also its reversal belongs to $\mathcal{L}(u)$.

Proposition 2.2.3. *Let u be an infinite uniformly recurrent word. If the language $\mathcal{L}(u)$ contains, for every $N \in \mathbb{N}$, a palindrome of length $n > N$, then $\mathcal{L}(u)$ is closed under reversal.*

Proof. For any factor w of the uniformly recurrent word u, any palindrome of length greater than $R(|w|)$ (defined in Section 2.2.4) contains w, and, consequently, contains also $\overline{w}$. □

The opposite implication is not true. Berstel *et al.* in [16] have constructed an infinite uniformly recurrent word such that its language is closed under reversal, however, contains only a finite number of palindromes. The precise definition and the description of its complexity can be found in Section 3.3.5; this word occurs in several other chapters as an illustrating example of the studied characteristics.

2.2.11 Fullness

Besides the study of the palindromic complexity, another interesting problem is to determine the number of palindromes in finite words. Droubay, Justin, and Pirillo have opened this question in [43]. They proved the following proposition.

Proposition 2.2.4. *For every finite word v, the number of different palindromes $P(v)$ (including the empty word) contained in v is at most $|v|+1$.*

Proof. Take an arbitrary palindrome v' contained in $v = v_1 \dots v_n$ and find its first occurrence k in v. Then v' is the longest palindromic suffix of $v_1 \dots v_{k+|v'|-1}$, otherwise k would not be the first occurrence of v' in v. Consequently,

$$P(v) = \#\{v' \mid v' \text{ is the longest palindromic suffix of } v_1 \dots v_l,\ 1 \leq l \leq n\} \leq n+1. \tag{2.17}$$

□

This result inspired the introduction and the study of the following notions. The difference between $|v|+1$ and the number of palindromes in a word v is called the *defect* of v. Keeping the terminology introduced by Brlek *et al.* in [23], we call a finite word v containing the maximal possible number $|v|+1$ of palindromes *full*.

Example: *The word $v = 01001010$ is full since it contains 9 palindromes: ε, 0, 1, 00, 010, 101, 1001, 01010, 010010, while the word $v' = 11001011$ is not full because the set of its palindromic factors is $\{\varepsilon, 0, 1, 00, 11, 010, 101, 1001\}$, thus the defect of v' is 1.*

The notion of fullness of finite words may be generalized to infinite words. An infinite word is called *full* if all its prefixes are full. (Glen *et al.* [62] use the term *rich in palindromes*, for both finite and infinite full words). Let us remark that the set of full infinite words does not change if, for the definition, we take into account all factors instead of prefixes; in [43], it is shown that if an infinite word is full, then all its factors are full. Obviously, a full infinite word contains infinitely many palindromes. According to Proposition 2.2.3, the language of a full uniformly recurrent infinite word is closed under reversal.

The notion of defect may be generalized to infinite words. The *defect* $D(u)$ of an infinite word u is equal to the maximal defect of factors of u. In fact, this definition may be simplified observing that if w is a factor of a word v, then $D(w) \leq D(v)$; thus $D(u) = \sup\{D(w) | w \text{ is a prefix of } u\}$. With this notion, finite or infinite full words are exactly those ones with zero defects.

2.2.12 Rauzy graphs

Rauzy graphs and factor complexity

Rauzy graphs (also called factor graphs) represent a great visualizing tool for languages of infinite words. The *Rauzy graph* Γ_n (of order n) of an infinite word u is a directed graph whose set of vertices is $\mathcal{L}_n(u)$ and set of edges is $\mathcal{L}_{n+1}(u)$. An edge $e = w_0 w_1 \dots w_{n-1} w_n$ starts in the vertex $w = w_0 w_1 \dots w_{n-1}$ and ends in the vertex $v = w_1 \dots w_{n-1} w_n$, as illustrated in Figure 2.2.

In Figure 2.3, the Rauzy graphs of the lowest orders of a Sturmian word are represented. It follows from the definition that the number of edges starting in a vertex $w \in \mathcal{L}_n(u)$ equals $\#Rext(w)$ and the number of edges ending in w is equal to $\#Lext(w)$. If we sum up, for every vertex, the number of all edges ending in this vertex, we obtain the total number of edges in Γ_n, thus

$$\mathcal{C}(n+1) = \#\mathcal{L}_{n+1}(u) = \sum_{w \in \mathcal{L}_n(u)} \#Lext(w).$$

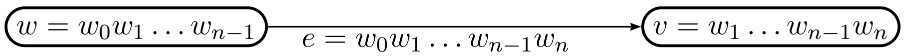


Fig. 2.2: Incidence relation between an edge and vertices in a Rauzy graph.

Subtracting $\mathcal{C}(n)$, i.e., the number of vertices in Γ_n, we get the formula for the first difference of complexity, valid for both recurrent and non-recurrent infinite words,

$$\Delta\mathcal{C}(n) = \sum_{w\in\mathcal{L}_n(u)} (\#Lext(w) - 1).$$

It is obvious that the Rauzy graphs of an infinite word u are strongly connected if and only if u is a recurrent word. (A directed graph is *strongly connected* if for every pair of vertices w, v, there exists a directed path starting in w and ending in v.)

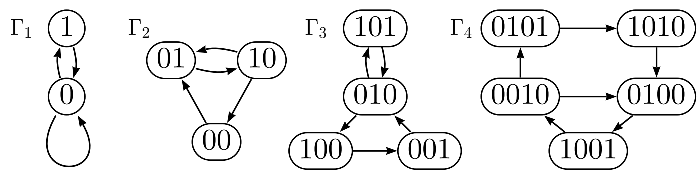


Fig. 2.3: Illustration of the Rauzy graphs of order $1, 2, 3$, and 4 of u_β coding β-integers $\mathbb{Z}_\beta$ for β being the simplest possible quadratic non-simple Parry unit, i.e., $d_\beta(1) = 21^\omega$. For β being a unit, u_β is known to be a Sturmian word. To construct the graphs, it is necessary to know that $\mathcal{L}_5(u_\beta) = \{00100, 00101, 01001, 01010, 10010, 10100\}$.

Kirchhoff's law in Rauzy graphs

Assume that the frequencies of all factors of u exist. We can label every edge e in the Rauzy graph Γ_n of u by the frequency $\rho(e)$. Such a graph is then called a *labeled Rauzy graph*. Frequencies in a Rauzy graph obey a similar law as current in a circuit. It follows from the definition of frequency that the frequency of a vertex w in Γ_n is equal to the sum of the frequencies of the edges starting in w, or, by symmetry, to the sum of the frequencies of the edges ending in w. Let us formalize this observation.

Lemma 2.2.5 (Kirchhoff's law)**.** *Let w be a factor of an infinite word u, then*

$$\rho(w) = \sum_{a\in Lext(w)} \rho(aw) = \sum_{a\in Rext(w)} \rho(wa).$$

Consequently, if we assume that each factor is extendable to the left, i.e., that u is recurrent, then, for any factor $w \in \mathcal{L}(u)$ which is neither LS nor RS, both the frequency of the unique edge starting in w and the frequency of the unique edge ending in w is equal to $\rho(w)$. Formally rewritten, this observation has the following reading.

Corollary 2.2.6. *Let u be an infinite recurrent word and let $w \in \mathcal{L}(u)$ be neither LS nor RS. Then $\rho(w) = \rho(aw) = \rho(wb)$, where a stands for the unique left extension of w and b for its unique right extension.*

Reduced Rauzy graphs

As already mentioned, recurrent words are either purely periodic or aperiodic. The factor frequencies of purely periodic words have been described in Section 2.2.6. From now on, we consider exclusively aperiodic recurrent infinite words.

Let us explain how labeled Rauzy graphs may be reduced in order to facilitate the study of frequencies. Assume again that the infinite word u is recurrent and that the frequencies of all factors of $\mathcal{L}(u)$ exist. Then the set of frequencies of factors in $\mathcal{L}_{n+1}(u)$ corresponds to the set of edge labels in Γ_n.

A *simple path* f in Γ_n is a factor of u of length at least $n+1$ such that the only special (RS or LS) factors of length n occurring in f are its prefix and its suffix of length n. If w is the prefix of f of length n and v is the suffix of f of length n, we say that the simple path f starts in w and ends in v. We put the *label of the simple path* equal to the frequency $\rho(f)$ of f. It is not difficult to see that for every factor w of an infinite aperiodic word, there exists a unique shortest BS factor containing w. Therefore, any edge e of Γ_n is a subword of a unique simple path f in Γ_n. Applying finitely many times Corollary 2.2.6, it follows that e and f have the same label, $\rho(e) = \rho(f)$.

The *reduced Rauzy graph* $\tilde{\Gamma}_n$ of u (of order n) is a directed graph whose set of vertices is formed by the LS and RS factors of $\mathcal{L}_n(u)$ and whose set of edges is given by the simple paths, i.e., two vertices w and v are connected with an edge f if there exists in Γ_n a simple path starting in w and ending in v. It follows that Γ_n and $\tilde{\Gamma}_n$ have the same set of edge labels.

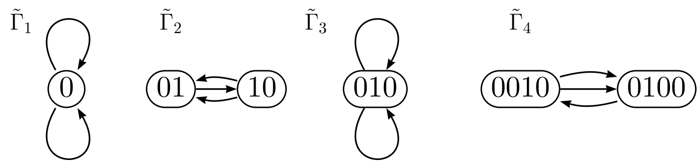


Fig. 2.4: Illustration of the reduced Rauzy graphs obtained from the Rauzy graphs in Figure 2.3.

2.2.13 Substitutions

A detailed overview on this topic is available in Pytheas Fogg [94].

Morphism and substitution

A *substitution* on $\mathcal{A}^*$ is a morphism $\varphi : \mathcal{A}^* \to \mathcal{A}^*$ such that there exists a letter $a \in \mathcal{A}$ and a non-empty word $w \in \mathcal{A}^*$ satisfying $\varphi(a) = aw$ and φ is *non-erasing*, i.e., $\varphi(b) \neq \varepsilon$ for all $b \in \mathcal{A}$. Since any morphism satisfies $\varphi(vw) = \varphi(v)\varphi(w)$ for all $v, w \in \mathcal{A}^*$, a substitution is uniquely determined by the images of letters. Instead of classical $\varphi(a) = w$, we sometimes write $a \to w$. A substitution can be naturally extended to an infinite word $u \in \mathcal{A}^{\mathbb{N}_0}$ by the prescription $\varphi(u) = \varphi(u_0)\varphi(u_1)\varphi(u_2)\ldots$ An infinite word u is said to be a *fixed point* of the substitution φ if it fulfills $u = \varphi(u)$. It is obvious that every substitution φ has at least one fixed point, namely $\lim_{n\to\infty} \varphi^n(a)$ (to be understood with respect to the topology introduced in Section 2.2.2).

Morphisms on $\mathcal{A}^*$, equipped with the operation of composition, form a monoid. Substitutions do not form a monoid for the simple fact that the identity is not a substitution. Nevertheless, if φ is a substitution, φ^n is also a substitution.

A substitution φ is called *uniform* if the images of letters have all the same length; that is, there exists $k \in \mathbb{N}$ such that $|\varphi(a)| = k$ for every $a \in \mathcal{A}$. It is easy to see that a uniform substitution φ is injective if and only if for all $a, b \in \mathcal{A}$, $\varphi(a) = \varphi(b)$ implies $a = b$. A substitution φ is said to be *marked* if the images of letters have mutually different first letters and mutually different last letters; that is, for all $a, b \in \mathcal{A}$, $a \neq b$, the first (last) letter of $\varphi(a)$ is different from the first (last) letter of $\varphi(b)$. Obviously, every marked substitution is injective. The set of letter images $\{\varphi(a) \mid a \in \mathcal{A}\}$ is called a *prefix code* if $\varphi(a)$ is not a prefix of $\varphi(b)$ for any pair $a, b \in \mathcal{A},\ a \neq b$. Analogously, it is called a *suffix code* if $\varphi(a)$ is not a suffix of $\varphi(b)$ for any pair $a, b \in \mathcal{A},\ a \neq b$. Clearly, every substitution whose letter images form a prefix or a suffix code is injective.

Ancestors and synchronization points of substitutions

This section is inspired by Frid [54]. To every substitution φ may be associated the mapping $\psi_{ij} : \mathcal{A}^* \to \mathcal{A}^*$ so that $\psi_{ij}(v)$ is obtained from $\varphi(v)$ by cutting the first i and the last j letters, $|\varphi(v)| > i + j$. Let $w \in \mathcal{A}^*$, $|w| \geq 2$, then the triple $s = (b_0 b_1 \ldots b_n, i, j)$ is an *interpretation* of w if

- either $n = 0$ and $w = \psi_{ij}(b_0)$,
- or $n \geq 1$ and $w = \psi_{ij}(b_0 b_1 \ldots b_n)$, where $|\varphi(b_0)| > i \geq 0$ and $|\varphi(b_n)| > j \geq 0$.

The word $b_0 b_1 \ldots b_n$ is then denoted $a(s)$ and is called the *ancestor* of the interpretation $s = (b_0 b_1 \ldots b_n, i, j)$ or an *ancestor* of w. Every interpretation $s = (b_0 b_1 \ldots b_n, i, j)$ has only one ancestor $b_0 b_1 \ldots b_n$. On the other hand, $b_0 b_1 \ldots b_n$ can be the ancestor of more interpretations (according to the parameters i and j), or, even, an ancestor of more distinct words. Clearly, a word w, $|w| \geq 2$, is a factor of $u = \varphi(u)$ if and only if at least one of its ancestors is a factor of u.

Another closely related term is a synchronization point. Let u be a fixed point of a substitution φ and let v be its factor, then we say that $(v^{(1)}, v^{(2)})$ is a *synchronization point* of v in u if $v = v^{(1)} v^{(2)}$ and whenever $z^{(1)} v z^{(2)} = \varphi(s)$ for some factors $z^{(1)}, z^{(2)}, s \in \mathcal{L}(u)$, then there exist factors $s^{(1)}, s^{(2)} \in \mathcal{L}(u)$ satisfying

$$s = s^{(1)} s^{(2)}, \quad z^{(1)} v^{(1)} = \varphi(s^{(1)}), \quad v^{(2)} z^{(2)} = \varphi(s^{(2)}).$$

Example 2.2.7. *Let φ be a substitution on $\{0, 1\}$ defined by $\varphi(0) = 01$, $\varphi(1) = 10$. This substitution is known as the Thue-Morse substitution. φ is uniform, marked, and $\{\varphi(0), \varphi(1)\}$ is both a prefix code and a suffix code. (More generally, every marked substitution φ on $\mathcal{A}$ satisfies that $\{\varphi(a) \mid a \in \mathcal{A}\}$ is both a prefix and a suffix code.) Furthermore, every factor of the form $waaw' \in \mathcal{L}(u)$, $a \in \mathcal{A}$, has the synchronization point (wa, aw'). It is not difficult to see that $waaw'$ has a unique interpretation, and, therefore, a unique ancestor. (It is a general truth for any fixed point of a uniform marked substitution that if a factor has a synchronization point, then it has a unique interpretation.)*

Substitution matrix

The following prescription associates to every substitution φ on an alphabet $\mathcal{A} = \{a_1, a_2, \ldots, a_d\}$ a non-negative integer $d \times d$ matrix, called the *substitution matrix* M_φ:

$$M_\varphi = \begin{pmatrix} |\varphi(a_1)|_{a_1} & |\varphi(a_1)|_{a_2} & \cdots & |\varphi(a_1)|_{a_d} \\ |\varphi(a_2)|_{a_1} & |\varphi(a_2)|_{a_2} & \cdots & |\varphi(a_2)|_{a_d} \\ \vdots & \vdots & \ddots & \vdots \\ |\varphi(a_d)|_{a_1} & |\varphi(a_d)|_{a_2} & \cdots & |\varphi(a_d)|_{a_d} \end{pmatrix}. \tag{2.18}$$

As an immediate consequence of the definition, it holds for any word w that

$$(|w|_{a_1}, |w|_{a_2}, \dots, |w|_{a_d})M_\varphi = (|\varphi(w)|_{a_1}, |\varphi(w)|_{a_2}, \dots, |\varphi(w)|_{a_d}). \tag{2.19}$$

The substitution matrix of the composition of substitutions $\varphi,\ \psi$ obeys the formula $M_{\varphi\circ\psi} = M_\psi M_\varphi$. We have, in particular,

$$M_{\varphi^k} = (M_\varphi)^k. \tag{2.20}$$

Example: *The substitution φ defined on $\{0,1,2\}$ by $\varphi(0) = 01,\ \varphi(1) = 120,\ \varphi(2) = 2$ has the following substitution matrix:*

$$M_\varphi = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix}.$$

Mind the fact that the same substitution matrix corresponds to several other substitutions; for instance, $\theta(0) = 10,\ \theta(1) = 102,\ \theta(2) = 2$.

Primitive substitutions

A substitution φ on an alphabet $\mathcal{A}$ is called *primitive* if there exists $k \in \mathbb{N}$ such that for any $a \in \mathcal{A}$, the word $\varphi^k(a)$ contains all letters of $\mathcal{A}$.

Proposition 2.2.8. *Any two fixed points of a primitive substitution φ generate the same language.*

Proof. Let $u^{(1)} = \lim_{n\to\infty} \varphi^n(a)$ and $u^{(2)} = \lim_{n\to\infty} \varphi^n(b)$ be two fixed points of φ on $\mathcal{A}$, $a, b \in \mathcal{A}$. Let us take any factor $w \in \mathcal{L}(u^{(1)})$, then there exists $n \in \mathbb{N}$ such that w is a subword of $\varphi^n(a)$. Since the substitution φ is primitive, there exists $k \in \mathbb{N}$ such that $\varphi^k(b)$ contains the letter a, consequently, $\varphi^n(a)$ is a subword of $\varphi^{k+n}(b)$. It follows that $w \in \mathcal{L}(u^{(2)})$. The opposite inclusion can be proved in a similar way. $\square$

Example: *Notorious primitive substitutions and their basic properties.*

- *Fibonacci substitution* $0 \to 01,\ 1 \to 0$ is injective, $\{\varphi(0), \varphi(1)\}$ is a suffix code, but not a prefix code.
- *Thue-Morse substitution* $0 \to 01,\ 1 \to 10$ is uniform, marked, injective, and $\{\varphi(0), \varphi(1)\}$ is both a prefix and a suffix code.

  It is easy to check that $\varphi^n(0) = S(\varphi^n(1))$, where S is the morphism exchanging letters, i.e., $S(0) = 1,\ S(1) = 0$.
- *Period-doubling substitution* $0 \to 01,\ 1 \to 00$ is uniform and injective.

Perron-Frobenius theorem

Let us recall a notion from matrix theory, which proves useful in the study of substitutions. A matrix M is called *primitive* if there exists $k \in \mathbb{N}$ such that all entries of M^k are positive. Applying Equation (2.20), we notice immediately that a substitution matrix is primitive if and only if the corresponding substitution is primitive. There is a powerful theorem treating primitive matrices, being thus relevant for primitive substitution matrices.

Theorem 2.2.9 (Perron-Frobenius)**.** *Let M be a $d \times d$ primitive matrix. Then:*

1. *the matrix M has a positive eigenvalue λ which is strictly greater than the modulus of any other eigenvalue,*
2. *the eigenvalue λ is algebraically simple, i.e., it is a single root of the characteristic polynomial,*
3. *to this eigenvalue corresponds an eigenvector with positive entries, while no other eigenvalue has an eigenvector with positive entries.*

The eigenvalue λ from the above theorem is called the *Perron-Frobenius eigenvalue* of M. If M is a substitution matrix, then, as a consequence of Item *1.* and of the fact that M is an integer matrix, λ is a Perron number (defined in Section 2.1.4). For fixed points of a primitive substitution φ on $\mathcal{A} = \{a_1, \ldots, a_d\}$, according to the result of Durand [45], the factor frequencies exist and the vector of letter frequencies is equal to the left eigenvector $(l_1,\ l_2, \ldots, l_d)$ of λ normalized by $\sum_{i=1}^{d} l_i = 1$, i.e.,

$$\big(\rho(a_1),\ \rho(a_2), \ldots, \rho(a_d)\big) = (l_1,\ l_2, \ldots, l_d). \tag{2.21}$$

Geometrical representation of substitutions

Every fixed point $u = u_0u_1u_2\ldots$ of a primitive substitution φ on $\mathcal{A} = \{a_1, \ldots, a_d\}$ with the substitution matrix M may be represented by a self-similar set $T = \{t_n \mid n \in \mathbb{N}_0\}$ constructed in the following way: Take a positive right eigenvector $r = (r_1, \ldots, r_d)$ of the Perron-Frobenius eigenvalue λ and define recurrently a sequence (t_n)

$$t_0 = 0 \quad \text{and} \quad t_{n+1} = t_n + r_i \quad \text{if } u_n = a_i.$$

Let v be a prefix of u, then, using the definition of (t_n), Equation (2.19), and the properties of the right eigenvector, it follows that

$$\begin{aligned} t_{|\varphi(v)|} &= (|\varphi(v)|_{a_1}, |\varphi(v)|_{a_2}, \ldots, |\varphi(v)|_{a_d})\, r^T \\ &= (|v|_{a_1}, |v|_{a_2}, \ldots, |v|_{a_d}) M r^T \\ &= \lambda(|v|_{a_1}, |v|_{a_2}, \ldots, |v|_{a_d}) r^T \\ &= \lambda t_{|v|}. \end{aligned}$$

Hence, $\lambda T \subset T$; in other words, T is a self-similar set with the self-similarity factor λ.

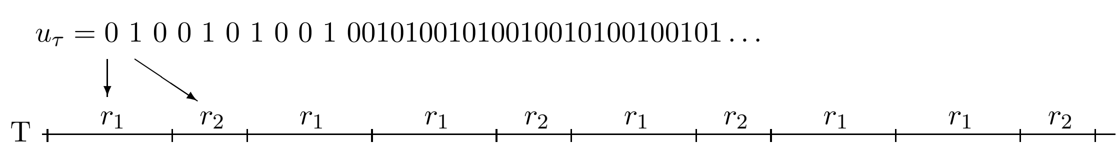


Fig. 2.5: Illustration of the self-similar set T with the self similarity factor $\lambda = \tau = \frac{1+\sqrt{5}}{2}$ associated with the fixed point u_τ of the Fibonacci substitution $\varphi(0) = 01,\ \varphi(1) = 0$. Any multiple of the vector $(1, \frac{1}{\tau})$ is a right eigenvector of τ. If we choose the vector $(r_1, r_2) = (1, \frac{1}{\tau})$, then T is equal to the set of non-negative τ-integers $\mathbb{Z}_\tau^+$ (as explained in Section 2.3).

Factor complexity of fixed points of substitutions

The complexity $\mathcal{C}$ of a fixed point of a substitution cannot be of any form, as brought to light by Pansiot in [90, 91]:

$$K_1 f(n) \leq \mathcal{C}(n) \leq K_2 f(n),$$

where K_1, K_2 are positive constants and $f(n)$ is one of the functions $1,\ n,\ n\log\log n,\ n\log n,\ n^2$.

In the sequel, let us explain that for fixed points of primitive substitutions, their complexity is even sublinear. Fixed points of primitive substitutions are known to be not only uniformly recurrent (Queffélec [95]), but Damanik and Zare in [39] have shown that they are even linearly recurrent. Finally, Durand has proved in [45] that for every linearly recurrent infinite word, thus, in particular, for every fixed point of a primitive substitution, there exists a constant K satisfying $\mathcal{C}(n) \leq Kn$ for every $n \in \mathbb{N}$.

2.3 Infinite words associated with beta-integers

With the background of combinatorics on words at hand, we can continue in the introduction of notions concerning the set $\mathbb{Z}_\beta$ of β-integers, initiated in Section 2.1. Here, our aim is to associate with β-integers infinite words which symbolically code distances between consecutive β-integers.

2.3.1 Parry numbers and infinite words u_β

From the formula for distances (2.8), we know that the number of distances between neighboring elements of $\mathbb{Z}_\beta$ is finite if and only if the Rényi expansion of unity $d_\beta(1)$ is eventually periodic; that is, if β is a Parry number.

- If $d_\beta(1)$ is finite, i.e., $d_\beta(1) = t_1 t_2 \dots t_m$, $t_m \neq 0$, β is said to be a *simple Parry number*, and the set of distances is $\{\Delta_0, \Delta_1, \dots, \Delta_{m-1}\}$, where all of the listed elements are mutually distinct.

- If $d_\beta(1)$ is eventually periodic, but not finite, β is a *non-simple Parry number*. Choose $r, m \in \mathbb{N}$ to be minimal such that $d_\beta(1) = t_1 t_2 \dots t_m (t_{m+1} \dots t_{m+r})^\omega$, then the set of all mutually distinct distances is $\{\Delta_0, \Delta_1, \dots, \Delta_{m+r-1}\}$.

Let us precisely define the infinite word $u_\beta = u_0 u_1 u_2 \dots$ associated with $\mathbb{Z}_\beta^+$ for a Parry number β. Let $\{\Delta_0, \dots, \Delta_{d-1}\}$ be the set of distances between neighboring β-integers and let $(b_n)_{n=0}^{\infty}$ be as defined in (2.7), then

$$u_n := i \quad \text{if} \quad b_{n+1} - b_n = \Delta_i. \tag{2.22}$$

2.3.2 Canonical substitutions for Parry numbers

Fabre in [49] has associated with Parry numbers canonical substitutions in the following way.

Let β be a simple Parry number, i.e., $d_\beta(1) = t_1 t_2 \dots t_m$, for $m \in \mathbb{N}$. Then the corresponding canonical substitution φ is defined on the alphabet $\{0, 1, \dots, m-1\}$ by

$$\begin{array}{rcl} \varphi(0) & = & 0^{t_1}1, \\ \varphi(1) & = & 0^{t_2}2, \\ & \vdots & \\ \varphi(m-2) & = & 0^{t_{m-1}}(m-1), \\ \varphi(m-1) & = & 0^{t_m}. \end{array} \tag{2.23}$$

Similarly, let β be a non-simple Parry number, i.e., $d_\beta(1) = t_1t_2 \dots t_m(t_{m+1} \dots t_{m+r})^\omega$. Then the associated canonical substitution φ is defined on the alphabet $\{0, 1, \dots, m + r - 1\}$ by

$$\begin{array}{rcl} \varphi(0) & = & 0^{t_1}1, \\ \varphi(1) & = & 0^{t_2}2, \\ & \vdots & \\ \varphi(m-1) & = & 0^{t_m}m, \\ & \vdots & \\ \varphi(m+r-2) & = & 0^{t_{m+r-1}}(m+r-1), \\ \varphi(m+r-1) & = & 0^{t_{m+r}}m. \end{array} \tag{2.24}$$

Each of these substitutions has a unique fixed point, namely $\lim_{n\to\infty} \varphi^n(0)$. Moreover, this fixed point turns out to coincide with u_β defined in (2.22). Both substitutions are primitive and $\varphi(\mathcal{A})$ is a suffix code in the case of simple Parry numbers (2.23) and a prefix code in the case of non-simple Parry numbers (2.24).

2.3.3 Combinatorial properties of u_β

The infinite words u_β associated with both simple and non-simple Parry numbers are uniformly recurrent due to the fact that they are fixed points of primitive substitutions.

In some aspects, languages closed under reversal are of particular interest – for instance, in the study of palindromes, as confirmed by Proposition 2.2.3. Let us specify how the Rényi expansion of unity $d_\beta(1)$ has to look like so that the language of u_β is closed under reversal.

Proposition 2.3.1 ([57])**.** *Let u_β be an infinite word associated with a simple Parry number β with $d_\beta(1) = t_1t_2 \dots t_m$. Then $\mathcal{L}(u_\beta)$ is closed under reversal if and only if $t_1 = \cdots = t_{m-1}$.*

A simple Parry number β with $d_\beta(1) = t_1t_2 \dots t_m$ satisfying $t_1 = \cdots = t_{m-1}$ is called a *confluent* Parry number.

Proposition 2.3.2 ([12])**.** *Let u_β be an infinite word associated with a non-simple Parry number β with $d_\beta(1) = t_1t_2 \dots t_m(t_{m+1} \dots t_{m+r})^\omega$, m, r chosen to be minimal. Then $\mathcal{L}(u_\beta)$ is closed under reversal if and only if $m = r = 1$.*

The previous proposition may be reformulated as follows:
Among non-simple Parry numbers β, $\mathcal{L}(u_\beta)$ is closed under reversal if and only if β is quadratic.

2.3.4 Quadratic Parry numbers

The base β being a quadratic Parry number is the simplest generalization of an integer base, with respect to the Rényi expansion of unity.

There are several other reasons for an exceptional position of quadratic numbers among Parry numbers. Firstly, they can be entirely characterized by their algebraic properties since the notions of Parry and Pisot number coincide for β being a quadratic number. Secondly, it results from Section 2.3.3 that an infinite word u_β has language closed under reversal for any quadratic Parry number β. Finally, if we search for Sturmian words among the infinite words u_β, it is meaningful to take into account only quadratic Parry numbers, for the simple reason that Sturmian words are binary.

1. **Simple quadratic Parry numbers**
   The Rényi expansion of unity is equal to $d_\beta(1) = pq$, where $p \geq q \geq 1$. Hence, β is the positive root of the polynomial $x^2 - px - q$. Only two distances occur between neighboring β-integers: the longer distance is always $\Delta_0 = 1$, the smaller one is equal to $\Delta_1 = \beta - p$. The associated substitution φ is given by

$$\varphi(0) = 0^p 1, \quad \varphi(1) = 0^q, \tag{2.25}$$

   and its fixed point is

$$u_\beta = \underbrace{\underbrace{0^p1 \ \dots \ 0^p1}_{p \text{ times}} \ 0^q \ \underbrace{0^p1 \ \dots \ 0^p1}_{p \text{ times}} \ 0^q \ \dots \ \underbrace{0^p1 \ \dots \ 0^p1}_{p \text{ times}}}_{p \text{ times}} \ 0^q \ \underbrace{0^p1 \ \dots \ 0^p1}_{q \text{ times}} \ \dots \tag{2.26}$$

   The substitution matrix is of the form $\begin{pmatrix} p & 1 \\ q & 0 \end{pmatrix}$ and it is easy to verify that the substitution is primitive.

   Example 2.3.3. *For $\beta = \tau = \frac{1+\sqrt{5}}{2}$, we know already that $d_\tau(1) = 11$. The substitution φ associated with τ is the Fibonacci substitution defined by $\varphi(0) = 01$, $\varphi(1) = 0$.*

2. **Non-simple quadratic Parry numbers**
   The Rényi expansion of unity is equal to $d_\beta(1) = pq^\omega$, where $p > q \geq 1$. Consequently, β is the larger root of the polynomial $x^2 - (p+1)x + p - q$. The set $\mathbb{Z}_\beta$ has again two distances between neighbors: $\Delta_0 = 1$ and $\Delta_1 = \beta - p$. The corresponding substitution is

$$\varphi(0) = 0^p 1, \quad \varphi(1) = 0^q 1, \tag{2.27}$$

   and its fixed point starts as follows

$$u_\beta = \underbrace{\underbrace{0^p1 \ \dots \ 0^p1}_{p \text{ times}} \ 0^q1 \ \underbrace{0^p1 \ \dots \ 0^p1}_{p \text{ times}} \ 0^q1 \ \dots \ \underbrace{0^p1 \ \dots \ 0^p1}_{p \text{ times}}}_{p \text{ times}} \ 0^q1 \ \underbrace{0^p1 \ \dots \ 0^p1}_{q \text{ times}} 0^q1 \ \dots \tag{2.28}$$

   The substitution matrix is $\begin{pmatrix} p & 1 \\ q & 1 \end{pmatrix}$ and φ is thus obviously primitive.

As an example, consider the infinite word u_β whose prefix is drawn in Figure 2.1 and that is the fixed point of the substitution $\varphi(0) = 0001$, $\varphi(1) = 01$.

To conclude, let us reveal the relation between infinite words associated with β-integers and Sturmian words, which is the topic of the next chapter.

Remark 2.3.4. *A result by Crisp et al. [33] concerning substitution matrices says that the only candidates for Sturmian words among the infinite words u_β are those ones with β being a quadratic unit. Conversely, such words u_β turn out to be Sturmian. Let us recall that among Parry numbers, β is a quadratic unit if,*

1. *in case of simple Parry numbers, β is a root of*

$$x^2 - px - 1, \quad p \in \mathbb{N}, \tag{2.29}$$

2. *in case of non-simple Parry numbers, β is a root of*

$$x^2 - (p+1)x + 1, \quad p \geq 2, \quad p \in \mathbb{N}. \tag{2.30}$$

2.4 Sturmian words

There exist plenty of publications on Sturmian words. We recommend Chapter 2 of the Lothaire book [84] for a self-contained survey.

2.4.1 Equivalent combinatorial definitions

Sturmian words are defined as words with the complexity $\mathcal{C}(n) = n + 1$ for all $n \in \mathbb{N}_0$. This condition requires a binary alphabet. Thanks to the remarkable fact that Sturmian words are aperiodic words with the lowest possible complexity, they have been always extensively studied. Naturally, several equivalent definitions of Sturmian words have been found out. The following theorem summarizes their well-known combinatorial characterizations (proved in [67], [107], [44]).

Theorem 2.4.1. *Let u be an infinite word. The properties listed below are equivalent:*

- *u is Sturmian,*
- *u is aperiodic and balanced,*
- *any factor of u has exactly two return words,*
- *u contains one palindrome of every even length and two palindromes of every odd length.*

The previous theorem implies immediately further properties of Sturmian words. They are uniformly recurrent, their language is closed under reversal, and each factor w contains exactly $|w| + 1$ palindromes; that is, Sturmian words are full.

2.4.2 Explicit arithmetical formulae

Hedlund and Morse have chosen the name *Sturmian sequence* because such sequences emerged when they were studying zeroes of the solutions of a differential equation of Sturm-Liouville type, more precisely, the number of zeroes of the solutions in the intervals $[n, n+1)$. They have shown that for any $0 < \alpha < 1$, the solution is of the form $\sin(\pi(\alpha x + \rho))$; hence, the number of zeroes in $[n, n+1)$ equals either $\overline{s}_{\alpha,\rho}(n)$ or $\underline{s}_{\alpha,\rho}(n)$, where

$$\overline{s}_{\alpha,\rho}(n) = \lceil \alpha(n+1) + \rho \rceil - \lceil \alpha n + \rho \rceil, \tag{2.31}$$

$$\underline{s}_{\alpha,\rho}(n) = \lfloor \alpha(n+1) + \rho \rfloor - \lfloor \alpha n + \rho \rfloor. \tag{2.32}$$

The sequence $\left(\overline{s}_{\alpha,\rho}(n)\right)_{n=0}^{\infty}$ is nowadays called an *upper mechanical word* and $\left(\underline{s}_{\alpha,\rho}(n)\right)_{n=0}^{\infty}$ a *lower mechanical word*. The below listed properties of mechanical words are easy to check

1. their alphabet is $\{0, 1\}$,
2. if α is rational, then they are periodic,
3. if α is irrational, then $\lceil \alpha n + \rho \rceil = \lfloor \alpha n + \rho \rfloor + 1$ whenever $\alpha n + \rho$ is not an integer, therefore
    - if $\rho \neq 0$, then $\overline{s}_{\alpha,\rho}(n) = \underline{s}_{\alpha,\rho}(n)$ for all $n \in \mathbb{N}_0$,
    - if $\rho = 0$, then $\overline{s}_{\alpha,0}(n) = \underline{s}_{\alpha,0}(n)$ for all $n \in \mathbb{N}$, however, $\overline{s}_{\alpha,0}(0) = 1$ and $\underline{s}_{\alpha,0}(0) = 0$.

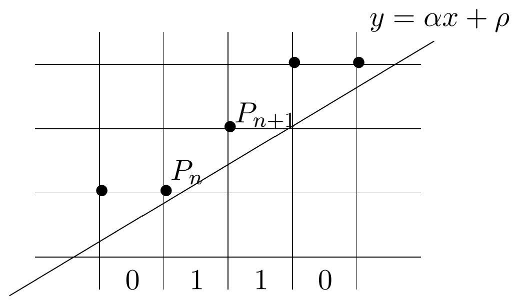


Fig. 2.6: Illustration of the construction of an upper mechanical word.

The parameter α is called the *slope* and ρ the *intercept* of the mechanical word since such a word may be visualized in the lattice $\mathbb{Z}^2$ using the line $y = \alpha x + \rho$.

To obtain the upper mechanical word, the lattice points P_n of $\mathbb{Z}^2$ just above the line are considered, their coordinates are $P_n = (n, \lceil \alpha n + \rho \rceil)$. If the line segment joining two consecutive lattice points P_n and P_{n+1} is horizontal, then $\overline{s}_{\alpha,\rho}(n) = 0$, if it is diagonal, then $\overline{s}_{\alpha,\rho}(n) = 1$. See Figure 2.6. The lower mechanical word can be constructed analogously, using the lattice points below the line instead.

The particular importance of mechanical words comes to light thanks to the following theorem proved by Hedlund and Morse [67].

Theorem 2.4.2. *An infinite word u is Sturmian if and only if u is a mechanical word with an irrational slope.*

The geometrical interpretation of mechanical words and the homogeneity of the lattice $\mathbb{Z}^2$ guarantee that the language of any Sturmian word depends only on the slope, not on the intercept.

2.4.3 Words coding 2-interval exchange transformation

Another synoptic algorithm providing Sturmian words is the *2-interval exchange transformation*. Take any $0 < \alpha < 1$ and make a partition of the unit interval $I = [0, 1)$ into two subintervals $[0, 1-\alpha)$ and $[1-\alpha, 1)$. Define the *interval exchange map* $T : [0, 1) \to [0, 1)$ by $T(x) = \{x + \alpha\}$ (see Figure 2.7). Choose a point $\rho \in I$ and write down the infinite word $u = u_0 u_1 u_2 \ldots$ given by

$$u_n := \begin{cases} 0 & \text{if } \ T^n(\rho) \ \in [0, 1-\alpha), \\ 1 & \text{if } \ T^n(\rho) \ \in [1-\alpha, 1). \end{cases}$$

The obtained word u is called a *2-interval exchange transformation coding word* and it is readily seen that u coincides with the lower mechanical word $\big(\underline{s}_{\alpha,\rho}(n)\big)_{n=0}^{\infty}$. The 2-interval exchange transformation may be visualized as the rotation of a chosen point ρ of the unit circle by an angle α. The circle is dissected into two disjoint arcs of lengths $1-\alpha$ and α. In order to get the 2-interval exchange transformation coding word, we write down 0 each time when the rotation moves ρ onto the arc of length $1-\alpha$, we note down 1 otherwise.

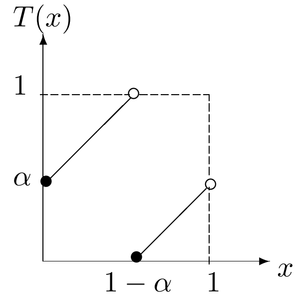


Fig. 2.7: Illustration of the interval exchange map T.

2.4.4 One-dimensional cut & project sets

Before we describe the construction of 1-dimensional C&P sets, let us recall that a general definition of higher-dimensional C&P sets as well as the construction of a 1-dimensional Fibonacci C&P set have been presented in the introductory part of the thesis.

Let ϵ, η be two distinct irrational numbers and Ω a bounded non-degenerated interval. Then the set

$$\Sigma_{\epsilon,\eta}(\Omega) = \{a + b\eta \mid a, b \in \mathbb{Z},\ a + b\epsilon \in \Omega\}$$

is called a *cut & project set with the acceptance window* Ω. It is easy to see that, up to a scaling factor, this set can be obtained by the projection of the lattice $\mathbb{Z}^2$ on the line $y = \epsilon x$ along the line $y = \eta x$ (as illustrated in Figure 2.8). We do not project all points of $\mathbb{Z}^2$, but only those ones belonging to a stripe parallel to the line $y = \epsilon x$. The position of the stripe is given by the interval Ω.

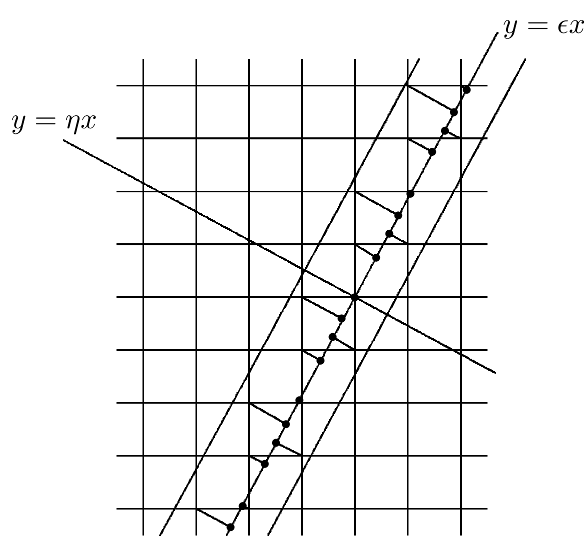


Fig. 2.8: Construction of a one-dimensional C&P set.

The results by Guimond, Masáková, and Pelantová from [65] detail the geometrical structure of $\Sigma_{\epsilon,\eta}(\Omega)$ and bring to light the relation between Sturmian words and words coding distances in C&P sets.

Theorem 2.4.3. *For any C&P set $\Sigma_{\epsilon,\eta}(\Omega)$, there exist two positive numbers Δ_1 and Δ_2 such that the distances between consecutive points in $\Sigma_{\epsilon,\eta}(\Omega)$ take values in $\{\Delta_1, \Delta_2, \Delta_1+\Delta_2\}$.*

Coding distances in $\Sigma_{\epsilon,\eta}(\Omega)$, we get a binary or ternary biinfinite word $\dots u_{-2}u_{-1}u_0u_1u_2\dots$. If the biinfinite word coding $\Sigma_{\epsilon,\eta}(\Omega)$ is binary, then its right-sided part $u_0u_1u_2\dots$ is a Sturmian word. In addition, it has been proved that parameters ϵ, η and the acceptance window Ω can be chosen so that the words coding the C&P set with such parameters coincide with mechanical words. More precisely, for $0<\alpha<1$, α irrational, $0 \le \rho < 1$, and $\eta > 0$, the distances between consecutive non-negative elements

- in the C&P set $\Sigma_{-\alpha,\eta}(\rho-1,\rho]$ form the sequence
$$\big(\eta + \lfloor \alpha(n+1)+\rho\rfloor - \lfloor \alpha n+\rho\rfloor\big)_{n=0}^{\infty};$$
hence, the lower mechanical word $\big(\underline{s}_{\alpha,\rho}(n)\big)_{n=0}^{\infty}$ coincides with the word coding the non-negative part of $\Sigma_{-\alpha,\eta}(\rho-1,\rho]$,
- in the C&P set $\Sigma_{-\alpha,\eta}[\rho,\rho+1)$ form the sequence
$$\big(\eta + \lceil \alpha(n+1)+\rho\rceil - \lceil \alpha n+\rho\rceil\big)_{n=0}^{\infty};$$
therefore, the upper mechanical word $\big(\overline{s}_{\alpha,\rho}(n)\big)_{n=0}^{\infty}$ coincides with the word coding the non-negative part of $\Sigma_{-\alpha,\eta}[\rho,\rho+1)$.

2.4.5 Generalizations of Sturmian words

We have seen that Sturmian words can be defined in many equivalent ways. As a matter of course, various generalizations to multilateral alphabets have been suggested and studied. We often refer to two of them (for details see [43] and [53], respectively).

Arnoux-Rauzy words (or *AR words* for simplicity) are infinite words over an m-letter alphabet containing exactly one LS factor w and one RS factor v of every length n, and both of these factors have m-extensions, i.e., $\#\mathit{Lext}(w) = \#\mathit{Rext}(v) = m$. The language of AR words turns out to be closed under reversal and AR words are uniformly recurrent. AR words form a subclass of extensively studied *episturmian words*, defined as infinite words that have language closed under reversal and contain at most one LS factor of every length.

Another possible generalization of Sturmian words (based on the definition from Section 2.4.3) is provided by *m-interval exchange transformation coding words*. Let us state their definition. Take positive numbers $\alpha_1,\dots,\alpha_m$ linearly independent over $\mathbb{Q}$ and such that $\sum_{i=1}^m \alpha_i = 1$. They define a partition of the interval $I=[0,1)$ into m subintervals
$$I_k = \Big[\sum_{i=1}^{k-1}\alpha_i, \sum_{i=1}^{k}\alpha_i\Big),\ k=1,2,\dots,m.$$
In general, the subintervals may be exchanged according to any permutation, however, the language of the word coding m-interval exchange transformation is closed under reversal only for the symmetric permutation $\pi(1)=m$, $\pi(2)=m-1,\dots,\pi(m)=1$. The interval exchange transformation associated with $\alpha_1,\dots,\alpha_m$ and π is the bijection $T:[0,1)\to[0,1)$ which exchanges the intervals I_k according to the permutation π, i.e.,
$$T(x) = x + \sum_{i>k}\alpha_i - \sum_{i<k}\alpha_i \quad \text{for} \quad x\in I_k.$$

The infinite word $u = u_0u_1u_2\dots$ over $\mathcal{A} = \{a_1, \dots, a_m\}$ associated with T is defined as

$$u_n := a_k \quad \text{if} \quad T^n(x) \in I_k$$

and is called an *m-interval exchange transformation coding word* (or an *m-iet word* for short). Its language does not depend on the position of the starting point x, but only on the transformation T. The 3-iet words can be geometrically represented by C&P sequences [65].

If we generalize the properties from Theorem 2.4.1 for an m-letter alphabet, they are never more characteristic, or, even, are not true for AR words and m-iet words. It will come to light in the forthcoming chapters that always start with a note on Sturmian words, AR words, and m-iet words for every studied combinatorial characteristics.

Chapter 3

Special factors and complexity

The computation of the factor complexity of infinite words (defined in (2.12) in Section 2.2.8) is a very complex problem, even for words with relatively low complexity.

As shown by Hedlund and Morse in [66], an infinite word is either eventually periodic and its complexity is bounded, or it is aperiodic and its complexity satisfies $\mathcal{C}(n) \geq n + 1$ for all $n \in \mathbb{N}_0$. So, for instance, $f(n) = \sqrt{n}$ cannot be the factor complexity of any infinite word. The periodic word a^ω has the complexity $\mathcal{C}(n) = 1$ for all $n \in \mathbb{N}_0$, while the Champernowne word $011011100101110111\ldots$, formed by concatenation of the binary expansions of non-negative integers, satisfies $\mathcal{C}(n) = 2^n$ for every $n \in \mathbb{N}_0$. These two examples are extreme; it holds for every infinite word over an alphabet $\mathcal{A}$ that $1 \leq \mathcal{C}(n) \leq (\#\mathcal{A})^n$ for all $n \in \mathbb{N}_0$. It is further evident that $\mathcal{C}(n)$ is a non-decreasing function satisfying $\mathcal{C}(m + n) \leq \mathcal{C}(m)\mathcal{C}(n)$. Nevertheless, in general, the question which functions may be the factor complexity of an infinite word is far from being answered. A detailed survey in this direction has been effected by Ferenczi in [50].

We present in this chapter, following mainly the survey by Cassaigne [27], special factors and some related terminology and tools, simplifying the derivation of factor complexity and being of great importance also in many consecutive chapters – for the study of palindromic complexity, recurrence function, and return words, or, factor frequencies. We consider separately the binary and multilateral case, firstly, since it is instructive to observe foremost the simpler case, secondly, since the infinite word u_β associated with a quadratic non-simple Parry number β, which is often in the center of our interest, is binary. Afterwards, as we concentrate in this thesis exclusively on infinite words with sublinear complexity, we sum up what is known about such infinite words. Moreover, we provide a summary of known results on special factors and complexity for some selected infinite words and classes of words with sublinear complexity – the Thue-Morse word, the period doubling word, the Rote word, a palindromeless reversal closed word, the infinite words associated with simple and non-simple Parry numbers – with an eye illustrating studied characteristics and methods in the forthcoming chapters for this "sample". As a new result, we describe the special factors and the factor complexity of u_β associated with a quadratic non-simple Parry number β.

3.1 Special factors over a binary alphabet

Let us first restrict our considerations to an infinite word u over a binary alphabet, say $\{0, 1\}$.

3.1.1 Classification of special factors

Three situations can come up for a BS factor $w \in \mathcal{L}(u)$, with respect to the number of elements of $\mathcal{L}(u) \cap \{0w0, 0w1, 1w0, 1w1\}$:

- If the cardinality is maximal, i.e., all four elements $0w0, 0w1, 1w0$, and $1w1$ are factors of u, then w is called a *strong* BS factor.
- If exactly three elements are factors of u, then w is called an *ordinary* BS factor.
- Finally, if only two elements are in the set, it means either $0w0, 1w1 \in \mathcal{L}(u)$ or $0w1, 1w0 \in \mathcal{L}(u)$, then w is called a *weak* BS factor.

Let us also classify LS factors and bring to light the connection between LS and BS factors. The classification of RS factors is analogous. A LS factor $w \in \mathcal{L}(u)$ belongs to one of the following types according to its extensibility to the right:

- If both $w0$ and $w1$ are LS, then w is a strong BS factor.
- If only one of the factors $w0$, $w1$ is LS, then w is called an *ordinary* LS factor. If w is moreover RS, then w is an ordinary BS factor.
- If neither $w0$ nor $w1$ is LS, then w is a weak BS factor. In the context of LS factors, w is usually called *maximal* LS factor (in order to express the impossibility of its extensibility to the right staying LS).

3.1.2 Infinite LS branches

Another important term concerning LS factors is an *infinite LS branch*, which is an infinite word whose all prefixes are LS factors of $\mathcal{L}(u)$. An *infinite RS branch* is defined symmetrically, so, it is a left-sided infinite word whose all suffixes are RS factors. Since every LS factor in $\mathcal{L}(u)$ is extendable to the right, it is either a prefix of a maximal LS factor or of an infinite LS branch.

3.1.3 Tree of LS factors

There exists a natural visualization tool of special factors- the *tree of LS factors* visualizing LS factors (growing to the right) and the *tree of RS factors* visualizing RS factors (growing to the left), respectively. Let us explain how the tree of LS factors is constructed. At the level n in the tree, branches starting in the root correspond to different LS factors of length n. According to the type of a LS factor, the following evolution can occur for a branch labeled with a LS factor w of length n:

- If w is an ordinary LS factor, then w can be uniquely extended to the right staying LS, and, hence, there is a unique branch of length $n+1$ starting in the root whose label has w as a prefix.
- If w is a maximal LS factor, then the branch w is truncated at the level n.
- If w is a strong BS factor, then there is a branching in the tree at the level n; that is, there are two branches of length $n+1$ whose labels have w as a prefix.

Let us discuss the form of the trees of LS and RS factors for eventually periodic and aperiodic words, both recurrent and non-recurrent.

Eventually periodic words: Since $\mathcal{C}(n)$ is bounded, there exists $n \in \mathbb{N}$ such that $\Delta\mathcal{C}(n) = 0$. For a recurrent word (it is necessarily periodic), applying Formula (2.15), we see that the tree of LS factors is finite. For a non-recurrent word u, we deduce from Remark 2.2.2 that the tree of LS factors contains exactly one infinite LS branch, and, possibly, a finite

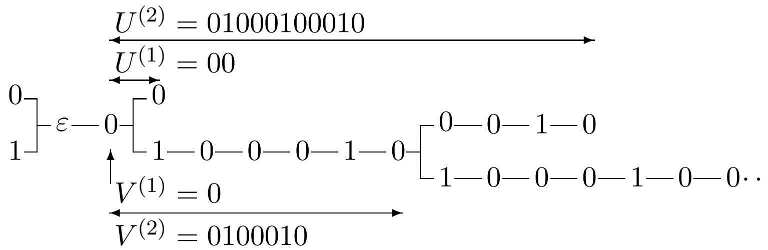


Fig. 3.1: Illustration of the tree of LS factors for the infinite word u_β being the fixed point of the substitution $\varphi(0) = 0001,\ \varphi(1) = 01$ (see also Example 2.1.5). The two shortest strong BS factors $V^{(1)},\ V^{(2)}$ as well as the two shortest maximal LS factors (or, equivalently, weak BS factors) $U^{(1)},\ U^{(2)}$ are pointed out.

number of truncated branches. More precisely, if $u = wv^\omega$, where w and v are chosen to be minimal, then the infinite LS branch is equal to v^ω.

Aperiodic words: Since $\Delta\mathcal{C}(n) \geq 1$ for every $n \in \mathbb{N}$, the tree of LS factors contains, for every $n \in \mathbb{N}$, at least one branch of length n, both for recurrent and non-recurrent words.

3.1.4 The first and the second difference of complexity

The formula for the first difference of complexity from (2.15) takes a simpler form in the case of a binary alphabet.

Proposition 3.1.1. *Let u be an infinite recurrent word on $\{0, 1\}$. Then, for every $n \in \mathbb{N}_0$,*

$$\Delta\mathcal{C}(n) \quad = \quad \#\{w \in \mathcal{L}_n(u) \mid w \text{ is LS}\} \quad = \quad \#\{w \in \mathcal{L}_n(u) \mid w \text{ is RS}\}. \tag{3.1}$$

To compute complexity, we have at disposal also the formula for *the second difference of complexity* $\Delta^2\mathcal{C}(n) = \Delta\mathcal{C}(n+1) - \Delta\mathcal{C}(n)$. Using Proposition 3.1.1, we obtain immediately $\Delta^2\mathcal{C}(n) = \#\{w \in \mathcal{L}_{n+1}(u) \mid w \text{ LS}\} - \#\{w \in \mathcal{L}_n(u) \mid w \text{ LS}\}$. From the description of the tree of LS factors, it is straightforward to deduce that the number of LS factors increases by 1 for every strong BS factor (branching) and decreases by 1 for every maximal LS factor = weak BS factor (truncated branch).

Proposition 3.1.2. *Let u be an infinite recurrent word, then, for every $n \in \mathbb{N}_0$,*

$$\Delta^2\mathcal{C}(n) = \#\{w \in \mathcal{L}_n(u) \mid w \text{ strong BS}\} - \#\{w \in \mathcal{L}_n(u) \mid w \text{ weak BS}\}. \tag{3.2}$$

3.2 Special factors over a multilateral alphabet

Suppose that u is an infinite word over a multilateral alphabet $\mathcal{A} = \{a_1, a_2, \ldots, a_m\}$. The situation gets more complicated since special factors have sometimes more than two letters in their extension, but not necessarily all m letters. Moreover, the number of right extensions and the number of left extensions of a BS factor are both at least two, but have no reason to be equal.

3.2.1 Classification of special factors

In order to get a classification of BS factors, we introduce the *bilateral order* $B(w)$ of a factor w:

$$B(w) := \#\left(\mathcal{L}(u) \cap \mathcal{A}w\mathcal{A}\right) - \#Rext(w) - \#Lext(w) + 1. \tag{3.3}$$

We deduce easily the following lower and upper bound on $B(w)$:

$$1 - \min\{\#Lext(w), \#Rext(w)\} \leq B(w) \leq (\#Lext(w) - 1)(\#Rext(w) - 1). \tag{3.4}$$

Since the cardinality of the alphabet $\mathcal{A}$ is m, we obtain immediately $1 - m \leq B(w) \leq (m-1)^2$. For a factor w that is not BS, the bilateral order $B(w) = 0$. For a binary alphabet, we recover three bilateral orders $-1, 0, 1$, corresponding to weak, ordinary, and strong BS factors, respectively. The classification of BS factors in the binary case may be generalized in the following way. Let w be a BS factor in $\mathcal{L}(u)$,

- if $B(w) > 0$, then w is called a *strong* BS factor,
- if $B(w) = 0$, then w is called an *ordinary* BS factor,
- if $B(w) < 0$, then w is called a *weak* BS factor.

Let us reformulate equivalently the definition of strong and weak BS factors, respectively. The inequality $B(w) > 0$, characterizing strong BS factors, can be rewritten as

$$\sum_{a \in Lext(w)} \big(\#Rext(aw) - 1\big) > \#Rext(w) - 1. \tag{3.5}$$

Analogously, the inequality $B(w) < 0$, characterizing weak BS factors, is equivalent with

$$\sum_{a \in Lext(w)} \big(\#Rext(aw) - 1\big) < \#Rext(w) - 1. \tag{3.6}$$

Let us generalize also the notion of a maximal LS factor. A LS factor $w \in \mathcal{L}(u)$ is called *maximal* if wa is not LS for any $a \in \mathcal{A}$. A maximal RS factor is defined analogously.

3.2.2 Infinite LS branches

An infinite LS branch v of an infinite word u is defined similarly as in the binary case, i.e., v is an infinite word whose each prefix is a LS factor of u. Clearly, since $\#Lext(w') \geq \#Lext(w)$ for every $w', w \in \mathcal{L}(u)$ such that w' is a prefix of w, the number of left extensions of all sufficiently large prefixes of v is constant. Thus, we can define the set of left extensions of an infinite LS branch v by

$$Lext(v) := \bigcap_{w \text{ prefix of } v} Lext(w). \tag{3.7}$$

3.2.3 Base of trees of LS factors

Evidently, it is inevitable to modify the notion of the tree of LS factors in the multilateral case. LS factors can loose some left extensions being extended to the right, though staying LS. Therefore, it makes sense to put in the same tree only LS factors having the same left extensions.

We construct, for every subset Σ of $\mathcal{A}$, a tree of LS factors such that all branches starting in the root correspond to LS factors having as left extensions all letters from Σ. We put aside the empty trees and we keep only the trees with Σ maximal, which means that no other subset of $\mathcal{A}$ containing Σ gives rise to the same tree. Following this recipe, we obtain the so-called *base* of the trees of LS factors. It is readily seen that to every weak or strong BS factor corresponds a branching or a truncated branch in at least one tree of the base. On the other hand, every branching and every truncated branch are labeled with a BS factor. Similarly as in the binary case, having the base of the trees of LS factors constructed, it is straightforward to compute the complexity.

3.2.4 The first and the second difference of complexity

We have two possibilities to compute complexity – using either the first (Equation (2.15)) or the second difference of complexity.

Proposition 3.2.1. *Let u be an infinite word, then, for all $n \in \mathbb{N}_0$, the second difference of complexity has the following form*

$$\Delta^2\mathcal{C}(n) = \sum_{w\in\mathcal{L}_n(u)} B(w). \tag{3.8}$$

Remark 3.2.2. *With Proposition 3.2.1 at disposal, let us discuss in more details how the first difference of complexity looks like in dependence on the type of BS factors. Obviously, $\Delta\mathcal{C}(0) = m-1$, where $m = \#\mathcal{A}$.*

If all BS factors are ordinary, then $\Delta\mathcal{C}(n) = m-1$ for all $n \in \mathbb{N}_0$. If u contains no weak BS factors, then $\Delta\mathcal{C}(n)$ is a non-decreasing function, thus $\Delta\mathcal{C}(n) \geq m-1$ for all $n \in \mathbb{N}_0$. Similarly, if u contains no strong BS factors, then $\Delta\mathcal{C}(n)$ is a non-increasing function, thus $\Delta\mathcal{C}(n) \leq m-1$ for all $n \in \mathbb{N}_0$.

3.3 Sublinear complexity

Infinite words with relatively low complexity, i.e., bounded by a polynomial of a small degree, are naturally better understood. Among words with sublinear complexity, we find besides eventually periodic words, also Sturmian words, Arnoux-Rauzy words, and m-interval exchange transformation coding words (defined in Section 2.4.5), or fixed points of primitive substitutions (Section 2.2.13: Factor complexity of fixed points of substitutions).

Cassaigne in [27] has constructed, for any pair of integers a, b such that either $a \geq 2$ and b arbitrary, or, $a \in \{0,1\}$ and $b > 0$, an infinite word whose complexity fulfills $\mathcal{C}(n) = an+b$ for all sufficiently large n. Moreover, he has proved that there exists an infinite word with $\mathcal{C}(n) = an+b$ for all $n \in \mathbb{N}_0$, $a \in \mathbb{N}_0$, $b \in \mathbb{Z}$, if and only if $a+b \geq 1$ and $2a+b \leq (a+b)^2$.

The same author in [28] has moreover shown for infinite words with a sublinear complexity that their first difference of complexity is bounded; that is, if there exists a constant $K > 0$ such that $\mathcal{C}(n) \leq Kn$ holds for all $n \in \mathbb{N}$, then there exists a constant $k > 0$ such that

$$\Delta\mathcal{C}(n) < k \quad \text{for all } n \in \mathbb{N}_0. \tag{3.9}$$

Let us write down a list of LS factors for some infinite words, being of particular interest in several other chapters. We complete this list by the description of BS factors and the exact formula for complexity, provided this information is known. All these words have sublinear complexity.

3.3.1 Sturmian words, AR words, and m-iet words

The formula for the complexity of Sturmian words, $\mathcal{C}(n) = n + 1$ for all $n \in \mathbb{N}_0$, ensures that for every $n \in \mathbb{N}_0$, there exists exactly one LS factor of length n. In consequence, the tree of LS factors of a Sturmian word u is reduced to one infinite LS branch. All BS factors are prefixes of this infinite LS branch and are necessarily ordinary. As u is uniformly recurrent, the language of u and of the infinite LS branch coincide (see Section 2.2.4). If, moreover, the LS branch of a Sturmian word u is u itself, then u is called *standard Sturmian*.

Similarly as for Sturmian words, the tree of LS factors of an AR word u over an m-letter alphabet consists of an infinite LS branch whose each prefix has exactly m left extensions. All BS factors are prefixes of this infinite LS branch and are ordinary. In consequence, $C(n) = (m-1)n+1$ for all $n \in \mathbb{N}_0$. As u is uniformly recurrent, the language of u and of the infinite LS branch are identical. We call an AR word u *standard* if u coincides with its infinite LS branch.

The complexity of m-iet words satisfies $\mathcal{C}(n) = (m-1)n + 1$ for all $n \in \mathbb{N}_0$. However, there exist $(m-1)$ LS factors of every length, hence, the sets of m-iet words and AR words are disjoint for $m > 2$. BS factors are prefixes of the $m-1$ infinite LS branches and are ordinary.

3.3.2 Thue-Morse word

The factor complexity of the Thue-Morse word u_{TM}, the fixed point – $\lim_{n\to\infty} \varphi^n(0)$ – of the substitution φ defined in Section 2.2.13 by $\varphi(0) = 01,\ \varphi(1) = 10$, has been determined independently by Brlek [22] and de Luca and Varricchio [86]. The details on the description of special factors are to consult in [27].

BS factors and the second difference of complexity

It is not difficult to verify the following lemma - the essential ingredient for the derivation of the complete list of BS factors.

Lemma 3.3.1. *Every BS factor $v \in \mathcal{L}(u_{TM})$ of length ≥ 4 has a unique interpretation $(w, 0, 0)$, i.e., $v = \varphi(w)$. Moreover, w is a BS factor of the same type as v.*

- STRONG BS factors

$$\begin{array}{ll} \varphi^n(01) & \text{for } n \in \mathbb{N}_0, \\ \varphi^n(10) & \text{for } n \in \mathbb{N}_0. \end{array} \tag{3.10}$$

  Also ε is a strong BS factor.

- WEAK BS factors

$$\begin{array}{ll} \varphi^n(010) & \text{for } n \in \mathbb{N}_0, \\ \varphi^n(101) & \text{for } n \in \mathbb{N}_0. \end{array} \tag{3.11}$$

  In more precise terms, for n odd,

$$0\varphi^n(010)0,\ 1\varphi^n(010)1 \in \mathcal{L}(u_{\mathrm{TM}}) \quad \text{and} \quad 0\varphi^n(101)0,\ 1\varphi^n(101)1 \in \mathcal{L}(u_{\mathrm{TM}}), \tag{3.12}$$

  for n even,

$$0\varphi^n(010)1,\ 1\varphi^n(010)0 \in \mathcal{L}(u_{\mathrm{TM}}) \quad \text{and} \quad 0\varphi^n(101)1,\ 1\varphi^n(101)0 \in \mathcal{L}(u_{\mathrm{TM}}). \tag{3.13}$$

- ORDINARY BS factors are 0 and 1.

According to Proposition 3.1.2 and having the length $|\varphi^n(0)| = 2^n$ computed, we see that the second difference of complexity obeys the following formula

$$\Delta^2\mathcal{C}(n) = \begin{cases} 1 & n = 0, \\ 2 & \text{if } \ n = 2^{k+1} \ \text{ for some } k \in \mathbb{N}_0, \\ -2 & \text{if } \ n = 3 \cdot 2^k \ \text{ for some } k \in \mathbb{N}_0, \\ 0 & \text{otherwise.} \end{cases}$$

LS factors and the first difference of complexity

There exist two infinite LS branches and two infinite sequences of maximal LS factors:

1. the first infinite LS branch is u_{TM} itself, having $\varphi^n(01)$ as the longest common prefix with the maximal LS factor $\varphi^n(010)$ for every $n \in \mathbb{N}_0$,

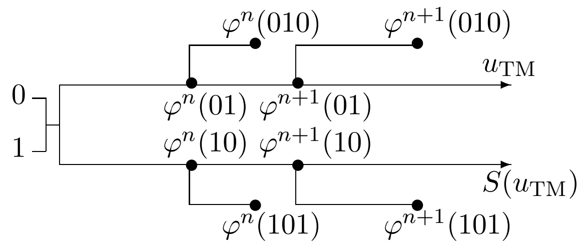


Fig. 3.2: Illustration of a sector of the tree of LS factors for u_{TM}. All branches of lengths between 2^{n+1} and $3 \cdot 2^{n+1}$ are plotted.

2. the second infinite LS branch is $S(u_{\mathrm{TM}})$ having $\varphi^n(10)$ as the maximal common prefix with the maximal LS factor $\varphi^n(101)$ for every $n \in \mathbb{N}_0$, where S is the morphism given by $S(0) = 1, \ S(1) = 0$.

Applying Equation (2.15), the explicit formula for the first difference of complexity is obtained

$$\Delta\mathcal{C}(n) = \begin{cases} 1 & \text{for } n = 0, \\ 4 & \text{if } \ 2^k < n \leq 3 \cdot 2^{k-1} \ \text{ for some } k \in \mathbb{N}, \\ 2 & \text{otherwise.} \end{cases}$$

Complexity

To complete this example, we mention the explicit formula for the factor complexity of u_{TM}:

$$\mathcal{C}(n) = \begin{cases} 1 & n = 0, \\ 2 & n = 1, \\ 4 & n = 2, \\ 4n - 2^k - 4 & \text{if } \ 2^k < n \leq 3 \cdot 2^{k-1} \quad \text{for some } k \in \mathbb{N}, \\ 2n + 2^{k+1} - 2 & \text{if } \ 3 \cdot 2^{k-1} < n \leq 2^{k+1} \quad \text{for some } k \in \mathbb{N}. \end{cases} \tag{3.14}$$

3.3.3 Period doubling word

The period doubling word u_{PD} is the unique fixed point of the substitution φ glanced already in Section 2.2.13. We recall that $\varphi(0) = 01, \ \varphi(1) = 00$. Properties of this infinite word that originates from the field of chaotic dynamics were first studied by Damanik [34]. The period doubling word has several peculiarities. It is a coding of the first difference of the Thue-Morse word, i.e.,

$$(u_{\mathrm{PD}})_k = (u_{\mathrm{TM}})_{k+1} - (u_{\mathrm{TM}})_k \mod 2 \quad \text{for every } k \in \mathbb{N}_0,$$

where $(u)_k$ denotes the $(k+1)$-st letter of the corresponding infinite word u. In addition, for every $n \in \mathbb{N}_0$, if we construct an infinite word writing down every n-th letter of u_{PD}, i.e., $(u_{\mathrm{PD}})_{n-1}(u_{\mathrm{PD}})_{2n-1}(u_{\mathrm{PD}})_{3n-1}\ldots$, we get again the period doubling word (possibly with permuted letters).

BS factors and the second difference of complexity

The essential tool for the description of BS factors is the following lemma, where $T_{\mathrm{PD}}(v) := \varphi(v)0$ for every word $v \in \{0,1\}^*$.

Lemma 3.3.2. *Every BS factor $v \in \mathcal{L}(u_{PD})$ containing at least one letter 1 has two interpretations $(w0,0,1)$ and $(w1,0,1)$ with ancestors $w0, w1$ in $\mathcal{L}(u_{PD})$, i.e., $v = T_{PD}(w)$. Moreover, w is a BS factor of the same type as v.*

- STRONG BS factors

$$\begin{array}{rcl} V^{(1)} & = & 0, \\ V^{(n)} & = & T_{\mathrm{PD}}(V^{(n-1)}) \quad \text{for } n \geq 2. \end{array} \tag{3.15}$$

- WEAK BS factors

$$\begin{array}{rcl} U^{(1)} & = & 00, \\ U^{(n)} & = & T_{\mathrm{PD}}(U^{(n-1)}) \quad \text{for } n \geq 2. \end{array} \tag{3.16}$$

- The only ORDINARY BS factor is ε.

Using Proposition 3.1.2 and having computed $|V^{(n)}| = 2^n - 1$ and $|U^{(n)}| = 3 \cdot 2^{n-1} - 1$, we get the second difference of complexity in the following form

$$\Delta^2 \mathcal{C}(n) = \begin{cases} 1 & \text{if } n = 2^k - 1 \text{ for some } k \in \mathbb{N}, \\ -1 & \text{if } n = 3 \cdot 2^{k-1} - 1 \text{ for some } k \in \mathbb{N}, \\ 0 & \text{otherwise.} \end{cases}$$

LS factors and the first difference of complexity

There exists a unique infinite LS branch $\lim_{n\to\infty} V^{(n)}$, having $V^{(n)}$ as the longest common prefix with the maximal LS factor $U^{(n)}$ for every $n \in \mathbb{N}$.

Applying Equation (2.15), the explicit formula for the first difference of complexity is obtained

$$\Delta \mathcal{C}(n) = \begin{cases} 2 & \text{if } 2^k \leq n < 3 \cdot 2^{k-1} \text{ for some } k \in \mathbb{N}, \\ 1 & \text{otherwise.} \end{cases}$$

Complexity

To conclude, let us provide the explicit formula for the factor complexity of u_{PD}:

$$\mathcal{C}(n) = \begin{cases} 1 & n = 0, \\ 2 & n = 1, \\ 2n - 2^{k-1} & \text{if } 2^k \leq n < 3 \cdot 2^{k-1} \text{ for some } k \in \mathbb{N}, \\ n + 2^k & \text{if } 3 \cdot 2^{k-1} \leq n < 2^{k+1} \text{ for some } k \in \mathbb{N}. \end{cases} \tag{3.17}$$

3.3.4 Rote word

Let us denote by u_{R} the fixed point of the non-primitive substitution φ defined by

$$\varphi(0) = 001, \ \varphi(1) = 111. \tag{3.18}$$

We call u_{R} the Rote word in order to recall Rote who was the first one to present a general method for constructing infinite words of complexity $2n$ and who introduced u_{R} as an example of such words (see [99]). The Rote word u_{R} is recurrent (it suffices to notice that the letter 0 occurs infinitely many times and that every factor is a subword of the prefix $\varphi^n(0)$ for some n), but not uniformly recurrent (there are blocks of 1's of arbitrary lengths).

BS factors and the second difference of complexity

Basic, however essential for determining BS factors is the description of blocks of 1's.

Observation 3.3.3. *Let $01^k0,\ k \in \mathbb{N}$, be a factor of u_R, then $k = \frac{3^n-1}{2}$ for some $n \in \mathbb{N}$.*

Proof. Suppose there exists $k \in \mathbb{N}$ different from $\frac{3^n-1}{2}$ for all $n \in \mathbb{N}$ such that $01^k0 \in \mathcal{L}(u_{\mathrm{R}})$. Take the smallest one of such numbers k, clearly $k > 1$. The form of φ implies that $(01, 1^{k-1}0)$ and $(01^k, 0)$ are synchronization points (defined in Section 2.2.13: Ancestors and synchronization points of substitutions). As φ is uniform (of length 3), we can write $01^k0 = 01\varphi(1^{\frac{k-1}{3}})0$. This is a contradiction with the minimality of k since $01^{\frac{k-1}{3}}0$ is a factor of u_{R} (it is the only ancestor of 01^k0) and $\frac{k-1}{3} \neq \frac{3^n-1}{2}$ for all $n \in \mathbb{N}$ (otherwise $k = \frac{3^{n+1}-1}{2}$). ☐

The main role in the description of BS factors is played by the following lemma, where $T_{\mathrm{R}}(v) := 1\varphi(v)$ for every word $v \in \{0,1\}^*$.

Lemma 3.3.4. *Every BS factor $v \in \mathcal{L}(u_R)$ containing the factor 00 has two interpretations $(0w, 2, 0)$ and $(1w, 2, 0)$ with ancestors $0w, 1w$ in $\mathcal{L}(u_R)$, i.e., $v = T_R(w)$. Moreover, w is a BS factor of the same type as v.*

- STRONG BS factors

$$\begin{aligned} V^{(1)} &= 1, \\ V^{(n)} &= T_{\mathrm{R}}(V^{(n-1)}) = 1^{\frac{3^n-1}{2}} \quad \text{for } n \geq 2. \end{aligned} \tag{3.19}$$

  Also ε is a strong BS factor.

- WEAK BS factors

$$\begin{aligned} U^{(1)} &= 0, \\ U^{(n)} &= T_{\mathrm{R}}(U^{(n-1)}) \quad \text{for } n \geq 2. \end{aligned} \tag{3.20}$$

- ORDINARY BS factors

$$\underbrace{11\ldots1}_{k-\text{times}}, \quad \text{where } k \neq \frac{3^n-1}{2} \text{ for all } n \in \mathbb{N}. \tag{3.21}$$

Applying Proposition 3.1.2 and taking into account that $|V^{(n)}| = |U^{(n)}| = \frac{3^n-1}{2}$, we get the second difference of complexity $\Delta^2\mathcal{C}(n) = 0$ for all $n \in \mathbb{N}$ and $\Delta^2\mathcal{C}(0) = 1$.

LS factors and the first difference of complexity

There exists a unique infinite LS branch $\lim_{n\to\infty} V^{(n)} = 1^\omega$, having $V^{(n)}$ as the longest common prefix with the maximal LS factor $U^{(n+1)}$ for every $n \in \mathbb{N}$.

Applying Equation (2.15), the formula for the first difference of complexity takes a simple form $\Delta\mathcal{C}(n) = 2$ for all $n \in \mathbb{N}$ and $\Delta\mathcal{C}(0) = 1$.

Complexity

To conclude, let us provide the explicit formula, obtained originally by Rote, for the factor complexity of u_{R}:

$$\mathcal{C}(n) = \begin{cases} 1 & n = 0, \\ 2n & n \in \mathbb{N}. \end{cases} \tag{3.22}$$

3.3.5 A palindromeless reversal closed word

An infinite word worth mentioning has been introduced by Berstel *et al.* in [16]. This word, say z, is defined as

$$z = \lim_{n\to\infty} z_n, \quad \text{where} \quad \begin{array}{l} z_{n+1} = z_n 01 \overline{z_n} \quad \text{for all} \quad n \in \mathbb{N}_0, \\ z_0 = 01. \end{array} \tag{3.23}$$

It is useful to compute the length $|z_n| = 2(2^{n+1} - 1)$. For illustration, let us write down a prefix of z

$$z = 0101100101101001010110100110100101011001011010010110100110 10\ldots \tag{3.24}$$

The peculiarity of this word consists in the fact that even if z is uniformly recurrent with language $\mathcal{L}(z)$ closed under reversal, z contains only palindromes of length ≤ 12. In other words, it shows that the opposite implication in Proposition 2.2.3 does not hold. The complexity of z may be quite easily derived using the following observation.

For every $n \geq 0$, the word z can be factorized over the alphabet $\{z_n, \overline{z_n}, 01, 10\}$ as

$$z = z_n 01 \overline{z_n} 01 z_n 10 \overline{z_n} 01 z_n 01 \overline{z_n} 10 z_n 10 \overline{z_n} 01 z_n 01 \overline{z_n} 01 z_n 10 \overline{z_n} 10 z_n 01 \overline{z_n} 10 z_n 10 \overline{z_n} \ldots; \tag{3.25}$$

that is, in such a way that z_n and $\overline{z_n}$ alternate regularly being separated either by 01 or by 10. It can be shown that for $n \geq 2$, the formula (3.25) determines all occurrences of z_n, respectively $\overline{z_n}$ in z. With this observation at disposal, we may prove that z is not only uniformly recurrent, but even linearly recurrent.

Proposition 3.3.5. *The infinite word z is linearly recurrent with constant $K = 31$.*

Proof. Let $w \in \{0, 1\}$, then every factor of length 3 contains w since z can be factorized over the alphabet $\{01, 10\}$. Let $|z_{n-1}| \leq |w| < |z_n|$, $n \geq 1$, then observing (3.25), it is readily seen that w is a factor of at least one of the following words: $z_n 01 \overline{z_n}$, $z_n 10 \overline{z_n}$, $\overline{z_n} 01 z_n$, or $\overline{z_n} 10 z_n$. By definition, both z_{n+3} and $\overline{z_{n+3}}$ contain all four previous words. Again by (3.25), every factor of z of length $2|z_{n+3}| + 1$ contains either z_{n+3} or $\overline{z_{n+3}}$, therefore it holds

$$\frac{R(|w|)}{|w|} \leq \frac{2|z_{n+3}| + 1}{|z_{n-1}|} = \frac{2^{n+4} - 1}{2^n - 1} \leq 31,$$

where $R(n)$ has been defined in Section 2.2.4. $\square$

BS factors and the second difference of complexity

- STRONG BS factors

$$\begin{array}{ll} \text{of length} < 14 & 01,\ 10,\ 0101,\ 1010,\ z_1,\ \overline{z_1}, \\ \text{of length} \geq 14 & z_n \quad \text{and} \quad \overline{z_n} \quad \text{for } n \geq 2. \end{array} \tag{3.26}$$

- WEAK BS factors

$$\begin{array}{ll} \text{of length} < 14 & 10101,\ 01010,\ 10100101,\ 100101101001, \\ \text{of length} \geq 14 & \overline{z_n}01z_n \quad \text{and} \quad \overline{z_n}10z_n \quad \text{for } n \geq 1. \end{array} \tag{3.27}$$

More precisely,

$$0\overline{z_n}01z_n0, 1\overline{z_n}01z_n1 \in \mathcal{L}(z) \quad \text{and} \quad 0\overline{z_n}10z_n0, 1\overline{z_n}10z_n1 \ \in \mathcal{L}(z).$$

- ORDINARY BS factors

$$0,\ 1,\ 010,\ 101,\ 0110,\ 1001,\ 100101,\ 101001. \tag{3.28}$$

Considering Proposition 3.1.2, the second difference of complexity is deduced

$$\Delta^2\mathcal{C}(n) = \begin{cases} 1 & n = 0, \\ 2 & n = 2, 4, 6, \\ -2 & n = 5, \\ -1 & n = 8, 12, \\ 0 & \text{otherwise.} \end{cases}$$

LS factors and the first difference of complexity

There exists one infinite LS branch $z = \lim_{n\to\infty} z_n$ and two infinite sequences of maximal LS factors $(\overline{z_n}01z_n)_{n\geq 1}$ and $(\overline{z_n}10z_n)_{n\geq 1}$.

The strong BS factor z_{n-1} is the maximal common prefix of z and $\overline{z_n}01z_n$, and, also, of z and $\overline{z_n}10z_n$, for all $n \geq 1$, while the strong BS factor $\overline{z_n}$ is the longest common prefix of $\overline{z_n}01z_n$ and $\overline{z_n}10z_n$, for all $n \in \mathbb{N}$.

Every LS factor of length $\geq |z_2| = 14$ is a prefix of z or of a maximal LS factor belonging to the above infinite sequences.

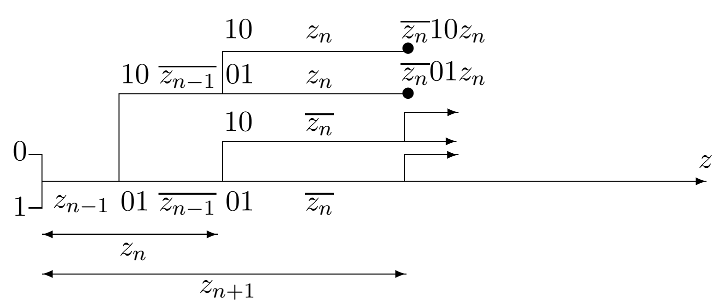


Fig. 3.3: Illustration of a sector of the tree of LS factors for the infinite word z. For $n \geq 2$, all branches of lengths between $|z_n|$ and $|z_{n+1}|$ are drawn down.

LS factors of length < 14 may be moreover prefixes of maximal LS factors - weak BS factors - listed in (3.27).

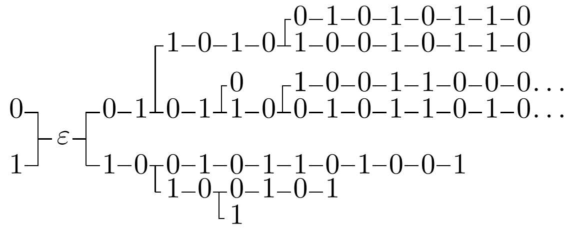


Fig. 3.4: Illustration of the tree of LS factors for the infinite word z up to the level 14.

Applying (2.15), a simple formula for the first difference of complexity is obtained

$$\Delta\mathcal{C}(n) = \begin{cases} 1 & n = 0, \\ 2 & n = 1, 2, \\ 5 & n = 9, 10, 11, 12, \\ 6 & n = 5, 7, 8, \\ 4 & \text{otherwise.} \end{cases}$$

Complexity

n	0	1	2	3	4	5	6	7	8	9	10	11	12	13	$n \geq 14$
$\mathcal{C}(n)$	1	2	4	6	10	14	20	24	30	36	41	46	51	56	$4(n+1)$

3.3.6 u_β associated with simple Parry numbers

As another example, let us present the description of special factors of infinite words u_β associated with simple Parry numbers, as derived by Frougny, Masáková, and Pelantová in [57]. Two cases of $d_\beta(1) = t_1 t_2 \dots t_m$ have been solved.

$$(a)\ t_1 = t_2 = \cdots = t_{m-1} = t, \quad t \geq t_m \geq 1 \quad (b)\ t_1 > \max\{t_2, \dots, t_{m-1}\},\ t_1 \geq t_m \geq 1. \tag{3.29}$$

The case (a) corresponds to the confluent Parry numbers β defined in Section 2.3.3.

BS factors and the second difference of complexity

The following list of BS factors with non-zero bilateral order (defined in (3.3)) is complete.

- STRONG BS factors form the set $(V^{(n)})_{n=1}^{\infty}$ given recurrently

$$\begin{array}{lrcl} (a) & V^{(1)} & = & 0^t, \\ \text{for } n \geq 2 & V^{(n)} & = & \varphi(V^{(n-1)})0^t, \end{array} \qquad \begin{array}{lrcl} (b) & V^{(1)} & = & 0^{t_1}, \\ \text{for } n \geq 2 & V^{(n)} & = & \varphi(V^{(n-1)})0^{t_j}, \\ & j & = & n \mod (m-1). \end{array} \tag{3.30}$$

  For every $n \in \mathbb{N}$, $\#Lext(V^{(n)}) = m$, $\#Rext(V^{(n)}) = 2$, and the bilateral order $B(V^{(n)}) = 1$.

- WEAK BS factors form the set $(U^{(n)})_{n=1}^{\infty}$ given by

$$\begin{array}{lrcl} (a) & U^{(1)} & = & 0^{t+t_m-1}, \\ \text{for } n \geq 2 & U^{(n)} & = & \varphi(U^{(n-1)})0^t, \end{array} \qquad \begin{array}{lrcl} (b) & U^{(1)} & = & 0^{t_1+t_m-1}, \\ \text{for } n \geq 2 & U^{(n)} & = & \varphi(U^{(n-1)})0^{t_j}, \\ & j & = & n \mod (m-1). \end{array} \tag{3.31}$$

  For every $n \in \mathbb{N}$, $\#Lext(U^{(n)}) = 2$, $\#Rext(U^{(n)}) = 2$, and $B(U^{(n)}) = -1$.

Applying Proposition 3.1.2, the formula for the second difference of complexity is obtained

$$\Delta^2\mathcal{C}(n) = \begin{cases} 1 & \text{if } \ n = |V^{(k)}| \ \text{ for some } k \in \mathbb{N}, \\ -1 & \text{if } \ n = |U^{(k)}| \ \text{ for some } k \in \mathbb{N}, \\ 0 & \text{otherwise.} \end{cases} \tag{3.32}$$

Using the formula (2.19), the lengths $|V^{(n)}|$, $|U^{(n)}|$ can be computed recurrently. It follows then that

$$|V^{(n)}| < |U^{(n)}| < |V^{(n+1)}| \quad \text{for all } n \in \mathbb{N}. \tag{3.33}$$

LS factors and the first difference of complexity

Let us give an exhaustive description of the base of trees of LS factors. There exists a unique infinite LS branch, namely u_β itself, satisfying $Lext(u_\beta) = \{0, 1, \ldots, m-1\}$.

If $t_m = 1$, then each LS factor is a prefix of u_β.

If $t_m \geq 2$, then each LS factor which is not a prefix of u_β has two left extensions and is a prefix of a weak BS factor. More precisely, besides the infinite LS branch u_β, there are the following m trees of LS factors. For every $i \in \{1, \ldots, m\}$, there exists a tree $v^{(i)}$ whose set of branches is $(U^{(i+km)})_{k\in\mathbb{N}_0}$ and whose left extensions are $Lext(v^{(i)}) = \{i-1 \mod m, \ i \mod m\}$. There is a branching in the tree $v^{(i)}$ if and only if the branch is labeled with $V^{(i+km)}$ for some $k \in \mathbb{N}_0$, as illustrated in Figure 3.5.

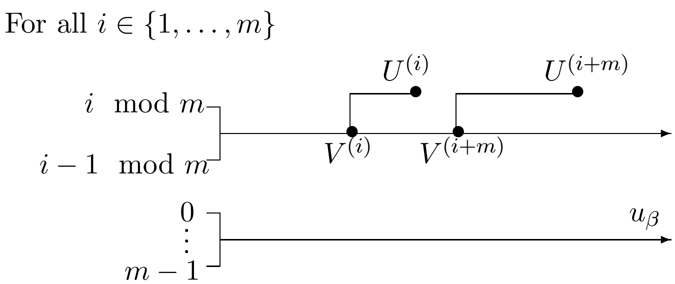


Fig. 3.5: Illustration of the base of the trees of LS factors for u_β associated with a simple Parry number β, $m > 2$. The base contains $m+1$ trees, m of them having two left extensions and one of them having m left extensions.

For $m = 2$, i.e., for a quadratic number β, the base of the trees of LS factors is reduced to one tree containing an infinite LS branch u_β and truncated branches - maximal LS factors - $U^{(n)}$ sharing with u_β the strong BS factors $V^{(n)}$ as the longest common prefixes. See Figure 3.6.

Applying Equation (2.15), the formula for the first difference of complexity is obtained.

For $t_m = 1$, we have $\Delta\mathcal{C}(n) = m - 1$ for every $n \in \mathbb{N}_0$.

For $t_m \geq 2$,

$$\Delta\mathcal{C}(n) = \begin{cases} m & \text{if } \ |V^{(k)}| < n \leq |U^{(k)}| \ \text{ for some } k \in \mathbb{N}, \\ m-1 & \text{otherwise.} \end{cases}$$

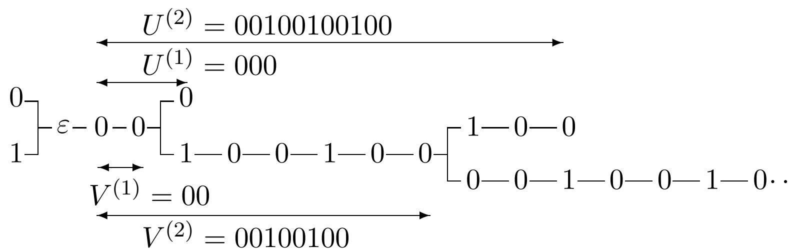


Fig. 3.6: Illustration of the tree of LS factors for the infinite word u_β with $d_\beta(1) = 22$, i.e., being the fixed point of the substitution $\varphi(0) = 001,\ \varphi(1) = 00$. The two shortest strong BS factors $V^{(1)},\ V^{(2)}$ as well as the two shortest maximal LS factors (or, equivalently, weak BS factors) $U^{(1)},\ U^{(2)}$ are pointed out.

Complexity

For $t_m = 1$, the complexity satisfies $\mathcal{C}(n) = (m-1)n + 1$. Proposition 2.3.1 implies that u_β is an Arnoux-Rauzy word if and only if β is a confluent Parry unit, i.e., $d_\beta(1) = t^{m-1}1$ for some $t \in \mathbb{N}$.

For $t_m \geq 2$, the precise formula is technical since it depends on the lengths of BS factors given by recurrent formulae. Let us just point out that in both considered cases of parameters (3.29), we have

$$(m-1)n + 1 \leq \mathcal{C}(n) \leq mn.$$

Another interesting question concerning complexity sounds: "For which simple Parry numbers β, the complexity of u_β associated with β is affine; that is, such that there exist constants A, B satisfying $C(n) = An + B$ for all $n \in \mathbb{N}_0$?" Bernat, Masáková, and Pelantová in [14] provide a complete answer in the following theorem.

Theorem 3.3.6. *Let u_β be the infinite word associated with a simple Parry number β with the Rényi expansion of unity $d_\beta(1) = t_1 t_2 \dots t_m$. Then the factor complexity of u_β is affine if and only if the coefficients $t_1, t_2, \dots, t_m$ satisfy $t_m = 1$ and $t_j \dots t_{m-1} t_1 \dots t_{j-1} \preceq t_1 \dots t_{m-1}$ for all $j \in \{2, \dots, m-1\}$, where $\preceq$ stands for 'lexicographically less or equal'.*

3.3.7 u_β associated with non-simple Parry numbers

According to Section 2.3.1, non-simple Parry numbers have an eventually periodic Rényi expansion of unity $d_\beta(1) = t_1 t_2 \dots t_m (t_{m+1} \dots t_{m+r})^\omega$, where $m, r \in \mathbb{N}$ are chosen to be minimal, and the associated infinite word u_β is the fixed point of the substitution (2.24). The determination of LS factors turns out to be even more complicated than in the case of simple Parry numbers and only infinite LS branches have been recovered by Frougny, Masáková, Pelantová in [58], under a rather restrictive assumption of all t_i's positive.

Infinite LS branches

Two very diverse situations occur in dependence on the period length r.

- If $r \geq 2$, the unique infinite LS branch is u_β itself and $Lext(u_\beta) = \{m, \dots, m+r-1\}$.

- If $r = 1$ and if we denote by $t := \min\{t_m, t_{m+r}\}$, there exist exactly m different LS branches
$$\begin{array}{rcl} v^{(1)} & = & 0^t m\varphi^m(0^t m)\varphi^{2m}(0^t m)\ldots, \\ v^{(2)} & = & \varphi(v^{(1)}), \\ & \vdots & \\ v^{(m)} & = & \varphi(v^{(m-1)}), \end{array}$$
each of them having only two left extensions, more precisely, $Lext(v^{(i)}) = \{i-1, i\}$.

3.4 Complexity of u_β associated with non-simple quadratic Parry numbers

Let us recall that the Rényi expansion of a non-simple quadratic Parry number β is of the form $d_\beta(1) = pq^\omega$, where $p > q \geq 1$, and u_β is the fixed point of the substitution φ given in (2.27).

$$u_\beta = \big(\underbrace{(0^p1)(0^p1)\ldots(0^p1)}_{p \text{ times}}0^q1\big)^p\underbrace{(0^p1)(0^p1)\ldots(0^p1)}_{q \text{ times}}0^q1\ldots \tag{3.34}$$

As stated in Remark 2.3.4, u_β is a Sturmian word if and only if $p = q+1$. In consequence, we can restrict our considerations to $p > q+1$, provided our aim is to determine the complexity.

We have seen in Section 3.3.7 that, so far, the special factors and the complexity of the infinite words u_β associated with general non-simple Parry numbers are not deeply understood.

Let us provide the case of the infinite word u_β associated with quadratic non-simple Parry numbers with a complete description of BS factors and the second difference of complexity, LS factors and the first difference of complexity, and, finally, an exact formula for the complexity.

First of all, some simple, but important properties of the substitution φ are observed.

Observation 3.4.1. *Let 10^k1 be a factor of u_β, then $k = p$ or $k = q$.*

Observation 3.4.2. *Let v be any word in $\mathcal{L}(u_\beta)$ containing at least one 1. One may rewrite v as $v = 0^{k_1}1v'$. Then, it is obvious that $(0^{k_1}1, v')$ is a synchronization point of v. Similarly, v may be rewritten as $v = v''10^{k_2}$ and $(v''1, 0^{k_2})$ is a synchronization point of v. This fact together with the injectivity of φ implies that there exists a unique factor $w \in \mathcal{L}(u_\beta)$ such that $v = 0^{k_1}1\varphi(w)0^{k_2}$. Thus, the set of ancestors of v is a subset of $\{0w0, 0w1, 1w0, 1w1\}$.*

Example: *Let $w = 010^q10^p10^p10^{q+1}$. Observing (3.34), we see that w is a factor of u_β. According to Observation 3.4.2, we may write $w = 01\varphi(100)0^{q+1}$ and the set of ancestors of w is $\{01000, 11000\}$. Since $01000 \in \mathcal{L}(u_\beta)$ and $11000 \notin \mathcal{L}(u_\beta)$, w has a unique ancestor 01000 in $\mathcal{L}(u_\beta)$.*

Of significant importance is the map $T : \{0,1\}^* \to \{0,1\}^*$ defined by

$$T(w) = 0^q1\varphi(w)0^q. \tag{3.35}$$

Lemma 3.4.3. *Let T be the map defined in (3.35). Then*

1. *$T(\mathcal{L}(u_\beta)) \subset \mathcal{L}(u_\beta)$.*
2. *Let w be a factor of u_β, then*
$$\{(a,b) \mid a,b \in \{0,1\},\ awb \in \mathcal{L}(u_\beta)\} = \{(a,b) \mid a,b \in \{0,1\},\ aT(w)b \in \mathcal{L}(u_\beta)\}.$$

3. *Let v be a BS factor of u_β containing at least one letter 1, then there exists a unique factor w of u_β such that $v = T(w)$.*

4. *Let w, v be factors of u_β, then w is a prefix of v if and only if $T(w)$ is a prefix of $T(v)$.*

Proof. 1. Take an arbitrary factor $w \in \mathcal{L}(u_\beta)$. Then w is extendable to the right, and, since u_β is recurrent, w is extendable also to the left. In other words, there exists $a, b \in \{0, 1\}$ such that awb is also a factor of u_β. As u_β is a fixed point of φ, the image $\varphi(awb)$ belongs to $\mathcal{L}(u_\beta)$. Finally, $T(w)$ is a factor of u_β because $T(w)$ is a subword of $\varphi(awb)$.

2. Let $1w1$ be a factor of $\mathcal{L}(u_\beta)$, then, since u_β is recurrent, there exists $a \in \{0, 1\}$ such that $a1w1$ is as well a factor of u_β. Applying φ, we learn that $\varphi(a1w1) = \varphi(a)T(w)1$ is a factor of u_β, which proves that $1T(w)1$ belongs to $\mathcal{L}(u_\beta)$. The other cases $0w0, 0w1, 1w0$ are analogous.

Let $0T(w)1 \in \mathcal{L}(u_\beta)$. Using Observation 3.4.1, the word $v = 0^p1\varphi(w)0^q1$ is also a factor of u_β. Applying Observation 3.4.2, v has a unique ancestor $0w1$, which is thus necessarily in $\mathcal{L}(u_\beta)$. All the other cases $0T(w)0, 1T(w)0, 1T(w)1$ are similar.

3. Observation 3.4.1 implies that each BS factor v containing at least one letter 1 has prefix 0^q1 and suffix 10^q. According to Observation 3.4.2, there exists a unique w such that $v = T(w)$.

4. The implication $\Rightarrow$ is obvious noticing that 0^q is prefix of $\varphi(a)$ for $a \in \{0, 1\}$. The opposite implication $\Leftarrow$ follows taking into account that $\{\varphi(0), \varphi(1)\}$ is a prefix code; that is, $\varphi(0)$ is not a prefix of $\varphi(1)$ and vice versa. □

BS factors and the second difference of complexity

Let us start the study of BS factors with the simplest ones - BS factors containing no letter 1.

Lemma 3.4.4. *Among factors that contain no letter 1, there are the following BS factors (with each factor w, the extension set $\{(a, b) |\ a, b \in \{0, 1\},\ awb \in \mathcal{L}(u_\beta)\}$ is written down, if not evident):*

one strong BS factor 0^q,	
one weak BS factor 0^{p-1},	$\{(0, 1), (1, 0)\}$,
ordinary BS factors 0^r, $r \in \{1, \dots, p-2\}$, $r \neq q$,	$\{(0, 0), (0, 1), (1, 0)\}$,
ordinary BS factor ε,	$\{(0, 0), (0, 1), (1, 0)\}$.

Proof. To verify that the above listed factors occur with the listed extensions in u_β, it is enough to observe the beginning of u_β in (3.34). To show afterwards that there are no other extensions, it suffices to take into account the form of blocks of zeros separating consecutive 1's (Observation 3.4.1) and the fact that $p > q + 1$. □

As an immediate consequence of Lemma 3.4.4, Items *2.* and *3.* of Lemma 3.4.3, and Observation 3.4.2, a complete list of BS factors is obtained.

Corollary 3.4.5. *Let u_β be the fixed point of the substitution φ defined by $\varphi(0) = 0^p1$, $\varphi(1) = 0^q1$, where $p - 1 > q \geq 1$. The set $(V^{(n)})_{n=1}^{\infty}$ of all strong BS factors is given recurrently by*

$$\begin{aligned} V^{(1)} &= 0^q, \\ V^{(n)} &= T(V^{(n-1)}) \quad \text{for } n \geq 2. \end{aligned} \tag{3.36}$$

The set $(U^{(n)})_{n=1}^{\infty}$ of all weak BS factors is

$$\begin{aligned} U^{(1)} &= 0^{p-1}, \\ U^{(n)} &= T(U^{(n-1)}) \quad \text{for } n \geq 2. \end{aligned} \tag{3.37}$$

The set of all ordinary BS factors $(W_r^{(n)})_{n=1}^{\infty}$, $r \in \{0, \dots, p-2\}$, $r \neq q$, *has the following form*

$$\begin{aligned} W_0^{(1)} &= \varepsilon, & & \\ W_r^{(1)} &= 0^r, & r &\neq 0, \\ W_r^{(n)} &= T(W_r^{(n-1)}) & & \textit{for } n \geq 2. \end{aligned} \tag{3.38}$$

According to Proposition 3.1.2, the second difference of complexity obeys the following formula

$$\Delta^2 \mathcal{C}(n) = \begin{cases} 1 & \text{if } \; n = |V^{(k)}| \; \text{ for some } k \in \mathbb{N}, \\ -1 & \text{if } \; n = |U^{(k)}| \; \text{ for some } k \in \mathbb{N}, \\ 0 & \text{otherwise.} \end{cases} \tag{3.39}$$

Recurrent formulae for the lengths of $V^{(n)}, U^{(n)}$

In order to compute lengths of weak and strong BS factors, we shall apply Equation (2.19). Let us recall that the substitution matrix of φ has been determined in Section 2.3.4. The recurrent definition of $V^{(n)}$ in (3.36) and $U^{(n)}$ in (3.37) leads to the following formulae for all $n \in \mathbb{N}$:

$$\begin{pmatrix} |V^{(n+1)}|_0 \\ |V^{(n+1)}|_1 \end{pmatrix} = \big(|V^{(n)}|_0, |V^{(n)}|_1\big) \begin{pmatrix} p & 1 \\ q & 1 \end{pmatrix} + \begin{pmatrix} 2q \\ 1 \end{pmatrix}, \text{ where } |V^{(1)}|_0 = q, \; |V^{(1)}|_1 = 0,$$

$$\begin{pmatrix} |U^{(n+1)}|_0 \\ |U^{(n+1)}|_1 \end{pmatrix} = \big(|U^{(n)}|_0, |U^{(n)}|_1\big) \begin{pmatrix} p & 1 \\ q & 1 \end{pmatrix} + \begin{pmatrix} 2q \\ 1 \end{pmatrix}, \text{ where } |U^{(1)}|_0 = p-1, \; |U^{(1)}|_1 = 0.$$

As a direct consequence of the above recurrent formulae, we deduce the ordering of the lengths of strong and weak BS factors:

$$|V^{(n)}| < |U^{(n)}| < |V^{(n+1)}| \quad \text{for all } n \in \mathbb{N}. \tag{3.40}$$

LS factors and the first difference of complexity

As each LS factor is the prefix of an infinite LS branch or of a maximal LS factor (or, equivalently, weak BS factor), it remains to find the infinite LS branches on order to have described all LS factors.

Lemma 3.4.6. *Let u_β be the fixed point of the substitution φ defined by $\varphi(0) = 0^p1$, $\varphi(1) = 0^q1$, where $p - 1 > q \geq 1$. Then, there exists at most one infinite LS branch of u_β.*

Proof. As the substitution φ is primitive, Section 3.3 claims that $\Delta\mathcal{C}(n)$ is bounded. Proposition 3.1.1 thus implies that the number of infinite LS branches of u_β is finite. Suppose there exists more infinite LS branches. Choose two of them, say $v^{(1)}$ and $v^{(2)}$, whose distance $d(v^{(1)}, v^{(2)})$ (defined in Section 2.2.2) is minimal. Nevertheless, in accordance with properties of the map T, the words $T(v^{(1)}) = \lim_{n\to\infty} T(v_0^{(1)} v_1^{(1)} v_2^{(1)} \dots v_n^{(1)})$ and $T(v^{(2)}) = \lim_{n\to\infty} T(v_0^{(2)} v_1^{(2)} v_2^{(2)} \dots v_n^{(2)})$ are also infinite LS branches of u_β and share a longer prefix, i.e., $d(v^{(1)}, v^{(2)}) > d\big(T(v^{(1)}), T(v^{(2)})\big)$, which is a contradiction. $\square$

Proposition 3.4.7. *The only infinite LS branch of u_β is $\lim_{n\to\infty} V^{(n)}$.*

Proof. The fact that $V^{(1)}$ is a proper prefix of $V^{(2)}$ together with Item *4.* of Lemma 3.4.3 and the completeness of the space $\mathcal{A}^* \cup \mathcal{A}^{\mathbb{N}_0}$ equipped with the metric d guarantees that $\lim_{n\to\infty} V^{(n)}$ is an infinite word. Clearly, it is an infinite LS branch since $V^{(n)}$ are LS factors of u_β. ☐

The tree of LS factors consists of the infinite LS branch $\lim_{n\to\infty} V^{(n)}$ and the truncated branches $U^{(n)}$ sharing with the infinite LS branch the strong BS factor $V^{(n)}$ as the maximal common prefix. See Figure 3.1. The formula for the first difference of complexity is straightforward:

$$\Delta\mathcal{C}(n) = \begin{cases} 2 & \text{if } \ |V^{(k)}| < n \leq |U^{(k)}| \ \text{ for some } k \in \mathbb{N}, \\ 1 & \text{otherwise.} \end{cases} \tag{3.41}$$

Complexity

To conclude, let us write down the formula for the factor complexity of u_β.

Theorem 3.4.8. *Let u_β be the fixed point of the substitution φ defined by $\varphi(0) = 0^p1,\ \varphi(1) = 0^q1$, where $p - 1 > q \geq 1$. Then*

$$\mathcal{C}(n+1) = \begin{cases} 2 + n & \text{if } \ n \leq |V^{(1)}|, \\ 2 + \sum_{i=1}^{k-1}(|U^{(i)}| - |V^{(i)}|) + 2n - |V^{(k)}| & \text{if } |V^{(k)}| < n \leq |U^{(k)}|,\ k \in \mathbb{N}, \\ 2 + \sum_{i=1}^{k}(|U^{(i)}| - |V^{(i)}|) + n & \text{if } |U^{(k)}| < n \leq |V^{(k+1)}|,\ k \in \mathbb{N}. \end{cases}$$

Remark 3.4.9. *Let us provide some details on the Sturmian case. It is known that any Sturmian word u has only one infinite LS branch and no maximal LS factors, thus, all BS factors of u are ordinary. For Sturmian words u_β, i.e., with parameters $p - 1 = q$, it is easy to show that Lemma 3.4.3 keeps its validity. As a direct consequence, the following set of BS factors is obtained:*

$$\{W_r^{(n)} \mid 0 \leq r \leq p-1,\ n \in \mathbb{N}\},$$

where $W_r^{(n)} = T(W_r^{(n-1)})$, $W_r^{(1)} = 0^r$ for $1 \leq r \leq p-1$ and $W_0^{(1)} = \varepsilon$, and, the extension set of $W_r^{(n)}$ is $\{(0,0),(0,1),(1,0)\}$ for $r < p-1$ and $\{(0,1),(1,0),(1,1)\}$ for $r = p-1$. Evidently, it holds for BS factors that $W_{r-1}^{(1)}$ is a prefix of $W_r^{(1)}$ and $W_{p-1}^{(1)}$ is a prefix of $W_1^{(2)}$. Thus, according to Item 4. of Lemma 3.4.3, all BS factors are prefixes of the infinite LS branch given by $\lim_{n\to\infty} W_1^{(n)}$.

Chapter 4

Palindromic complexity

Palindromes, words that remain the same when read backwards, is a popular linguistic game. The longest palindrome listed in the Oxford Dictionary is “tattarrattat”. This word is a neologism created by James Joyce to express *tap on the door* in his novel Ulysses. Not only words, but also palindromic numbers have been attracting attention for ages. Such numbers appear already in a sanskrit manuscript Ganitasarasâmgraha dated around 850 AD. The most famous king of Bohemia – Charles IV – seems to have been fascinated by palindromes as well. He inaugurated the Charles Bridge in Prague on the 9th of July 1357 at 5 o’clock 31 minutes. The palindrome obtained writing down year-day-month-hour-minutes of the inauguration consists moreover uniquely of odd numbers going from 1 to 9 and back.

However, palindromes occur in serious disciplines as well. For instance, nucleotides in most of human genomes form palindromic sequences, or infinite words rich in palindromes are suitable models for the potential of Schröodinger operators linked with quasicrystalline materials (see the paper of Hof, Knill, and Simon [70]).

In this chapter, we study the palindromic complexity of infinite words, which describes how rich an infinite word is in palindromes of a fixed length. After an extension of basics from Section 2.2.10, facilitating the study of palindromic complexity, we recall the palindromic complexity for infinite words in our illustrative sample (introduced in Chapter 3). Newly, we deduce an exact formula for the palindromic complexity of u_β associated with a quadratic non-simple Parry number.

4.1 Extended preliminaries

In order to investigate the palindromic complexity of an infinite word u over an alphabet $\mathcal{A}$, defined in Section 2.2.10, it is suitable to introduce some further notions. Intuitive terms are those ones of central factors and centers of palindromes. A palindrome w' is a *central factor* of a palindrome w if there exists a finite word v such that $w = \overline{v}w'v$. A letter a is a *center* of a palindrome w if it is its central factor. The center of a palindrome of an even length is the empty word ε. We say that $a \in \mathcal{A}$ is a *palindromic extension* of a palindrome $w \in \mathcal{L}(u)$ if awa belongs to $\mathcal{L}(u)$. A palindrome $w \in \mathcal{L}(u)$ is called *maximal* if $awa \notin \mathcal{L}(u)$ for any letter $a \in \mathcal{A}$, or, in other words, if the only palindrome in $\mathcal{L}(u)$ having w as its central factor is w itself.

A complement concept to a maximal palindrome is an infinite palindromic branch. Let $v = v_0v_1v_2\ldots$ be an infinite word over the alphabet $\mathcal{A}$ and let $a \in \{\varepsilon\} \cup \mathcal{A}$. Denote by $\overline{v}$ the left-sided infinite word $\overline{v} = \ldots v_2v_1v_0$. If, for every $n \in \mathbb{N}_0$, the palindrome $w = v_nv_{n-1}...v_0av_0v_1...v_n$ belongs to $\mathcal{L}(u)$, then the biinfinite word $\overline{v}av$ is called an *infinite palindromic branch* of u with the center a; we also say that the palindrome w is a central factor of the infinite palindromic branch $\overline{v}av$.

We will often use the fact (valid thanks to the completeness of the metric space $\mathcal{A}^* \cup \mathcal{A}^{\mathbb{N}_0}$) that any sequence $(w^{(n)})_{n\in\mathbb{N}}$ of palindromes of strictly increasing length such that $w^{(n)}$ is a central factor of $w^{(n+1)}$ for all $n \in \mathbb{N}$ determines uniquely an infinite palindromic branch.

Example: *For the infinite word $u = (010)^\omega$, the only maximal palindrome is 0 and there are two infinite palindromic branches, one of them with the center ε and of the form $\overline{v}v$ and the other one with the center 1 and of the form $\overline{v}010v$, where $v = (010)^\omega$.*

Since every palindrome is either a central factor of a maximal palindrome or of an infinite palindromic branch, once all maximal palindromes and infinite palindromic branches described, the palindromic complexity is fully determined.

4.2 Bounds on palindromic complexity

A nice survey on the palindromic complexity of several concrete infinite words and some larger classes of infinite words by Allouche *et al.* is to consult in [3]. It is natural to study the relation between factor complexity and palindromic complexity. The authors of [3] have derived an upper bound on the palindromic complexity of aperiodic words in terms of their factor complexity:

$$\mathcal{P}(n) < \tfrac{16}{n}\mathcal{C}(n + \lfloor \tfrac{n}{4} \rfloor) \quad \text{for all } n \in \mathbb{N}. \tag{4.1}$$

For infinite uniformly recurrent words, the following upper bound on the palindromic complexity using the first difference of complexity has been obtained by Baláži, Masáková, and Pelantová in [10]:

$$\mathcal{P}(n) + \mathcal{P}(n+1) \leq \Delta\mathcal{C}(n) + 2 \quad \text{for all } n \in \mathbb{N}_0. \tag{4.2}$$

Remark 4.2.1. *This estimate holds even for infinite words with language closed under reversal that are not necessarily uniformly recurrent. We recall that closeness under reversal implies recurrence and recurrent words have strongly connected Rauzy graphs (see Section 2.2.12). Closeness under reversal and strongly connected Rauzy graphs were sufficient for the proof of* (4.2) *in [10].*

This upper bound is better than the general one from (4.1) for infinite words with language closed under reversal and with factor complexity equal to a polynomial of degree ≤ 16. Infinite words that realize the equality in (4.2) is the object of our further study.

Definition 4.2.2. *An infinite word realizing the equality in* (4.2) *is called opulent in palindromes.*

Hereinafter, we start as usually with the known results on palindromes of Sturmian, AR, and m-iet words. They represent the best-known examples of words opulent in palindromes.

We mention what is known about palindromes and the palindromic complexity for the infinite words whose special factors and complexity have been described in Section 3.3. Since the estimate (4.2) together with Equation (3.9) guarantees that infinite words with sublinear complexity have bounded palindromic complexity, it follows that the palindromic complexity of each infinite word in our sample is bounded. We decide moreover for each sample word whether it is opulent in palindromes or not. (We show later that also the infinite words u_β associated with quadratic non-simple Parry numbers are opulent in palindromes.)

4.2.1 Sturmian words, AR words, and m-iet words

Every Sturmian word has one palindrome of every even length and two palindromes of every odd length (Theorem 2.4.1). Similarly, both AR words of order m (as proved by Damanik and Zamboni in [40]) and m-iet words (as shown by Baláži, Masáková, and Pelantová in [10]) have one palindrome of every even length and m palindromes of every odd length. The palindromic complexity together with their first difference of complexity (Section 3.3.1) implies that all these words are opulent in palindromes.

4.2.2 Thue-Morse word

Palindromes of the Thue-Morse word were originally determined by de Luca and Varricchio in [86]. Crucial for the determination of palindromes in u_{TM} is the following lemma.

Lemma 4.2.3. *Let w be a factor of u_{TM}. Then w is a palindrome if and only if $\varphi^2(w)$ is a palindrome. Moreover, w and $\varphi^2(w)$ has the same number of palindromic extensions.*

Maximal palindromes

The word u_{TM} contains only two maximal palindromes of odd length:

$$010, \ 101,$$

while there exist two infinite sequences of maximal palindromes of even length:

$$\left(\varphi^{2n}(010)\right)_{n\geq 1} \quad \text{and} \quad \left(\varphi^{2n}(101)\right)_{n\geq 1}.$$

Infinite palindromic branches

There are two infinite palindromic branches of u_{TM} given by the following sequences of their central factors

$$v^{(1)} = \left(\varphi^{2n}(1)\right)_{n\geq 1} \quad \text{and} \quad S(v^{(1)}) = \left(\varphi^{2n}(0)\right)_{n\geq 1},$$

where the maximal palindrome $\varphi^{2n}(010)$ shares with the infinite palindromic branch $v^{(1)}$ as the longest common central factor $\varphi^{2n}(1)$, and $\varphi^{2n}(101)$ shares with $S(v^{(1)})$ the central factor $\varphi^{2n}(0)$ as illustrated in Figure 4.1.

Palindromic complexity

We have

$$\begin{array}{ll} \text{for } n \text{ odd} & \mathcal{P}(1) = 2, \ \mathcal{P}(3) = 2, \ \mathcal{P}(n) = 0 \text{ for } n \geq 5, \\ \text{for } n \text{ even} & \mathcal{P}(n) = \begin{cases} 4 & \text{if } 4^k < n \leq 3 \cdot 4^k \text{ for some } k \in \mathbb{N}, \\ 2 & \text{otherwise.} \end{cases} \end{array} \tag{4.3}$$

Let us remark that the Thue-Morse word is not opulent in palindromes. For instance, if we set $n := 2\cdot 4^k, \ k \in \mathbb{N}$, then $\mathcal{P}(n+1)+\mathcal{P}(n) = 4$ and $\Delta\mathcal{C}(n) = 4$, hence $\mathcal{P}(n+1)+\mathcal{P}(n) < \Delta\mathcal{C}(n)+2$.

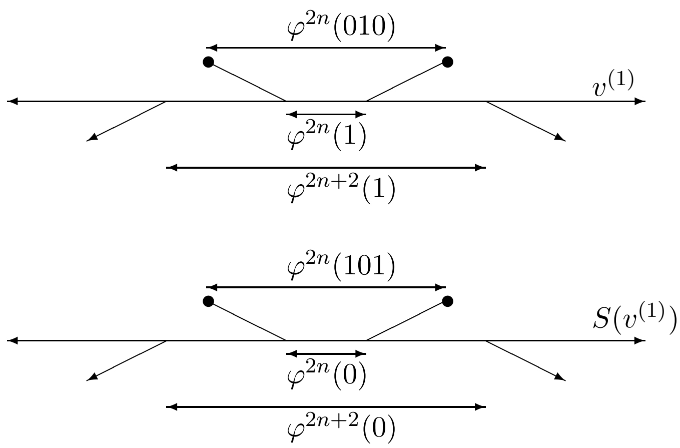


Fig. 4.1: Illustration of a sector of the infinite palindromic branches and of the maximal palindromes of u_{TM} between lengths $|\varphi^{2n}(0)| = 4^n$ and $|\varphi^{2n+2}(0)| = 4^{n+1}$.

4.2.3 Period doubling word

The description of the palindromic structure of u_{PD} has been provided by Damanik [34]. The essential role for the determination of palindromes in u_{PD} is played by the following lemma.

Lemma 4.2.4. *Let w be a factor of u_{PD}. Then w is a palindrome if and only if $T_{PD}(w) = \varphi(w)0$ is a palindrome. Moreover, w has the same number of palindromic extensions as $T_{PD}(w)$.*

Maximal palindromes

The word u_{PD} has only one maximal palindrome of even length:

$$U^{(1)} = 00,$$

and there exists an infinite sequence of maximal palindromes of odd length $(U^{(n)})_{n\in\mathbb{N}}$. (See Section 3.3.3 for the definition of $U^{(n)},\ V^{(n)}$.)

There are two infinite palindromic branches of u_{PD} given by the following sequences of their central factors

$$v^{(1)} = \left(V^{(2n-1)}\right)_{n\geq 1}, \quad v^{(2)} = \left(V^{(2n)}\right)_{n\geq 1}.$$

The center of $v^{(1)}$ is 0 and $v^{(1)}$ shares $V^{(2n-1)}$ as the longest central factor with the maximal palindrome $U^{(2n)}$ for every $n \in \mathbb{N}$. The center of $v^{(2)}$ is 1 and $v^{(2)}$ shares $V^{(2n)}$ as the longest central factor with the maximal palindrome $U^{(2n+1)}$ for every $n \in \mathbb{N}$.

Palindromic complexity

We deduce

$$\begin{aligned} &\text{for } n \text{ even} \quad \mathcal{P}(0) = 1,\ \mathcal{P}(2) = 1,\ \mathcal{P}(n) = 0 \text{ for } n \geq 4,\\ &\text{for } n \text{ odd} \quad \mathcal{P}(n) = \begin{cases} 2 & \text{if } n = 1,\\ 4 & \text{if } 2^k < n \leq 3\cdot 2^{k-1} - 1 \text{ for some } k \in \mathbb{N},\ k \geq 2,\\ 3 & \text{otherwise.} \end{cases} \end{aligned} \tag{4.4}$$

Comparing with the formula for the first difference of complexity from Section 3.3.3, we get $\mathcal{P}(n) + \mathcal{P}(n+1) = \Delta\mathcal{C}(n) + 2$. The period doubling word is thus another example of an infinite word opulent in palindromes.

4.2.4 Rote word

Similarly as in the previous cases, the most important tool is a lemma revealing some relation between palindromes and their images.

Lemma 4.2.5. *Let w be a factor of u_R. Then w is a palindrome if and only if $T_R(w) = 1\varphi(w)$ is a palindrome. Moreover, w and $T_R(w)$ have the same number of palindromic extensions.*

As a first observation, let us point out that $\mathcal{L}(u_{\mathrm{R}})$ is closed under reversal. The explanation is as follows. Any factor w occurs in $\varphi^n(0)$ for some n, it is then not difficult to see that $\varphi^n(0)$ is a suffix of $T_{\mathrm{R}}^n(0)$, which is a palindromic factor of u_{R}. Hence, $\overline{w}$ is also a factor of u_{R}.

Maximal palindromes

The word u_R has only one maximal palindrome with the center 0:

$$U^{(1)} = 0,$$

and one with central factor 00:

$$U^{(2)} = 1001,$$

there exists an infinite sequence $(U^{(n)})_{n\in\mathbb{N}}$ of maximal palindromes with either the center 1, if n is odd, or the central factor 11, if n is even.

There are two infinite palindromic branches of u_R given by the following sequences of their central factors

$$v^{(1)} = \left(V^{(2n-1)}\right)_{n\geq 1}, \quad v^{(2)} = \left(V^{(2n)}\right)_{n\geq 1}.$$

The center of $v^{(1)}$ is 1 and $v^{(1)}$ shares $V^{(2n-1)}$ as the longest central factor with the maximal palindrome $U^{(2n+1)}$ for every $n \in \mathbb{N}$. The center of $v^{(2)}$ is ε and $v^{(2)}$ shares $V^{(2n)}$ as the longest central factor with the maximal palindrome $U^{(2n+2)}$.

Palindromic complexity

We derive a nice formula for the palindromic complexity

$$\mathcal{P}(n) = 2 \quad \text{for all } n \in \mathbb{N} \qquad \text{and} \qquad \mathcal{P}(0) = 1. \tag{4.5}$$

Comparing with the formula for the first difference of complexity from Section 3.3.4, we deduce $\mathcal{P}(n) + \mathcal{P}(n+1) = \Delta\mathcal{C}(n) + 2$. The Rote word is thus a further example of an infinite word opulent in palindromes.

4.2.5 A palindromeless reversal closed word

As another example, we consider the infinite word z (defined by (3.23)). We find all factors of length 13 and 14, which is a simple task thanks to the linear recurrence of z with constant 31 (Proposition 3.3.5). By inspection, we see that no palindromes of length > 12 are contained in z. More precisely, the complete list of the maximal palindromes of z is: 10101, 01010, 10100101, 100101101001.

4.2.6 u_β associated with simple Parry numbers

The palindromic structure of u_β has been studied by Ambrož *et al.* in [4] for confluent Parry numbers since it is the only case for which $\mathcal{L}(u_\beta)$ is closed under reversal (see Proposition 2.3.1), and, therefore, u_β may have an infinite number of palindromes. Let us recall that such an infinite word u_β is the fixed point of the substitution

$$\varphi(0) = 0^t1,\ \varphi(1) = 0^t2, \ldots,\ \varphi(m-2) = 0^t(m-1),\ \varphi(m-1) = 0^s, \tag{4.6}$$

where $t \geq s \geq 1$.

If $s = 1$, then according to Section 3.3.6, the word u_β is an Arnoux-Rauzy word, and, consequently, its palindromic complexity is known (consult Section 4.2.1).

In the sequel, we provide the list of maximal palindromes and infinite palindromic branches. The basic observation for the derivation of this list is the following lemma, which moreover guarantees that u_β contains infinitely many palindromes.

Lemma 4.2.6. *Let u_β be an infinite word associated with a confluent Parry number β and let w be its factor. Then w is a palindrome if and only if $\varphi(w)0^t$ is a palindrome.*

Maximal palindromes and palindromes with two palindromic extensions

The set of all maximal palindromes coincides with the set of all weak BS factors $\{U^{(n)} | n \in \mathbb{N}\}$, defined in (3.31), and the set of all palindromes with two palindromic extensions is equal to the set of all strong BS factors $\{V^{(n)} | n \in \mathbb{N}\}$, defined in (3.30). The other palindromes have exactly one palindromic extension. This fact together with the formula for the second difference of complexity from (3.32) implies the equality

$$\mathcal{P}(n+2) - \mathcal{P}(n) = \Delta^2\mathcal{C}(n) \quad \text{for all } n \in \mathbb{N}_0.$$

Performing a simple calculation, one gets finally

$$\mathcal{P}(n) + \mathcal{P}(n+1) = \Delta\mathcal{C}(n) + 2 \quad \text{for every } n \in \mathbb{N}_0.$$

In other words, u_β associated with a confluent Parry number β is an example of an infinite word opulent in palindromes.

Infinite palindromic branches

We write down not only infinite palindromic branches, but also the longest common central factors they share with the maximal palindromes having the same center. The situation is diversified in dependence on the parity of parameters t and s.

- If t is even and s even, then u_β has a unique infinite palindromic branch which is given by the sequence of its central factors $\left(V^{(n)}\right)_{n\geq 1}$ and has the center ε. For every $n \in \mathbb{N}$, $V^{(n)}$ is the longest common central factor of the infinite palindromic branch and the maximal palindrome $U^{(n+m)}$. Every palindrome with the center $k-1$ is the central factor of the maximal palindrome $U^{(k)}$, $k \in \{1, 2, \ldots, m\}$.
- If t is even and s odd, then there exist $m+1$ infinite palindromic branches, namely: $\left(V^{(n)}\right)_{n\geq 1}$ with the center ε and having the common central factor $V^{(n)}$ with $U^{(n)}$ for every $n \in \mathbb{N}$, and, for $k \in \{1, 2, \ldots, m\}$, $\left(W_1^{(k+mn)}\right)_{n\geq 0}$ with the center $k-1$, defined by $W_1^{(1)} = 0,\ W_1^{(n)} = \varphi(W_1^{(n-1)})0^t$ for all $n \in \mathbb{N}$.

- If t is odd and s even, then there are m infinite palindromic branches, namely: for $k \in \{1, 2, \dots, m\}$, the branch $\left(V^{(k+mn)}\right)_{n \geq 1}$ has the center $k-1$ and the central factor $V^{(k+mn)}$ in common with $U^{(k+mn+1)}$ for all $n \in \mathbb{N}_0$. All palindromes of even length are central factors of $U^{(1)}$.
- If t is odd and s odd, then u_β possesses $m+1$ infinite palindromic branches, namely: $\left(V^{(k+(m+1)n)}\right)_{n \geq 0}$ for $k \in \{1, 2, \dots, m+1\}$ with the center $k-1$ if $k \neq m+1$ and ε if $k = m+1$, and sharing the central factor $V^{(k+(m+1)n)}$ with $U^{(k+(m+1)n)}$ for all $n \in \mathbb{N}_0$.

Palindromic complexity

The exact formula for the palindromic complexity is straightforward with the previous paragraph in hand, however, it is rather technical. In consequence, we prefer to summarize that for n large and

$$\begin{array}{llcl}
t \text{ even, } s \text{ even,} & m+1 \leq \mathcal{P}(2n) \leq m+2 & \text{and} & \mathcal{P}(2n+1) = 0, \\
t \text{ even, } s \text{ odd,} & 1 \leq \mathcal{P}(2n) \leq 2 & \text{and} & \mathcal{P}(2n+1) = m, \\
t \text{ odd, } s \text{ even,} & \mathcal{P}(2n) = 0 & \text{and} & m+1 \leq \mathcal{P}(2n+1) \leq m+2, \\
t \text{ odd, } s \text{ odd,} & 1 \leq \mathcal{P}(2n) \leq 2 & \text{and} & m \leq \mathcal{P}(2n+1) \leq m+1.
\end{array}$$

4.3 Palindromic complexity of u_β associated with quadratic non-simple Parry numbers

For the study of the palindromic complexity of infinite words u_β associated with non-simple Parry numbers β, it is meaningful to restrict the considerations to the quadratic numbers. The word u_β associated with a non-simple Parry number β may have infinitely many palindromes only if β is a quadratic number (combine Propositions 2.2.3 and 2.3.2). We shall see immediately that the infinite words associated with quadratic non-simple Parry numbers contain indeed an infinite number of different palindromes.

Let us recall that the infinite word u_β is the fixed point of the substitution φ defined in (2.27) by $\varphi(0) = 0^p1$, $\varphi(0) = 0^q1$, $p > q \geq 1$. In reference to Remark 2.3.4, u_β is a Sturmian word if and only if $p = q+1$. The palindromic complexity of Sturmian words is known, therefore, we restrict our considerations to $p > q+1$.

Similarly as in the study of special factors and complexity, the map T defined in (3.35) plays an essential role in the determination of palindromic complexity.

Lemma 4.3.1. *Let T be the map defined in* (3.35) *and let w be a factor of u_β. Then w is a palindrome if and only if $T(w)$ is a palindrome. Moreover, w has the same palindromic extensions as $T(w)$.*

Proof. To prove both implications, it suffices to notice that $1\varphi(a) = \overline{\varphi(a)}1$ for $a \in \{0, 1\}$. The implication $\Leftarrow$ follows using in addition the fact that $\{\varphi(0), \varphi(1)\}$ is a prefix code.

The second statement is an immediate consequence of Item *2.* of Lemma 3.4.3. ∎

Proposition 4.3.2. *Let u_β be the fixed point of the substitution φ defined by $\varphi(0) = 0^p1$, $\varphi(1) = 0^q1$, where $p-1 > q \geq 1$, and let w be a palindromic factor of u_β. Then*

1. *w is a maximal palindrome $\Leftrightarrow$ $w = U^{(n)}$ for a positive integer n.*
2. *w has two palindromic extensions $\Leftrightarrow$ $w = V^{(n)}$ for a positive integer n.*
3. *w has one palindromic extension $\Leftrightarrow$ $w \neq U^{(n)} \wedge w \neq V^{(n)}$ for all $n \in \mathbb{N}$.*

Proof. *1.* ($\Rightarrow$): Let w be a maximal palindrome, then the set of extensions $\{(a,b)|\ a,b \in \{0,1\}, awb \in \mathcal{L}(u_\beta)\}$ is a subset of $\{(0,1),(1,0)\}$. On the other hand, since the infinite word u_β is recurrent and its language $\mathcal{L}(u_\beta)$ is closed under reversal, the sets even coincide $\{(a,b)|\ a,b \in \{0,1\}, awb \in \mathcal{L}(u_\beta)\} = \{(0,1),(1,0)\}$. Thus, w is a weak BS factor and is therefore necessarily equal to $U^{(n)}$ for some $n \in \mathbb{N}$. ($\Leftarrow$): The fact that all weak BS factors are palindromes is guaranteed by Lemma 4.3.1.
2. ($\Rightarrow$): Let w be a palindrome with two palindromic extensions, then Corollary 3.4.5 together with Lemma 3.4.4 and Item *2.* of Lemma 3.4.3 state that w is a strong BS factor, hence, w is equal to $V^{(n)}$ for some $n \in \mathbb{N}$. ($\Leftarrow$): Again, the fact that all strong BS factors are palindromes follows from Lemma 4.3.1.
3. is obvious - there are no other possibilities for palindromic extensions over a binary alphabet. □

It is interesting to notice that sequences $U^{(n)}$ of weak BS factors and $V^{(n)}$ of strong BS factors play an important role not only in computing the factor complexity, but also in determining the palindromic complexity. For illustration, consider the example from Figure 3.1 in Section 3.4 and check that the strong and weak BS factors illustrated there are indeed palindromes.

Using the inequality $|V^{(n)}| < |U^{(n)}| < |V^{(n+1)}|$ from (3.40) for all $n \in \mathbb{N}$, we obtain the following corollary of Proposition 4.3.2.

Corollary 4.3.3. *Let u_β be the fixed point of the substitution φ defined by $\varphi(0) = 0^p1$, $\varphi(1) = 0^q1$, where $p-1 > q \geq 1$. Then*

$$\mathcal{P}(n+2) - \mathcal{P}(n) = \begin{cases} 1 & \textit{if } \ n = |V^{(k)}| \textit{ for some } k \in \mathbb{N}, \\ -1 & \textit{if } \ n = |U^{(k)}| \textit{ for some } k \in \mathbb{N}, \\ 0 & \textit{otherwise.} \end{cases}$$

Combining with the formula from (3.39), we can derive a simple connection of palindromic complexity with the second difference of complexity:

$$\Delta^2\mathcal{C}(n) = \mathcal{P}(n+2) - \mathcal{P}(n)\,.$$

This relation is essential in order to show that the word u_β is another example of an infinite word opulent in palindromes.

Corollary 4.3.4. *Let u_β be the fixed point of the substitution φ defined by $\varphi(0) = 0^p1$, $\varphi(1) = 0^q1$, where $p-1 > q \geq 1$. Then*

$$\mathcal{P}(n+1) + \mathcal{P}(n) = \Delta\mathcal{C}(n) + 2 \qquad \textit{for all } n \in \mathbb{N}_0\,. \tag{4.7}$$

Proof. We have

$$\begin{aligned} \mathcal{P}(n+1) + \mathcal{P}(n) &= \mathcal{P}(0) + \mathcal{P}(1) + \sum_{i=1}^{n}\big(\mathcal{P}(i+1) - \mathcal{P}(i-1)\big) = \\ &= 1 + 2 + \sum_{i=1}^{n}\Delta^2\mathcal{C}(i-1) = \\ &= 3 + \sum_{i=1}^{n}\big(\Delta\mathcal{C}(i) - \Delta\mathcal{C}(i-1)\big) = \\ &= 3 + \Delta\mathcal{C}(n) - \Delta\mathcal{C}(0) = \\ &= \Delta\mathcal{C}(n) + 2. \end{aligned}$$

□

A direct consequence of the above corollary and the formula (3.41) is an upper bound on the palindromic complexity of u_β in the form $\mathcal{P}(n+1) + \mathcal{P}(n) \leq 4$.

4.3.1 Centers of palindromes

We have seen that the set of palindromes of u_β is closed under the map $w \mapsto T(w) = 0^q 1\varphi(w)0^q$. Let us study how T acts on the central factors of palindromes.

Lemma 4.3.5. *Let w, v be palindromes in u_β. If w is a central factor of v, then $T(w)$ is a central factor of $T(v)$.*

Proof. Let $v = w'0w0\overline{w'}$ for a $w' \in \mathcal{L}(u_\beta)$. Then $T(v) = 0^q 1\varphi(w')0^p 1\varphi(w)0^p 1\varphi(\overline{w'})0^q$. According to Lemma 4.3.1, $T(v)$ is a palindrome, and clearly, $T(w) = 0^q 1\varphi(w)0^q$ is its central factor. The proof is similar for $v = w'1w1\overline{w'}$. □

Now, using Lemma 4.3.5, we can describe how the center of the palindrome $T(w)$ depends on the center of the palindrome w.

Lemma 4.3.6. *Let w be a palindromic factor of u_β.*

(i) If w has the center ε, then $T(w)$ has the center 1.

(ii) If w has the center 0, then $T(w)$ has the center $\begin{cases} 0 & \text{for } p \text{ odd,} \\ \varepsilon & \text{for } p \text{ even.} \end{cases}$

(iii) If w has the center 1, then $T(w)$ has the center $\begin{cases} 0 & \text{for } q \text{ odd,} \\ \varepsilon & \text{for } q \text{ even.} \end{cases}$

Proof. Let us verify for example the statement (ii). Using Lemma 4.3.5, it is evident that if w has the center 0, then $T(w)$ has the central factor $T(0) = 0^q 10^p 10^q$. Consequently, the center of $T(w)$ is either 0 if p is odd, or ε if p is even. The other statements can be proved analogously. □

Lemmas 4.3.5 and 4.3.6 allow us to describe the centers of palindromes with two palindromic extensions $V^{(n)}$ and the centers of maximal palindromes $U^{(n)}$.

Proposition 4.3.7. *The centers and central factors of palindromes $V^{(n)}$ with two palindromic extensions depend on the values of parameters p and q.*

(i) Let q be even. Then $V^{(n)}$ is a central factor of $V^{(n+2)}$ for all $n \in \mathbb{N}$. Moreover, $V^{(2n)}$ has the center 1 and $V^{(2n-1)}$ has the center ε.

(ii) Let q be odd and p even. Then $V^{(n)}$ is a central factor of $V^{(n+3)}$ for all $n \in \mathbb{N}$. Moreover, $V^{(3n)}$ has the center 1, $V^{(3n-1)}$ has the center ε, and $V^{(3n-2)}$ has the center 0.

(iii) Let both q and p be odd. Then $V^{(n)}$ is a central factor of $V^{(n+1)}$ for all $n \in \mathbb{N}$ and has the center 0.

Proof. In order to show the statement (i), it suffices to verify that $V^{(1)}$ is a central factor of $V^{(3)}$ and that $V^{(1)}$ has the center ε and $V^{(2)}$ has the center 1. The statement (i) then follows by induction on $n \in \mathbb{N}$ using Lemma 4.3.5. Since q is even, $V^{(1)} = 0^q$ has the center ε. By Lemma 4.3.6, $V^{(2)}$ has the center 1. Applying Lemma 4.3.5, one can see that $V^{(3)}$ has the central factor $T(1) = 0^q 10^q 10^q$, i.e., it has also $V^{(1)}$ as its central factor.

Proofs of statements (ii) and (iii) are analogous. □

Proposition 4.3.8. *The centers and central factors of maximal palindromes $U^{(n)}$ depend on the values of parameters p and q.*

(i) Let q be even and p odd. Then $V^{(n)}$ is a central factor of $U^{(n)}$ for all $n \in \mathbb{N}$. Moreover, $U^{(2n-1)}$ has the center ε and $U^{(2n)}$ has the center 1.

(ii) Let both q and p be even. Then $U^{(1)} = 0^{p-1}$ is the only maximal palindrome with the center 0. *For all $n \in \mathbb{N}$, $V^{(n)}$ is a central factor of $U^{(n+1)}$. Moreover, $U^{(2n)}$ has the center ε and $U^{(2n+1)}$ has the center* 1.

(iii) Let q be odd and p even. Then $V^{(n)}$ is a central factor of $U^{(n)}$ for all $n \in \mathbb{N}$. Moreover, $U^{(3n-2)}$ has the center 0*, $U^{(3n-1)}$ has the center ε, and $U^{(3n)}$ has the center* 1.

(iv) Let both q and p be odd. The only maximal palindrome with the center ε is $U^{(1)} = 0^{p-1}$. The only maximal palindrome having the center 1 *is $U^{(2)}$. For $n \geq 3$, $U^{(n)}$ has the center* 0 *and the central factor $V^{(n-2)}$.*

Proof. Let us show for example the statement (ii). Since p is even, $U^{(1)} = 0^{p-1}$ has the center 0. Lemma 4.3.6 implies that $U^{(2)}$ has the center ε and the central factor $T(0) = 0^q 1 0^p 1 0^q$. Consequently, $V^{(1)} = 0^q$ is also a central factor of $U^{(2)}$, q being even. Applying Lemma 4.3.6, we obtain that $U^{(3)}$ has the center 1. The statement follows by the induction on $n \in \mathbb{N}$, applying Lemma 4.3.5. □

4.3.2 Infinite palindromic branches

We have already described maximal palindromes, therefore the remaining task in order to derive the palindromic complexity is to find infinite palindromic branches. First, let us show that there may be only a few infinite palindromic branches.

Lemma 4.3.9. *Let $a \in \{\varepsilon, 0, 1\}$. Then there exists at most one infinite palindromic branch with the center a.*

Proof. We show the statement by contradiction. Suppose that there are two different infinite palindromic branches given by the sequences of their central factors $(w^{(n)})_{n\in\mathbb{N}}$ and $(v^{(n)})_{n\in\mathbb{N}}$ with the same center a having w as the maximal common central factor. By applying the map T, we obtain two different infinite palindromic branches $(T(w^{(n)}))_{n\in\mathbb{N}}$ and $(T(v^{(n)}))_{n\in\mathbb{N}}$ with a longer common central factor $T(w)$. Repeating this procedure, we can construct infinitely many different infinite palindromic branches, which is a contradiction with boundedness of the palindromic complexity. □

Using Propositions 4.3.7 and 4.3.8, we now describe, for each $a \in \{\varepsilon, 0, 1\}$, the infinite palindromic branch of u_β with the center a (provided it exists) and the common central factors of this branch with maximal palindromes having the same center a. With this in hand, we will be able to summarize the values of the palindromic complexity. Note that the candidate for the longest common prefix of a maximal palindrome and an infinite palindromic branch with the same center is a palindrome, which has two palindromic extensions, thus one of the palindromes $V^{(n)}$.

Proposition 4.3.10. *Let u_β be the fixed point of the substitution $\varphi(0) = 0^p 1$, $\varphi(1) = 0^q 1$, $p-1 > q \geq 1$.*

(i) Let q be even and p odd. There exists an infinite palindromic branch with the center a for all $a \in \{\varepsilon, 1, 0\}$, namely:

$$\begin{array}{ll} \left(V^{(2n-1)}\right)_{n\in\mathbb{N}} & \textit{having the center } \varepsilon, \\ \left(V^{(2n)}\right)_{n\in\mathbb{N}} & \textit{having the center } 1, \\ \left(W_1^{(n)}\right)_{n\in\mathbb{N}} & \textit{where } W_1^{(1)} = 0, W^{(n)} = T(W_1^{(n-1)}), \\ & \textit{having the center } 0. \end{array}$$

For $n \in \mathbb{N}$, the longest common central factor of the maximal palindrome $U^{(n)}$ and the infinite palindromic branch with the same center is $V^{(n)}$.

(ii) Let both q and p be even. There exists an infinite palindromic branch with the center a for $a \in \{\varepsilon, 1\}$, namely:

$$\begin{array}{ll} \left(V^{(2n-1)}\right)_{n\in\mathbb{N}} & \textit{having the center } \varepsilon, \\ \left(V^{(2n)}\right)_{n\in\mathbb{N}} & \textit{having the center } 1. \end{array}$$

There is no infinite palindromic branch with the center 0. For $n \in \mathbb{N}$, $n \geq 2$, the longest common central factor of the maximal palindrome $U^{(n)}$ and the infinite palindromic branch with the same center is $V^{(n-1)}$.

(iii) Let q be odd and p even. There exists an infinite palindromic branch with the center a for $a \in \{0, \varepsilon, 1\}$, namely:

$$\begin{array}{ll} \left(V^{(3n-2)}\right)_{n\in\mathbb{N}} & \textit{having the center } 0, \\ \left(V^{(3n-1)}\right)_{n\in\mathbb{N}} & \textit{having the center } \varepsilon, \\ \left(V^{(3n)}\right)_{n\in\mathbb{N}} & \textit{having the center } 1. \end{array}$$

For $n \in \mathbb{N}$, the longest common central factor of the maximal palindrome $U^{(n)}$ and the infinite palindromic branch with the same center is $V^{(n)}$.

(iv) Let both q and p be odd. There exists one infinite palindromic branch, namely:

$$\left(V^{(n)}\right)_{n\in\mathbb{N}} \qquad \textit{having the center } 0.$$

There is neither an infinite palindromic branch with the center ε, nor with the center 1. For $n \in \mathbb{N}$, $n \geq 3$, the longest common central factor of the maximal palindrome $U^{(n)}$ and the infinite palindromic branch is $V^{(n-2)}$.

Proof. It follows from Lemma 4.3.9 that there is at most one infinite palindromic branch with the center a for each $a \in \{\varepsilon, 0, 1\}$. It suffices to use Proposition 4.3.7, or Lemma 4.3.5, to see that the listed sequences determine infinite palindromic branches, i.e., are sequences of palindromes of strictly growing length and such that these palindromes are central factors of one another. Let us explain why in cases (ii) and (iv) one does not have an infinite palindromic branch with every center.

(ii) Let q and p be even, suppose that there is a palindromic branch with the center 0. Necessarily, this branch has a block of the form 0^p or 0^q as its central factor. It is impossible owing to the fact that both p and q are even.

(iv) Let both q and p be odd, suppose that there is an infinite palindromic branch with the center ε. Then it has a block of the form 0^p or 0^q as its central factor. It is impossible since both p and q are odd. Suppose now that there exists an infinite palindromic branch with the center 1. Take a central factor of this palindromic branch of the form $T(w)$ for a palindrome w

containing at least two letters 1. Using Lemma 4.3.6, w must have the center ε, and, thus, have the central factor 0^p or 0^q, which is impossible.

The statements about the maximal common central factors of maximal palindromes and infinite palindromic branches is a consequence of Proposition 4.3.8. $\square$

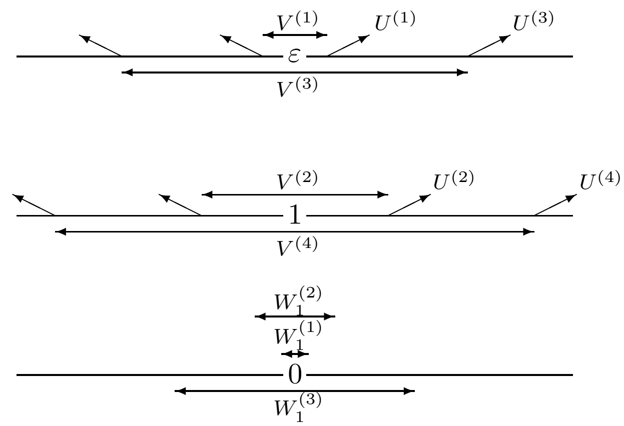


Fig. 4.2: Illustration of maximal palindromes and infinite palindromic branches for q even and p odd. There is one infinite branch with the center ε, one with the center 1, and one with the center 0. There are infinitely many maximal palindromes with the center ε and 1.

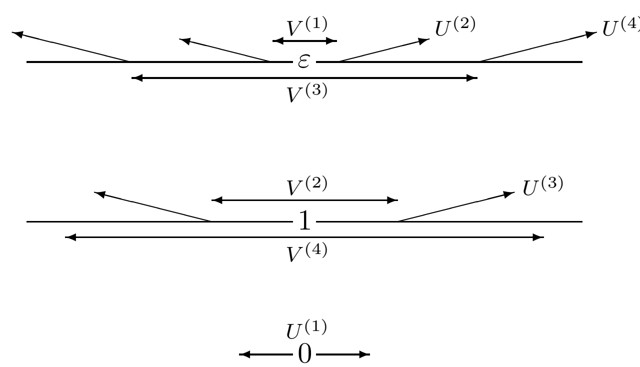


Fig. 4.3: Illustration of maximal palindromes and infinite palindromic branches for p and q even. There is one infinite branch with the center ε and one with the center 1. There are infinitely many maximal palindromes with the center ε and 1. There is only one maximal palindrome with the center 0.

4.3.3 Explicit values of the palindromic complexity of u_β

We are now in position to derive explicitly the values of the palindromic complexity of the infinite word u_β dependently on the parity of parameters p, q of the Rényi expansion of unity $d_\beta(1) = pq^\omega$. We have investigated maximal palindromes, infinite palindromic branches, and their centers. The determination of the complexity is easy with the use of Figures 4.2–4.5, which

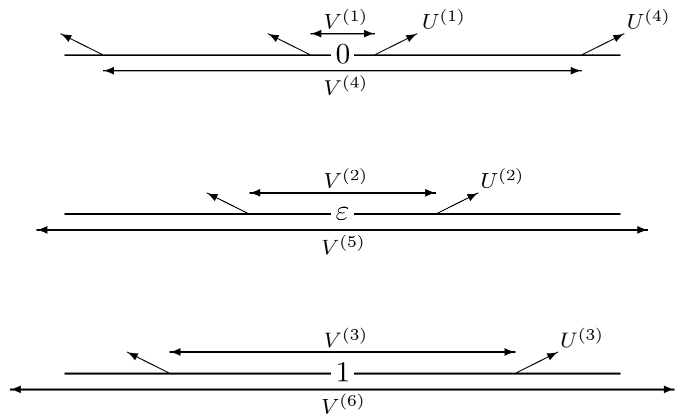


Fig. 4.4: Illustration of maximal palindromes and infinite palindromic branches for q odd and p even. There are infinite branches and infinitely many maximal palindromes with the centers $0, 1, \varepsilon$.

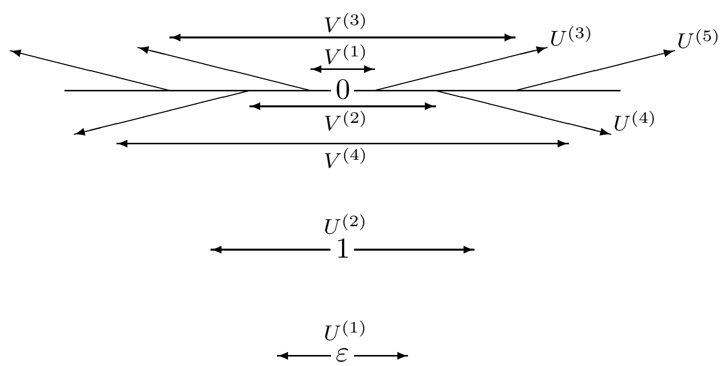


Fig. 4.5: Illustration of maximal palindromes and infinite palindromic branches for p and q odd. The only infinite palindromic branch has the center 0. There are infinitely many maximal palindromes with the center 0. There is only one maximal palindrome with the center ε and one with the center 1.

visualize the structure of maximal palindromes and of infinite palindromic branches, according to Proposition 4.3.10.

Theorem 4.3.11. *Let u_β be the fixed point of the substitution $\varphi(0) = 0^p1,\ \varphi(1) = 0^q1,\ p-1 > q \geq 1$. Then 4 cases appear according to the values of parameters p and q, $n \in \mathbb{N}_0$:*

(i) Let q be even and p odd.

$$\mathcal{P}(2n) = \begin{cases} 2 & \textit{if } |V^{(2k-1)}| < 2n \leq |U^{(2k-1)}| \textit{ for some } k \in \mathbb{N}, \\ 1 & \textit{otherwise.} \end{cases}$$

$$\mathcal{P}(2n+1) = \begin{cases} 3 & \textit{if } |V^{(2k)}| < 2n+1 \leq |U^{(2k)}| \textit{ for some } k \in \mathbb{N}, \\ 2 & \textit{otherwise.} \end{cases}$$

(ii) Let both q and p be even.

$$\mathcal{P}(2n) = \begin{cases} 2 & \textit{if } \ |V^{(2k-1)}| < 2n \leq |U^{(2k)}| \textit{ for some } k \in \mathbb{N}\,, \\ 1 & \textit{otherwise.} \end{cases}$$

$$\mathcal{P}(2n+1) = \begin{cases} 2 & \textit{if } \quad 2n+1 \leq |U^{(1)}| = p-1\,, \\ 2 & \textit{if } \ |V^{(2k)}| < 2n+1 \leq |U^{(2k+1)}| \textit{ for some } k \in \mathbb{N}\,, \\ 1 & \textit{otherwise.} \end{cases}$$

(iii) Let q be odd and p even.

$$\mathcal{P}(2n) = \begin{cases} 2 & \textit{if } \ |V^{(3k-1)}| < 2n \leq |U^{(3k-1)}| \textit{ for some } k \in \mathbb{N}\,, \\ 1 & \textit{otherwise.} \end{cases}$$

$$\mathcal{P}(2n+1) = \begin{cases} 3 & \textit{if } |V^{(k)}| < 2n+1 \leq |U^{(k)}| \textit{ for some } k \in \mathbb{N},\ k \not\equiv 2 \bmod 3, \\ 2 & \textit{otherwise.} \end{cases}$$

(iv) Let both q and p be odd. We have

$$\mathcal{P}(2n) = \begin{cases} 1 & \textit{if } \ 0 \leq 2n \leq |U^{(1)}| = p-1, \\ 0 & \textit{otherwise.} \end{cases}$$

$$\mathcal{P}(2n+1) = \begin{cases} 2 & \textit{if } \ 2n+1 \leq |V^{(1)}| = q, \\ 4 & \textit{if } \ |V^{(k)}| < 2n+1 \leq |U^{(k)}| \textit{ for some } k \geq 2, \\ 3 & \textit{otherwise.} \end{cases}$$

Note that we can either derive the values of the palindromic complexity, for both even and odd n, directly from Proposition 4.3.10, or we can determine only $\mathcal{P}(2n)$ and then use the relation (4.7) between palindromic complexity and the first difference of factor complexity,

$$\mathcal{P}(2n+1) = \triangle\mathcal{C}(2n) + 2 - \mathcal{P}(2n),$$

knowing the first difference of factor complexity from (3.41).

Chapter 5

Fullness

Let us open anew the investigation of palindromes to which the entire Chapter 4 has been already devoted. This time, the study is initiated from another point of view: We are interested in the degree of "saturation" of an infinite word by palindromes – the smaller the defect the more saturated the word. The infinite words the most saturated by palindromes are thus those ones with zero defect, baptized full words in Section 2.2.11.

The first ones to tackle this problem were Droubay, Justin, and Pirillo [43]; they have shown that Sturmian and episturmian words are full. Brlek *et al.* [23] provide an insight in the defects of periodic words. In particular, in the context of fullness of infinite words, the following result is worth mentioning: An infinite periodic word $u = w^{\omega}$, where w is minimal, has an infinite number of palindromes if and only if w is a concatenation of two palindromes, i.e., $w = w^{(1)}w^{(2)}$, where $w^{(1)}, w^{(2)}$ are palindromes. If it is the case, then $u = w^{\omega}$ is full if its prefix of length $|w| + \lfloor \frac{||w^{(1)}|-|w^{(2)}||}{3} \rfloor$ is full. Recently, Glen *et al.* [62] have completed the above result by the proof that an infinite periodic word $u = w^{\omega}$, where w is minimal, has bounded defect if and only if w is a concatenation of two palindromes.

In the center of our attention are two distinct measures of palindromic variety – palindromic complexity and defects. A recent result of Bucci *et al.* [25] shed some light on their relation. They have proved for a uniformly recurrent infinite word u that u is full if and only if u is opulent in palindromes (see Definition 4.2.2). In this chapter, we provide a simpler elegant proof of this equivalence, valid even for infinite words with language closed under reversal that are not necessarily uniformly recurrent.

5.1 Measures of palindromic variety

Two different measures of palindromic variety in an infinite word u are the most frequently studied – **palindromic complexity** (determining, for any given length n, the number of distinct palindromes of length n occurring in the language of u) and **defects** of prefixes of u (counting, for any given prefix of length n of u, the difference between the utmost number $n+1$ and the actual number of palindromes of all possible lengths occurring in the prefix). A natural question to be settled is: "Do the sets of infinite words with maximal palindromic complexity and of full infinite words coincide?" This question has been answered affirmatively for uniformly recurrent words in [25]. We answer it affirmatively even for words with language closed under reversal that are not necessarily uniformly recurrent. The keynote of our proof is a meticulous inspection of complete return words of factors of full infinite words and the application of some basic graph theory.

5.1.1 Full infinite words

Fullness of finite and infinite words has been defined in Section 2.2.11. Here, let us recall a definition and a result from [43] which supplies us with an equivalent and more hands-on formulation of fullness. We say that a finite word v satisfies *Property Ju* (or *Ju* for short) if there exists a palindromic suffix of v which occurs exactly once in v, or, equivalently, if the longest palindromic suffix of v occurs exactly once in v.

Proposition 5.1.1. *Let u be an infinite word. Then u is full if and only if each prefix v of u satisfies Ju.*

Proof. It is a direct consequence of the formula (2.17) for $P(v)$ in the proof of Proposition 2.2.4. □

Let us introduce several lemmas, concerning mainly occurrences of factors and their reversals, which turn out to be useful for our aim to prove the equivalence of infinite words with maximal palindromic variety, according to each one of the two measures. As a by-product, we get a useful equivalent characterization of full infinite words (Proposition 5.1.3), proved already by Glen *et al.* in [62].

Lemma 5.1.2. *Let u be a full infinite word and w and $v = u_n u_{n+1} \dots u_{m-1} u_m$ be factors of u such that: 1) w is a prefix and $\overline{w}$ is a suffix of v and 2) neither w nor $\overline{w}$ occurs in $u_{n+1} \dots u_{m-1}$. Then v is a palindrome.*

Proof. Let us prove it by contradiction. Assume that there exists a pair of factors w and $v = u_n u_{n+1} \dots u_{m-1} u_m$ satisfying *1)* and *2)* such that v is not a palindrome.

Choose the smallest n with this property and find s such that $u_s u_{s+1} \dots u_m$ is the longest palindromic suffix of $u_0 u_1 \dots u_m$. Since v is not a palindrome $s \neq n$. The assumption $s < n$ leads to a contradiction with the choice of n, since already the pair of factors $u_s u_{s+1} \dots u_{s+m-n}$ and w satisfies *1)* and *2)* with $u_s u_{s+1} \dots u_{s+m-n}$ non-palindromic. If $n < s < m - |w|$, then s is an occurrence of w in $u_{n+1} \dots u_{m-1}$, which is impossible. If $m - |w| \leq s < m$, then the longest palindromic suffix of $u_0 u_1 \dots u_m$ occurs twice: at the positions s and n, i.e., Property Ju does not hold. □

Proposition 5.1.3. *An infinite word u is full if and only if complete return words of any palindromic factor of u are palindromes.*

Proof. One implication is an immediate consequence of the previous lemma if $w = \overline{w}$. To prove the opposite implication, suppose that u is not full. There exists a prefix u' of u which does not fulfill Ju. Therefore, the longest palindromic suffix of u', denote it by v, occurs in u' at least twice. Clearly, the most righthand complete return word of v contained in u' is not a palindrome. □

Lemma 5.1.4. *Let u be a full infinite word and w its non-palindromic factor. Then occurrences of w and its mirror image $\overline{w}$ alternate, i.e., any complete return word of w contains the factor $\overline{w}$ and any complete return word of $\overline{w}$ contains the factor w.*

Proof. Let us denote by $(o_n)_{n\in\mathbb{N}}$ the strictly increasing sequence of integers such that any element of the sequence is an occurrence of w or $\overline{w}$ and any occurrence of w or $\overline{w}$ appears in the sequence. For any $n \in \mathbb{N}$, we want to prove

$$o_n \text{ is an occurrence of } w \iff o_{n+1} \text{ is an occurrence of } \overline{w}.$$

Let us suppose the contrary and find the smallest n for which both o_n and o_{n+1} are occurrences of the same factor, say w. Let us consider the prefix u' of u of length $o_{n+1} + |w| - 1$ and denote by v the longest palindromic suffix of u'. The choice of the length of u' guarantees that the factor w is a suffix of u'. The fullness of u implies that v occurs in u' exactly once; we denote its occurrence by s.
If $s \geq o_{n+1}$, then v is a suffix of w, and, therefore, v occurs in u' twice, which is a contradiction with Ju.
The situation $o_n \leq s < o_{n+1}$ is impossible because s is an occurrence of $\overline{w}$ and w is not a palindrome.
Let us discuss the situation $s < o_n$. We know that s and $s + o_{n+1} - o_n$ are occurrences of $\overline{w}$. Since the factor $\overline{w}$ does not occur between o_n and o_{n+1} and v is a palindrome, there are no occurrence of w between s and $s + o_{n+1} - o_n$, which is a contradiction with the choice of n. □

Lemma 5.1.5. *Let u be a full infinite word, w and z be factors of u of the same length ℓ such that $w \neq z, \overline{z}$. Then there exists a unique factor $v = v_0 v_1 \dots v_q$ of u with the properties:*

- *w or $\overline{w}$ is a prefix of v,*
- *z or $\overline{z}$ is a suffix of v,*
- *factors w, $\overline{w}$, z, and $\overline{z}$ do not occur in $v_1 \dots v_{q-1}$.*

Proof. Let us denote by $(o_n)_{n \in \mathbb{N}}$ the strictly increasing sequence of integers such that any element of the sequence is an occurrence of w or $\overline{w}$ and any occurrence of w or $\overline{w}$ appears in the sequence. According to Lemma 5.1.2, the factors

$$U_n := u_{o_n} u_{o_n+1} \dots u_{o_{n+1}+\ell-1}$$

are palindromes for any $n \in \mathbb{N}$. Therefore the number of occurrences of the factor z and the number of occurrences of the factor $\overline{z}$ in U_n coincide. Let us find two indices $n < m$ such that U_n and U_m contain z at least once, and U_k does not contain z for any $k \in \mathbb{N}$, $n < k < m$.

Let us denote by $o_n + i$ the smallest occurrence of one of the factors z and $\overline{z}$ in U_n. WLOG suppose that o_n is an occurrence of w and $o_n + i$ is an occurrence of z. Similarly, denote by $o_m + j$ the smallest occurrence of one of the factors z and $\overline{z}$ in U_m. Our choice guarantees that both segments $u_{o_n} \dots u_{o_n+i+\ell-1}$ and $u_{o_m} \dots u_{o_n+j+\ell-1}$ have the properties imposed on the factor v in Lemma 5.1.5, and, moreover, they are the closest neighbors behaving as v. To prove Lemma 5.1.5, it is enough to show that they coincide.

Since U_n is a palindrome, $o_{n+1} - i$ is an occurrence of $\overline{z}$. With respect to Lemma 5.1.4, the index $o_m + j$ is an occurrence of z. Due to Lemma 5.1.2, the factor $u_{o_{n+1}-i} \dots u_{o_m+j+\ell-1}$ which starts with $\overline{z}$ and ends with z is a palindrome. Therefore the segment $u_{o_{n+1}-i} \dots u_{o_{n+1}+\ell-1}$ (its prefix is $\overline{z}$ and its suffix is $\overline{w}$) is the mirror image of the segment $u_{o_m} \dots u_{o_m+j+\ell-1}$, and $i = j$. As U_n itself is a palindrome, the suffix $u_{o_{n+1}-i} \dots u_{o_{n+1}+\ell-1}$ of U_n is as well the mirror image of the prefix $u_{o_n} \dots u_{o_n+i+\ell-1}$. So, we have shown $u_{o_n} \dots u_{o_n+i+\ell-1} = u_{o_m} \dots u_{o_m+j+\ell-1}$, as desired. □

5.1.2 Infinite words opulent in palindromes

For infinite words with language closed under reversal, opulence in palindromes may be reformulated as a condition on a modified reduced Rauzy graph. To formulate this condition, we employ the notion of a simple path (introduced in Section 2.2.12). Let u be an infinite word with language closed under reversal and n be a given positive integer. We will denote by G_n an undirected graph whose set of vertices is formed by unordered pairs $(w, \overline{w})$ such that $w \in \mathcal{L}_n(u)$ is RS or LS. We connect two vertices $(w, \overline{w})$ and $(v, \overline{v})$ by an unordered pair $(e, \overline{e})$ if e or $\overline{e}$ is a simple path starting in w or $\overline{w}$ and ending in v or $\overline{v}$. Note that the graph G_n may have multiple edges and loops. With this in hand, we may formulate a lemma resulting from the proof of (4.2) in [10].

Lemma 5.1.6. *Let u be an infinite word with language closed under reversal. Then u is opulent in palindromes if and only if both of the following conditions are satisfied:*

1. *The graph G_n, after removing loops, is a tree.*
2. *Any simple path forming a loop in the graph G_n is a palindrome.*

Corollary 5.1.7. *Let u be an infinite word with language closed under reversal. If u is opulent in palindromes, then complete return words of any palindromic factor of u are palindromes.*

Proof. Assume the contrary. Let $w = w_1w_2 \dots w_k$ be a palindrome and let v be its complete return word which is not a palindrome. Remark that the length of any non-palindromic return word of a palindrome w is $> 2|w|$. Hence, there exist factors t, v' (possibly empty) and two different letters x and y such that $v = wtxv'y\overline{t}w$.

Let us consider the graph G_n, where n is the length of the factor $z := wt$. Since the language of u is closed under reversal, the factor z is right special - the letters x and y belong to its right extensions.

If the complete return word v contains no other right or left special factors, then the non-palindromic v is a simple path which starts in $z = wt$ and ends in $\overline{z} = \overline{t}w$, which is a contradiction with the condition *2.* in Lemma 5.1.6.

Let v contain other left or right special factors. We find the prefix of v which is a simple path. This simple path starts in z, its ending point is a special factor, we denote it by A. Since v is a complete return word of w, we have $A \neq z, \overline{z}$. So, in the graph G_n, the vertices $(z, \overline{z})$ and $(A, \overline{A})$ are connected with an edge. Similarly, we find the suffix of v which is a simple path, and we denote its starting point by B, its ending point is $\overline{z}$. Again, $B \neq z, \overline{z}$ and the vertices $(z, \overline{z})$ and $(B, \overline{B})$ are connected with an edge. So, in the graph G_n, we have a path with two edges which connects $(A, \overline{A})$ and $(B, \overline{B})$ and the vertex $(z, \overline{z})$ is its intermediate vertex.

Since A and B are factors of $w_2 \dots w_k txv'y\overline{t}w_k \dots w_2$, we have, in the Rauzy graph with the set of vertices $\mathcal{L}_n(u)$, an oriented walk from the vertex A to B. To be precise, it means that in the graph G_n there exists a walk, and, therefore, a path[1] as well, between vertices $(A, \overline{A})$ and $(B, \overline{B})$, which does not use the vertex $(z, \overline{z})$.

Finally, if $(A, \overline{A})$ and $(B, \overline{B})$ coincide, then we have, in the graph G_n, a multiple edge. If $(A, \overline{A}) \neq (B, \overline{B})$, then, in the graph G_n, there are two different paths connecting $(A, \overline{A})$ and $(B, \overline{B})$. In any event, we have a contradiction with the condition *1.* in Lemma 5.1.6. $\square$

Theorem 5.1.8. *Let u be an infinite word with language closed under reversal. The word u is full if and only if u is opulent in palindromes, i.e., for any $n \in \mathbb{N}$, we have*

$$\mathcal{P}(n) + \mathcal{P}(n+1) = \Delta\mathcal{C}(n) + 2\,.$$

[1] Along a walk, vertices may occur with repetition, in a path, any vertex appears at most once.

Proof. The implication ($\Leftarrow$) results from Corollary 5.1.7 and Proposition 5.1.3. To prove the opposite implication, we use Lemma 5.1.6. At first, we have to show that the graph G_n, after removing loops, is a tree. Let us recall that an undirected graph without loops is a tree if and only if any two different vertices of G_n are connected with a unique path. This property of G_n follows from the definition of G_n and Lemma 5.1.5. The second condition of Lemma 5.1.6 follows from Lemma 5.1.2.

$\square$

Remark 5.1.9. *Let us correct the following example given in [25]. The word u generated by the substitution $a \to aba$, $b \to bb$ is recurrent, however not uniformly recurrent (by a similar argument as the one from Section 3.3.4), and u is closed under reversal (by a similar argument as in Section 4.2.4). By inspection of the complete return words of palindromic factors, applying Proposition 5.1.3, it may be proved that u is full. According to Theorem 5.1.8, u is also opulent in palindromes. The authors of [25] claimed that $\mathcal{P}(2) + \mathcal{P}(3) \neq \Delta\mathcal{C}(2) + 2$. This mistake is however based on the fact that $\mathcal{C}(3) = 5$ and not 6.*

Example 5.1.10. *We have seen in Chapter 4 that the m-iet words, the Rote word, the period-doubling word, the infinite word u_β associated with a confluent simple Parry number, and the infinite word u_β associated with a quadratic non-simple Parry number are opulent in palindromes. Thanks to Theorem 5.1.8, we see that all these words are full.*

Let us clarify that Theorem 5.1.8 is slightly stronger than the equivalence of fullness and opulence in palindromes for uniformly recurrent words, proved in [25]. In other words, the following statement is a corollary of Theorem 5.1.8.

Corollary 5.1.11. *Let u be a uniformly recurrent infinite word. Then u is full if and only if u is opulent in palindromes.*

Proof. If $\mathcal{L}(u)$ is closed under reversal, then the statement follows from Theorem 5.1.8. If $\mathcal{L}(u)$ is not closed under reversal, then Proposition 2.2.3 claims that u contains only a finite number of palindromes. It is then readily seen that u is neither full, nor opulent in palindromes. $\square$

Let us mention as an open problem the following question. “Is it possible to extend the equivalence of fullness and opulence in palindromes for a larger class of words than words with languages closed under reversal?”

- It does not hold for non-recurrent infinite words in general. In [25], the infinite word ab^ω is given as an example of a full non-recurrent infinite word (with language of course not closed under reversal), which is not opulent in palindromes.
- Notice that both full infinite words and infinite words opulent in palindromes contain infinitely many palindromes. Moreover, if u is full and recurrent, then u is closed under reversal (Glen in [62], Proposition 2.11).
  - In order to disprove the general validity of the equivalence of fullness and opulence in palindromes for recurrent words, it suffices to find a recurrent word opulent in palindromes with infinitely many palindromes and language not closed under reversal.
  - On the other hand, if we prove that any recurrent infinite word opulent in palindromes has language closed under reversal, then the answer to the above question is affirmative for recurrent words.

Chapter 6

Return words

Recently, return words (defined in Section 2.2.5) have turned out to be useful in many disciplines: symbolic dynamical systems, combinatorics on words, and number theory. This notion was introduced by Durand [47] in order to give a nice characterization of primitive substitutive sequences. A slightly different definition of return words was used by Ferenczi, Mauduit, and Nogueira [52] in the investigation of dynamical systems associated with primitive substitutions. One may be also interested in the ordering of return words in an infinite word. This leads to the study of the so-called derivated words encoding the unique decomposition of an infinite word in terms of return words. A characterization of words derivated from standard Sturmian words can be found in [6].

We preface the study of return words by the description of some simple ideas facilitating the task. We explain that in order to describe return words of all factors, it is sufficient to take into account only BS factors. The so-called tree of return words is introduced as a useful visualization tool. A factor and its image under a symmetry are shown to have the same number of return words and the relation between their return words is described in details. Finally, a closer look is focused onto the fixed points of substitutions - some relation between (complete) return words of factors and (complete) return words of their ancestors is pointed out.

As a practical application of these useful rules, we determine return words of factors of several infinite words in our illustrative sample.

Furthermore, an insight into the characterization of infinite words with a constant number of return words for every factor is provided. The last topic linked with return words is the recurrence function which to every n associates the minimal length $R(n)$, provided it exists, such that every segment of length $R(n)$ of the infinite word in question contains all factors of length n. We derive the recurrence function of the infinite word u_β associated with a quadratic non-simple Parry number.

6.1 Handy tools for the study of return words

6.1.1 Restriction to BS factors

If a factor w of an infinite word u is not RS, denote its unique right extension b. Then the sets of occurrences of w and wb coincide, and $Ret(w) = Ret(wb)$. If a factor w has a unique left extension a, then j is an occurrence of w in the infinite word u if and only if $j-1$ is an occurrence of aw. This statement does not hold for $j = 0$. Nevertheless, if u is a recurrent infinite word, then the set of return words of w stays the same no matter whether we include the return word corresponding to the prefix w of u or not. Consequently, we have $Ret(aw) = aRet(w)a^{-1} = \{ava^{-1} \mid v \in Ret(w)\}$, where ava^{-1} means that the word v is extended to the left by the letter a and it is shortened from the right by erasing the letter a (which is always the suffix of v for $v \in Ret(w)$). For an aperiodic recurrent infinite word u, every factor w can be uniquely extended to the left and to the right to the shortest BS factor containing w. To describe the cardinality and the structure of $Ret(w)$ for all factors w, it suffices therefore to consider BS factors w.

6.1.2 Tree of return words

A useful visualization tool of return words is a tree constructed in the following way: Label the root with a factor w, and attach $\#Rext(w)$ children, with labels wb, $b \in Rext(w)$. Repeat this recursively with every vertex labeled by v, except if w is a suffix of v. If u is uniformly recurrent, then this algorithm stops, and it is easy to see that the labels of the leaves of this tree are exactly the complete return words of w. Therefore, we have

$$\#Ret(w) = \#\{\text{leaves}\} = 1 + \sum_{\text{non-leaves } v} (\#Rext(v) - 1). \tag{6.1}$$

In particular, if w is the unique RS factor of its length, then the only branching in the tree takes place in the root, all non-root vertices have just one child, thus $\#Ret(w) = \#Rext(w)$.

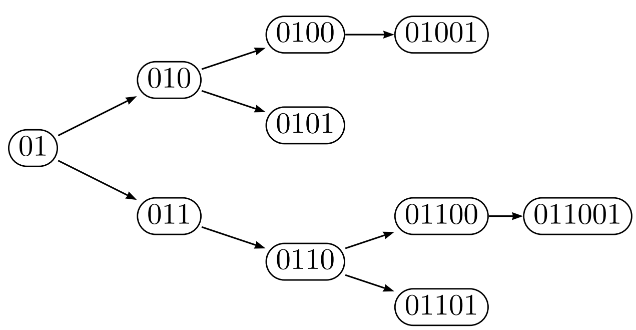


Fig. 6.1: The tree of return words of 01 in the Thue-Morse word.

A similar construction can be done with left extensions, yielding similar formulae. Since we can restrict our considerations to special factors by Section 6.1.1, we obtain the following proposition.

Proposition 6.1.1. *Let u be a recurrent word and $m \in \mathbb{N}$. Suppose that for every $n \in \mathbb{N}_0$, at least one of the following conditions is satisfied:*

1. *There is a unique LS factor $w \in \mathcal{L}_n(u)$, and $\#Lext(w) = m$.*
2. *There is a unique RS factor $w \in \mathcal{L}_n(u)$, and $\#Rext(w) = m$.*

Then every factor of u has exactly m return words.

Definition 6.1.2. *An infinite word u satisfies the property $\mathcal{R}_m$ if every of its factors has exactly m return words.*

As an immediate consequence of Proposition 6.1.1, the number of return words of every factor for Arnoux-Rauzy words may be determined.

Corollary 6.1.3. *Arnoux-Rauzy words of order m satisfy $\mathcal{R}_m$, in particular, Sturmian words satisfy $\mathcal{R}_2$.*

6.1.3 Symmetries

Let us focus on maps which preserve in a certain way factor occurrences in an infinite word u. We say that a map $S : \mathcal{L}(u) \to \mathcal{L}(u)$ is a *symmetry* of $\mathcal{L}(u)$ if S fulfills two properties:

1. S is a bijective map.
2. For every $w, v \in \mathcal{L}(u)$,

$$\#\{\text{occurrences of } w \text{ in } v\} = \#\{\text{occurrences of } S(w) \text{ in } S(v)\}.$$

Lemma 6.1.4. *Let u be an infinite word over an alphabet $\mathcal{A} = \{a_1, \ldots, a_m\}$ and let S be a symmetry of $\mathcal{L}(u)$. Then it holds $S\big(\mathcal{L}_n(u)\big) = \mathcal{L}_n(u)$ for every $n \in \mathbb{N}$, i.e., $|S(w)| = |w|$ for all $w \in \mathcal{L}(u)$.*

Proof. It clearly holds that $\#\{\text{occurrences of } S(w) \text{ in } S(\varepsilon)\} = \#\{\text{occurrences of } w \text{ in } \varepsilon\} = 0$, for every $w \in \mathcal{L}(u)$. As S is a bijection, it follows that $\#\{\text{occurrences of } v \text{ in } S(\varepsilon)\} = 0$ for every $v \in \mathcal{L}(u)$. Hence, $S(\varepsilon) = \varepsilon$. Since S is a bijection, for each letter $a \in \mathcal{A}$, there exists $w \in \mathcal{L}(u)$ such that $S(w) = a$, where $w \neq \varepsilon$. Take $b \in \mathcal{A}$ such that $\#\{\text{occurrences of } b \text{ in } w\} > 0$. Then $\#\{\text{occurrences of } S(b) \text{ in } S(w) = a\} > 0$. Therefore, $S(b) = a$. In other words, taking into account that S is a bijection, we have deduced that there exists a permutation $\pi \in S_m$ such that $S(a_k) = a_{\pi(k)}$ for all $k \in \{1, \ldots, m\}$. Let us now take an arbitrary $w \in \mathcal{L}(u)$, then, for every $a \in \mathcal{A}$, it holds $\#\{\text{occurrences of } a \text{ in } w\} = \#\{\text{occurrences of } S(a) \text{ in } S(w)\}$. As $S(\mathcal{A}) = \mathcal{A}$, it follows

$$|w| = \sum_{a \in \mathcal{A}} \#\{\text{occurrences of } a \text{ in } w\} = \sum_{a \in \mathcal{A}} \#\{\text{occurrences of } S(a) \text{ in } S(w)\} = |S(w)|.$$

□

In fact, a language cannot have too many symmetries. We know already from the proof of Lemma 6.1.4 that there exists a permutation $\pi \in S_m$ such that $S(a_k) = a_{\pi(k)}$ for all $k \in \{1, \ldots, m\}$. Moreover, since a symmetry preserves the number of letter occurrences, it is readily seen for every $w = w_1 w_2 \ldots w_n \in \mathcal{L}_n(u)$ that the following equation is valid

$$S(w_1 w_2 \ldots w_n) = S(w_{\sigma(1)}) S(w_{\sigma(2)}) \ldots S(w_{\sigma(n)}) \tag{6.2}$$

for some permutation $\sigma \in S_n$. We shall see in the sequel that the permutation σ is necessarily either the identical permutation $(1\ 2\ \ldots\ n)$ or the symmetric permutation $(n\ \ldots\ 2\ 1)$. In other words, every symmetry S is a letter permutation extended to a morphism on $\mathcal{A}^*$ (words with such symmetry are called *complementation-symmetric*), or, the composition of this morphism with the mirror map.

Lemma 6.1.5. *Let S be a symmetry of the language of an infinite word u. Then either $S(w) = S(w_1)S(w_2)\ldots S(w_n)$ for every $w = w_1 w_2 \ldots w_n \in \mathcal{L}_n(u)$, or $S(w) = S(w_n)\ldots S(w_2)S(w_1)$ for every $w = w_1 w_2 \ldots w_n \in \mathcal{L}_n(u)$.*

Proof. Let us proceed by induction on the length n of w. For $n = 2$, suppose a contradiction, i.e., there exist factors $v_1 v_2$ and $z_1 z_2$ in $\mathcal{L}_2(u)$, with $v_1 \neq v_2$ and $z_1 \neq z_2$, such that $S(v_1 v_2) = S(v_2)S(v_1)$ and $S(z_1 z_2) = S(z_1)S(z_2)$. Then, obviously, it is possible to find a factor $w_1 w_2 w_3$ of length 3 in u, with $w_1 \neq w_2$ and $w_2 \neq w_3$, satisfying

1. either $S(w_1 w_2) = S(w_1)S(w_2)$ and $S(w_2 w_3) = S(w_3)S(w_2)$,

2. or $S(w_1w_2) = S(w_2)S(w_1)$ and $S(w_2w_3) = S(w_2)S(w_3)$.

Assume that 1. holds (the proof for the case 2. is an analogy). Using the fact that for all $i, j \in \{1, 2, 3\}$, we have $\#\{\text{occurrences of } w_iw_j \text{ in } w_1w_2w_3\} = \#\{\text{occurrences of } S(w_iw_j) \text{ in } S(w_1w_2w_3)\}$, and taking into account that $w_1 \neq w_2$ and $w_2 \neq w_3$, we deduce

$$S(w_1w_2w_3) = S(w_1w_2)S(w_3) \quad \text{or} \quad S(w_1w_2w_3) = S(w_3)S(w_1w_2)$$

and

$$S(w_1w_2w_3) = S(w_1)S(w_2w_3) \quad \text{or} \quad S(w_1w_2w_3) = S(w_2w_3)S(w_1).$$

Assume that $S(w_1w_2w_3) = S(w_1w_2)S(w_3)$ and $S(w_1w_2w_3) = S(w_1)S(w_2w_3)$. Using 1., we get $S(w_1)S(w_2)S(w_3) = S(w_1)S(w_3)S(w_2)$, which is a contradiction with $w_2 \neq w_3$. Analogously, we obtain contradictions in all the other cases. To sum up, we have proved that either $S(w) = S(w_1)S(w_2)$ for every $w = w_1w_2 \in \mathcal{L}_2(u)$, or $S(w) = S(w_2)S(w_1)$ for every $w = w_1w_2 \in \mathcal{L}_2(u)$. Suppose that $S(w) = S(w_1)S(w_2)\dots S(w_k)$ for every $w = w_1w_2\dots w_k \in \mathcal{L}_k(u)$, $2 \leq k < n$. Take an arbitrary factor $w = w_1w_2\dots w_n \in \mathcal{L}_n(u)$. Then, as S is a symmetry, $S(w_2\dots w_n)$ is a factor of $S(w_1w_2\dots w_n)$, in more precise terms, $S(w_2\dots w_n)$ is either a prefix or a suffix of $S(w_1\dots w_n)$. Moreover, if w_1 occurs in $w_2\dots w_n$ l-times, w_1 occurs in $w_1w_2\dots w_n$ $(l+1)$-times. Since S is a symmetry, it follows that $S(w_1)$ occurs then l-times in $S(w_2\dots w_n)$ and $(l+1)$-times in $S(w_1w_2\dots w_n)$. These two observations result in

$$S(w_1w_2\dots w_n) = S(w_1)S(w_2\dots w_n) \quad \text{or} \quad S(w_1w_2\dots w_n) = S(w_2\dots w_n)S(w_1).$$

Similar reasoning leads to

$$S(w_1w_2\dots w_n) = S(w_n)S(w_1\dots w_{n-1}) \quad \text{or} \quad S(w_1w_2\dots w_n) = S(w_1\dots w_{n-1})S(w_n)$$

Let us show in detail that $S(w) = S(w_1)S(w_2)\dots S(w_n)$ for all cases which can occur.

(a) Suppose that $S(w) = S(w_1)S(w_2\dots w_n)$ and $S(w) = S(w_n)S(w_1\dots w_{n-1})$. Applying the induction hypothesis, this is equivalent with $S(w_1)S(w_2)\dots S(w_n) = S(w_n)S(w_1)\dots S(w_{n-1})$. Hence, this case occurs only for $w_1 = w_2 = \cdots = w_n$. Then, $S(w) = S(w_1)S(w_2)\dots S(w_n)$.

(b) Suppose that $S(w) = S(w_1)S(w_2\dots w_n)$ and $S(w) = S(w_1\dots w_{n-1})S(w_n)$. Applying the induction hypothesis, we see that $S(w) = S(w_1)S(w_2)\dots S(w_n)$.

(c) Suppose that $S(w) = S(w_2\dots w_n)S(w_1)$ and $S(w) = S(w_1\dots w_{n-1})S(w_n)$. Applying the induction hypothesis, we learn that this case occurs only for $w_1 = w_2 = \cdots = w_n$. Then, $S(w) = S(w_1)S(w_2)\dots S(w_n)$.

(d) Suppose that $S(w) = S(w_2\dots w_n)S(w_1)$ and $S(w) = S(w_n)S(w_1\dots w_{n-1})$. Applying the induction hypothesis, this is equivalent with $S(w_2)\dots S(w_n)S(w_1) = S(w_n)S(w_1)\dots S(w_{n-1})$. If n is odd, then it implies $w_1 = w_2 = \cdots = w_n$, thus $S(w) = S(w_1)S(w_2)\dots S(w_n)$. If n is even, say $n = 2l$, then it follows that $w_{2k-1} = w_1$ and $w_{2k} = w_2$ for all $k \leq l$. Thus $w_1w_2\dots w_n = (w_1w_2)^l$ and $S(w_1w_2\dots w_n) = (S(w_2)S(w_1))^l$. Using again that S is a symmetry, $\#\{\text{occurrences of } w_1w_2 \text{ in } (w_1w_2)^l\} = \#\{\text{occurrences of } S(w_1)S(w_2) \text{ in } (S(w_2)S(w_1))^l\}$. This is possible only for $w_1 = w_2$. Therefore, $S(w) = S(w_1)S(w_2)\dots S(w_n)$.

With the same reasoning, we deduce that if $S(w) = S(w_k)\dots S(w_2)S(w_1)$ for every $w = w_1w_2\dots w_k \in \mathcal{L}_k(u)$, $k < n$, then $S(w) = S(w_n)\dots S(w_2)S(w_1)$ for every $w = w_1w_2\dots w_n \in \mathcal{L}_n(u)$. $\square$

Theorem 6.1.6. *Let S be a symmetry of the language $\mathcal{L}(u)$ of an infinite word u. Then, the complete return words of any factor w of u and of its symmetrical image $S(w)$ obey the following relation*

$$Ret\big(S(w)\big)S(w) = S\big(Ret(w)w\big).$$

Proof. Let v be a return word of a factor $w \in \mathcal{L}(u)$, then, using Lemma 6.1.5, $S(vw)$ contains $S(w)$ only twice - as prefix and suffix, thus, $S(vw)$ is a complete return word of $S(w)$. The other inclusion is obvious since S^{-1} is also a symmetry. □

Corollary 6.1.7. *If the symmetry S of an infinite word u is a morphism, i.e., S is a letter permutation extended to a morphism, then the relation between the return words of a factor w and the return words of its image by S reads*

$$Ret\big(S(w)\big) = S\big(Ret(w)\big).$$

6.1.4 Respect for ancestors

If an infinite word u is a fixed point of a substitution φ, then some relation between return words of a factor and return words of its ancestors can be revealed. See Section 2.2.13 (Ancestors and synchronization points of substitutions), for the definition of an ancestor and a synchronization point.

Proposition 6.1.8. *Let u be a fixed point of an injective substitution φ, and let v be a factor of u. Assume:*

1. *There exist factors $t, t', w \in \mathcal{L}(u)$ such that $v = t\varphi(w)t'$ and $(t\varphi(w), t')$ and $(t, \varphi(w)t')$ are synchronization points of v.*
2. *The factor $\varphi(w)$ occurs only as subword of v.*

Then the following relation binds the complete return words of v and w

$$Ret(v)v = t\varphi\big(Ret(w)w\big)t'.$$

Proof. Let v' be a complete return word of v, then, according to Assumption *1.*, there exists $w' \in \mathcal{L}(u)$ such that $v' = t\varphi(w')t'$. Since φ is injective, w' contains w as prefix and suffix. Moreover, w' contains w exactly twice, otherwise, using Assumption *2.*, v' would contain v more than twice. Thus, we have shown the inclusion $\subset$.

On the other hand, let w' be a complete return word of w. Then, applying Assumption *2.*, $v' = t\varphi(w')t'$ is a factor of $\mathcal{L}(u)$ and v is a prefix and a suffix of v'. The factor v' is a complete return word of v, otherwise, with respect to Assumption *1.* and the injectivity of φ, w' would contain w more than twice. □

Let us remark that the injectivity of φ implies

$$\#Ret(v) = \#Ret(w).$$

Corollary 6.1.9. *Let u be a fixed point of an injective substitution φ and let v be a factor of u. If v is of the form $\varphi(w)$, where $s = (w, 0, 0)$ is the unique interpretation of v with $w \in \mathcal{L}(u)$, then $Ret(v) = \varphi\big(Ret(w)\big)$.*

6.1.5 Return words of several infinite words

We recall return words of the Thue-Morse word (determined by Cassaigne in [30]). Furthermore, we derive return words of infinite words u_β associated with quadratic non-simple Parry numbers β, return words of the period doubling word, and of the Rote word.

According to Section 6.1.1, we can restrict our considerations to BS factors if we want to describe the set of return words of an aperiodic recurrent infinite word.

Thue-Morse word

The list of BS factors of u_{TM} is at disposal in Section 3.3.2. We can combine Corollary 6.1.9 from Section 6.1.4 and Lemma 3.3.1 from Section 3.3.2 and we learn that in order to obtain return words of BS factors, it suffices to determine return words of BS factors of length less than 4. Non-empty BS factors of length ≤ 3 are: $\{0, 1, 01, 10, 010, 101\}$. Moreover, Corollary 6.1.7 implies that if $Ret(w)$ is the set of return words of a factor w, then $S\big(Ret(w)\big)$ is the set of return words of $S(w)$, where S is the morphism defined by $S: 0 \to 1,\ 1 \to 0$. It is easy to show that

$$\begin{aligned} Ret(0) &= \{0, 01, 011\}, \\ Ret(01) &= \{01, 010, 011, 0110\}, \\ Ret(010) &= \{010, 01011, 0100110, 010110011\}. \end{aligned}$$

Corollary 6.1.10. *Every factor of the Thue-Morse word has either* 3 *or* 4 *return words. The complete list of return words of non-empty BS factors has the following form:*

Return words of strong BS factors

$$\begin{aligned} Ret\big(\varphi^n(01)\big) &= \{\varphi^n(01), \varphi^n(010), \varphi^n(011), \varphi^n(0110)\}, \\ Ret\big(\varphi^n(10)\big) &= \{\varphi^n(10), \varphi^n(101), \varphi^n(100), \varphi^n(1001)\}. \end{aligned}$$

Return words of weak BS factors

$$\begin{aligned} Ret\big(\varphi^n(010)\big) &= \{\varphi^n(010), \varphi^n(01011), \varphi^n(0100110), \varphi^n(010110011)\}, \\ Ret\big(\varphi^n(101)\big) &= \{\varphi^n(101), \varphi^n(10100), \varphi^n(1011001), \varphi^n(101001100)\}. \end{aligned}$$

Return words of ordinary BS factors

$$\begin{aligned} Ret(0) &= \{0, 01, 011\}, \\ Ret(1) &= \{1, 10, 100\}. \end{aligned}$$

u_β associated with quadratic non-simple Parry numbers

In Section 3.4, the description of BS factors of u_β is provided. Moreover, Observation 3.4.2 and Item *3.* of Lemma 3.4.3 together with Proposition 6.1.8 proves that to determine return words of BS factors, it is sufficient to determine return words of BS factors containing no letter 1. More precisely, for every BS factor v containing at least one letter 1, there exists a unique BS factor w such that $v = T(w)$ and $Ret(v)v = t\varphi\big(Ret(w)w\big)t' = 0^q1\varphi\big(Ret(w)w\big)0^q = T\big(Ret(w)w\big)$.

Non-empty BS factors containing no letter 1 are: $0^r,\ 1 \leq r \leq p-1$. Their complete return words are easy to derive.

$$\begin{aligned} Ret(0^r)0^r &= \{0^{r+1}, 0^r10^r\}, & 1 \leq r \leq q, \\ Ret(0^r)0^r &= \{0^{r+1}, 0^r10^r, 0^r10^q10^r\}, & q < r \leq p-1. \end{aligned}$$

Corollary 6.1.11. *Every factor of u_β associated with quadratic non-simple Parry numbers has either 2 or 3 return words. The list of complete return words of non-empty BS factors has the following form:*

Complete return words of strong BS factors

$$Ret\big(V^{(n)}\big)V^{(n)} = \{T^{n-1}(0^{q+1}), T^{n-1}(0^q10^q)\}.$$

Complete return words of weak BS factors

$$Ret\big(U^{(n)}\big)U^{(n)} = \{T^{n-1}(0^p), T^{n-1}(0^{p-1}10^{p-1}), T^{n-1}(0^{p-1}10^q10^{p-1})\}.$$

Complete return words of ordinary BS factors

for $1 \le r < q$

$$Ret\big(W_r^{(n)}\big)W_r^{(n)} = \{T^{n-1}(0^{r+1}), T^{n-1}(0^r10^r)\},$$

for $q < r < p-1$

$$Ret\big(W_r^{(n)}\big)W_r^{(n)} = \{T^{n-1}(0^{r+1}), T^{n-1}(0^r10^r), T^{n-1}(0^r10^q10^r)\}.$$

Period doubling word

The list of BS factors of u_{PD} has been deduced in Section 3.3.3. Relating Proposition 6.1.8 from Section 6.1.4 and Lemma 3.3.2 from Section 3.3.3, we see that for every BS factor v containing the letter 1, there exists a unique BS factor w such that $v = T_{\mathrm{PD}}(w)$ and $Ret(v)v = t\varphi\big(Ret(w)w\big)t' = \varphi\big(Ret(w)w\big)0 = T_{\mathrm{PD}}\big(Ret(w)w\big)$.

Therefore, we need to describe only complete return words of non-empty BS factors containing no letter 1, i.e., of factors 0, and 00. This is simple.

$$\begin{aligned} Ret(0)0 &= \{00, 010\}, \\ Ret(00)00 &= \{000, 00100, 001010100\}. \end{aligned}$$

Corollary 6.1.12. *Every factor of the period doubling word has either 2 or 3 return words. The list of complete return words of non-empty BS factors has the following form:*

Complete return words of strong BS factors

$$Ret\big(V^{(n)}\big)V^{(n)} = \{T_{PD}^{n-1}(00), T_{PD}^{n-1}(010)\}.$$

Complete return words of weak BS factors

$$Ret\big(U^{(n)}\big)U^{(n)} = \{T_{PD}^{n-1}(000), T_{PD}^{n-1}(00100), T_{PD}^{n-1}(001010100)\}.$$

Rote word

Let us recall that the Rote word u_{R} is recurrent, however, u_{R} is not uniformly recurrent. Thus, we will not be surprised that some BS factors have infinitely many return words. The list of BS factors of u_{R} has been deduced in Section 3.3.4. Relating Proposition 6.1.8 from Section 6.1.4 and Lemma 3.3.4 from Section 3.3.4, we learn that for every BS factor v containing 00 as a factor, there exists a unique BS factor w such that $v = T_{\mathrm{R}}(w)$ and $Ret(v)v = t\varphi\big(Ret(w)w\big)t' = 1\varphi\big(Ret(w)w\big) = T_{\mathrm{R}}\big(Ret(w)w\big)$. Consequently, it remains to describe return words of non-empty

BS factors which do not contain the factor 00 in order to have all return words determined. BS factors which do not contain 00 are: 0 and $1^k,\ k \in \mathbb{N}$.

The complete return words of the factor 0 are obtained using Observation 3.3.3 (notice that there are infinitely many of them):

$$Ret(0)0 = \{00\} \cup \{01^k0 \mid k = \tfrac{3^j-1}{2},\ j \in \mathbb{N}\}.$$

To determine complete return words of blocks of 1's, two observations are necessary. The first one is a direct consequence of Observation 3.3.3, the second one of Proposition 6.1.8.

Observation 6.1.13. *Return words of 1^k, where $\frac{3^{n-1}-1}{2} < k < \frac{3^n-1}{2}$ for some $n \in \mathbb{N}$, distinct from 1 are in a one-to-one correspondence with return words of $V^{(n)} = \frac{3^n-1}{2}$, more precisely,*

$$Ret\big(V^{(n)}\big) = 1^{\frac{3^n-1}{2}-k} Ret(1^k).$$

Observation 6.1.14. *The complete return words of $V^{(n)},\ n \geq 2$, containing the letter 0 satisfy*

$$Ret(V^{(n)})V^{(n)} = T_R\left(Ret(V^{(n-1)})V^{(n-1)}\right).$$

With the previous observations in hand, it is straightforward to determine the searched complete return words of blocks of 1's.

Corollary 6.1.15. *The list of complete return words of BS factors has the following form:*

Complete return words of strong BS factors

$$Ret\big(V^{(n)}\big)V^{(n)} \quad = \quad \{V^{(n)}1, T_R^{n-1}(1001)\}.$$

Complete return words of weak BS factors

$$Ret\big(U^{(n)}\big)U^{(n)} = \{T_R^{n-1}(00),\ T_R^{n-1}(01^k0) \mid k = \tfrac{3^j-1}{2},\ j \in \mathbb{N}\}.$$

Complete return words of ordinary BS factors

$$Ret\big(1^k\big)1^k = \{1^{k+1}\} \cup \{1^{k-\frac{3^n-1}{2}} T_R^{n-1}(1001)1^{k-\frac{3^n-1}{2}}\},$$

where $n \in \mathbb{N}$ is such that $\frac{3^{n-1}-1}{2} < k < \frac{3^n-1}{2}$.

6.2 Infinite words with a constant number of return words

An interesting task is to characterize infinite words with a constant number of return words, i.e., infinite words satisfying the property $\mathcal{R}_m$ for some $m \in \mathbb{N}$ (see Definition 6.1.2). Vuillon in [107] has proved that the set of infinite words satisfying $\mathcal{R}_2$ coincides with the set of Sturmian words. Consequently, infinite words fulfilling $\mathcal{R}_m$ represent another generalization of Sturmian words. This generalization includes Arnoux-Rauzy words (as shown by Justin and Vuillon [74]) and words coding m-interval exchange transformation (Vuillon [108]).

Both AR words and m-iet words satisfy $\mathcal{C}(n) = (m-1)n+1$ for all $n \in \mathbb{N}_0$. However, already Vuillon noticed that this assumption on complexity is not sufficient for a word to have $\mathcal{R}_m$ for $m \geq 3$; the fixed point of a certain recoding of the Chacon substitution that has complexity $2n+1$ (as shown by Ferenczi [51]) contains factors with more than 3 return words.

A closer look brings to light that both AR words and m-iet words have not only a constant first difference of complexity, but the bilateral order (defined in Section 3.2.1) of every their factor is equal to zero. We prove that this condition is sufficient for an infinite word over an m-letter alphabet to have $\mathcal{R}_m$. More precisely, we show a stronger statement: If an infinite word does not contain weak BS factors, i.e., factors with negative bilateral orders, then $\mathcal{R}_m$ is equivalent with $\mathcal{C}(n) = (m-1)n + 1$ for all $n \in \mathbb{N}_0$.

If a word satisfies $\mathcal{R}_3$, then we can show that no factor is weak BS. Therefore, the words with $\mathcal{R}_3$ are characterized by complexity $2n+1$ and the absence of weak BS factors, or, equivalently, by the fact that all their BS factors have zero bilateral order.

For $m \geq 4$, neither the complexity $\mathcal{C}(n) = (m-1)n + 1$ nor the absence of weak BS factors are necessary conditions for an infinite word to fulfill $\mathcal{R}_m$. Steiner [11] has constructed a word satisfying $\mathcal{R}_4$ with an even number of factors of every positive length, thus, $\mathcal{C}(n) \neq 3n+1$ for n even, $n \geq 1$, and containing infinitely many weak BS factors. The problem to find a nice characterization of words with $\mathcal{R}_m$ for $m \geq 4$ thus remains open.

We conclude the study of infinite words with a constant number of return words by determining which infinite words among words u_β associated with Parry numbers β satisfy $\mathcal{R}_m$.

6.2.1 Sufficient conditions for $\mathcal{R}_m$

The main objective of this section is to study sufficient conditions guaranteeing for an infinite word u the property $\mathcal{R}_m$, however, we mention first two evident necessary conditions. If u has $\mathcal{R}_m$, then:

1. The alphabet $\mathcal{A}$ of u must have m letters since the occurrences of the empty word ε are all integers $n \in \mathbb{N}_0$, and its return words are therefore all letters.
2. Furthermore, u must be uniformly recurrent since every factor has a return word and only finitely many of them.

Combining Item 1. and Remark 3.2.2, we derive the following lemma.

Lemma 6.2.1. *If an infinite word u satisfies $\mathcal{R}_m$ and no factor is weak BS, then $\Delta\mathcal{C}(n) \geq m-1$ for all $n \in \mathbb{N}_0$.*

The number of return words may be bounded from below and from above with the help of the following lemmas.

Lemma 6.2.2. *If u is an infinite uniformly recurrent word with no weak BS factor, then $\#Ret(w) \geq \Delta\mathcal{C}(|w|) + 1$ for every factor $w \in \mathcal{L}(u)$.*

Proof. Let $w \in \mathcal{L}(u)$ and denote by $v^{(1)}, v^{(2)}, \ldots, v^{(r)}$ the RS factors of length $|w|$. Since no factor is weak BS and u is uniformly recurrent, every $v^{(j)}$ can be extended to the left without decreasing the total amount of "right branching" until w is reached. More precisely, we have (mutually different) RS factors $v_1^{(j)}, v_2^{(j)}, \ldots, v_{s_j}^{(j)}$ with suffix $v^{(j)}$, prefix w, and no other occurrence of w such that $\#Rext(v^{(j)}) - 1 \leq \sum_{i=1}^{s_j} \big(\#Rext(v_i^{(j)}) - 1\big)$. The construction implies that the set $\{v_i^{(j)} \mid 1 \leq j \leq r,\ 1 \leq i \leq s_j\}$ is equal to the set of vertices in the tree of return words of w and $v_i^{(j)} \neq v_{i'}^{(j')}$ for $(j,i) \neq (j',i')$. Consequently, we can use Equation (6.1) and obtain

$$\#Ret(w) = 1 + \sum_{j=1}^{r} \sum_{i=1}^{s_j} \big(\#Rext(v_i^{(j)}) - 1\big) \geq 1 + \sum_{j=1}^{r} \big(\#Rext(v^{(j)}) - 1\big) = 1 + \Delta\mathcal{C}(|w|).$$

$\square$

Lemma 6.2.3. *If an infinite uniformly recurrent word u has no weak BS factor and $\Delta\mathcal{C}(n) < m$ for all $n \in \mathbb{N}_0$, then $\#Ret(w) \leq m$ for every factor $w \in \mathcal{L}(u)$.*

Proof. Let $v^{(1)}, v^{(2)}, \dots, v^{(r)}$ denote the RS factors which are labels of non-leave vertices in the tree of return words of a factor w, and put $n := \max_{1 \leq j \leq r} |v^{(j)}|$. Since no BS factor is weak, every $v^{(j)}$ can be extended to the left to factors of length n without decreasing the total amount of "right branching". More precisely, we have (mutually different) RS factors $v_1^{(j)}, v_2^{(j)}, \dots, v_{s_j}^{(j)}$ of length n with suffix $v^{(j)}$ such that $\#Rext(v^{(j)}) - 1 \leq 1 + \sum_{i=1}^{s_j} \big(\#Rext(v_i^{(j)}) - 1\big)$. Since w occurs in $v^{(j)}$ only as prefix, no $v^{(j)}$ can be a proper suffix of $v^{(j')}$. Hence, we have $v_i^{(j)} \neq v_{i'}^{(j')}$ for $(j,i) \neq (j',i')$ and

$$\#Ret(w) = 1 + \sum_{j=1}^{r} \big(\#Rext(v^{(j)} - 1\big) \leq 1 + \sum_{j=1}^{r} \sum_{i=1}^{s_j} \big(\#Rext(v_i^{(j)}) - 1\big) \leq \Delta\mathcal{C}(n) + 1 \leq m.$$

□

For words with no weak BS factors, the previous three lemmas give a very simple characterization of the property $\mathcal{R}_m$.

Theorem 6.2.4. *If u is a uniformly recurrent word with no weak BS factor, then it satisfies $\mathcal{R}_m$ if and only if $\mathcal{C}(n) = (m-1)n + 1$ for all $n \in \mathbb{N}_0$.*

It is easy to see that the following two statements are equivalent.

1. The complexity of u obeys the formula $\mathcal{C}(n) = (m-1)n + 1$ for all $n \in \mathbb{N}_0$ and u contains no weak BS factors.

2. The word u is defined over an m-letter alphabet and u contains only ordinary BS factors.

Using the equivalence of the above statements, we may reformulate the sufficient condition.

Corollary 6.2.5. *Let u be a uniformly recurrent word over $\mathcal{A}$ with $\#\mathcal{A} = m$. If u contains only ordinary BS factors, then u fulfills $\mathcal{R}_m$.*

6.2.2 Known characterization of $\mathcal{R}_2$ and new characterization of $\mathcal{R}_3$

For $m = 2$ and $m = 3$, words with the property $\mathcal{R}_m$ can be completely characterized.

Definition 6.2.6. *Let v be a return word of $w \in \mathcal{L}(u)$. We say that the return word v starts with b if wb is a prefix of the complete return word vw and that it ends with a if aw is a suffix of vw.*

Lemma 6.2.7. *If w is a maximal RS factor of a recurrent word u such that for any $b \in Rext(w)$, there exists a unique $v \in Ret(w)$ starting with b, then u is eventually periodic.*

Proof. Denote the return words of w by $v^{(1)}, v^{(2)}, \dots, v^{(r)}$, where $v^{(j)}$ starts with b_j, ends with a_j, and b_{j+1} is the only letter in $Rext(a_j w)$ for $1 \leq j < r$. Then b_1 is the only letter in $Rext(a_r w)$ and $u = u'(v^{(1)} v^{(2)} \dots v^{(r)})^\omega$ for some prefix u'. □

Corollary 6.2.8. *If u satisfies $\mathcal{R}_2$, then it has no maximal RS factor.*

Proof. Assume that w is a maximal RS factor. Then the two return words of w have different starting letters, hence u is eventually periodic by Lemma 6.2.7 and $\#Ret(wa) = 1$. □

Over a binary alphabet, the notions of weak BS and maximal RS factor coincide. Therefore, Corollaries 6.1.3, 6.2.8, Lemma 6.2.2 provide a short proof of the following theorem.

Theorem 6.2.9 (Vuillon [107])**.** *An infinite word u satisfies $\mathcal{R}_2$ if and only if u is Sturmian.*

In order to characterize words with the property $\mathcal{R}_3$, we need one more lemma.

Lemma 6.2.10. *Let u be a recurrent word.*

1. *Let w be a weak BS factor of u with a unique $a \in Lext(w)$ such that more than one return word of w starts with a letter in $Rext(aw)$. Then $\#Ret(aw) < \#Ret(w)$.*

2. *Similarly, let w be a weak BS factor of u with a unique $b \in Rext(w)$ such that more than one return word of w ends with a letter in $Lext(wb)$. Then $\#Ret(wb) < \#Ret(w)$.*

Proof. 1. Any return word of aw has the form $av^{(1)}v^{(2)} \dots v^{(r)}a^{-1}$ for some $r \geq 1$ and $v^{(j)} \in Ret(w)$, $1 \leq j \leq r$. If $v^{(1)}$ ends with a, then $r = 1$. If $v^{(1)}$ ends with $a' \neq a$, then the assumption of the lemma implies that there is a unique return word of w starting with a letter in $Rext(a'w)$ (and $\#Rext(a'w) = 1$). Therefore, $v^{(2)}$ and inductively the sequence of words $v^{(2)}, \dots, v^{(r)}$ are completely determined by the choice of $v^{(1)}$. This implies that $\#Ret(aw)$ equals the number of return words of w starting with a letter in $Rext(aw)$. Since w is weak BS, we have $\#Rext(aw) < \#Rext(w)$, and, thus, $\#Ret(aw) < \#Ret(w)$.

2. Any return word of wb has the form $v^{(1)}v^{(2)} \dots v^{(r)}$ for some $r \geq 1$ and $v^{(j)} \in Ret(w)$, $1 \leq j \leq r$. If $v^{(r)}$ starts with b, then $r = 1$. If $v^{(r)}$ starts with $b' \neq b$, then there is a unique return word of w ending with a letter in $Lext(wb')$ (and $\#Lext(wb') = 1$). Thus, $v^{(r-1)}$ and inductively the sequence of words $v^{(1)}, \dots, v^{(r-1)}$ are completely determined by the choice of $v^{(r)}$. This means that $\#Ret(wb)$ equals the number of return words of w ending with a letter in $Lext(wb)$. Since w is weak BS, we have $\#Lext(wb) < \#Lext(w)$, and, consequently, $\#Ret(wb) < \#Ret(w)$.

□

Remark 6.2.11. *There are two cases for Item 1. of Lemma 6.2.10: Either aw is RS or there is more than one return word of w starting with the unique right extension of aw.*

Corollary 6.2.12. *If u satisfies $\mathcal{R}_3$, then it has no weak BS factor.*

Proof. Assume that w is a weak BS factor.

- If $\#Rext(w) = 3$, then every return word of w starts with a different letter in $Rext(w)$. Either w is a maximal RS factor, which causes a contradiction to $\mathcal{R}_3$ applying Lemma 6.2.7, or, there exists a unique $a \in Lext(w)$ such that the factor aw is RS, then we obtain a contradiction to $\mathcal{R}_3$ by *Item 1.* of Lemma 6.2.10.

- If $Rext(w) = \{b, b'\}$, then either $Lext(w) = \{a, a'\}$, $Rext(aw) = \{b\}$, and $Rext(a'w) = \{b'\}$. Then, w.l.o.g., two return words of w start with b and one starts with b' and we obtain a contradiction to $\mathcal{R}_3$ by *Item 1.* of Lemma 6.2.10. Or, $\#Lext(w) = 3$ and, w.l.o.g., two return words ends with a letter in $Lext(wb)$, then we have again a contradiction to $\mathcal{R}_3$ by *Item 2.* of Lemma 6.2.10.

□

By combining Corollary 6.2.12 and Theorem 6.2.4, we obtain the following theorem.

Theorem 6.2.13. *A uniformly recurrent word u satisfies $\mathcal{R}_3$ if and only if $\mathcal{C}(n) = 2n+1$ for all $n \in \mathbb{N}_0$ and u has no weak BS factor.*

Using Corollary 6.2.5, the theorem can be reformulated.

Corollary 6.2.14. *Let u be a uniformly recurrent word over $\mathcal{A}$ with $\#\mathcal{A} = 3$. Then u has $\mathcal{R}_3$ if and only if u contains only ordinary BS factors.*

Let us give several remarks:

- Theorem 6.2.13 remains true if "weak BS factor" is replaced by "maximal RS factor": If $\Delta\mathcal{C}(n) = 2$ for all $n \in \mathbb{N}_0$, then every factor w with $\#Rext(w) = 3$ is the unique RS factor of its length, and it cannot be weak BS. If $\#Rext(w) = 2$, then the two notions coincide.
- By symmetry, "weak BS factor" can be replaced by "maximal LS factor".
- The condition on weak BS factors cannot be omitted. Ferenczi in [51] showed that the fixed point $\lim_{n\to\infty} \varphi^n(1)$ of the substitution given by $\varphi : 1 \to 12,\ 2 \to 312,\ 3 \to 3312$, a recoding of the Chacon substitution, has complexity $2n+1$ and it contains weak BS factors.

6.2.3 Comments on $\mathcal{R}_m,\ m \geq 4$

The characterization of $\mathcal{R}_m$ for $m = 3$ introduced in Theorem 6.2.13 cannot be easily generalized for $m \geq 4$. The following example due to Steiner [11] shows that $\mathcal{C}(n)$ need not be $(m-1)n+1$ for all $n \in \mathbb{N}_0$ if u satisfies $\mathcal{R}_m$, $m \geq 4$.

Example 6.2.15. *Define the substitution φ by*

$$\begin{aligned} \varphi : 1 &\to 13231 \\ 2 &\to 13231424131 \\ 3 &\to 42324131424 \\ 4 &\to 42324 \end{aligned}$$

and denote its fixed point $u = \lim_{n\to\infty} \varphi^n(1)$.

The first observation to do is that the language $\mathcal{L}(u)$ has a symmetry: the morphism S defined by $S : 1 \leftrightarrow 4,\ 2 \leftrightarrow 3$. Since factors w and $S(w)$ are different (provided $w \neq \varepsilon$) but of the same length, there exists an even number of different factors of every length. Therefore $\mathcal{C}(n) \neq 3n+1$ for any $n > 1$, n even.

Now let us show that u satisfies $\mathcal{R}_4$. By Section 6.1.1, it is sufficient to consider BS factors of u. Let us determine them, using the fact that if w is a BS factor, then $S(w)$ is a BS factor of the same bilateral order. Observing the substitution φ, we learn that the following table shows LS and RS factors of lengths between 1 and 7, if we add their images by S, we obtain a complete list of LS and RS factors of lengths between ≤ 7.

length	1	2	3	4	5	6	7
LS's	1, 2	23, 24	241	2413	24131, 24132	241314, 241323	2413142 , 2413231
RS's	1, 2	32, 42	142	3142	13142, 23142	413142, 323142	2413142 , 1323142

Thus, the only BS factors of length ≤ 7 are weak BS factors 1 *and* 4, 23 *and* 32, 2413142 *and* 3142413, *and strong BS factors* 2 *and* 3, 2413 *and* 3142. *Every BS factor of length > 7 has* *either* 2413231 *or* 3142324 *as prefix and either* 1323142 *or* 4232413 *as suffix. Consequently, it is easy to see that every BS factor* v *of length* > 7 *satisfies Proposition 6.1.8 with decomposition* $v = t\varphi(w)t'$, *where* $t \in \{24, 31\}$, $t' \in \{1323142, 4232413\}$, *provided* $w \neq \varepsilon$.

Therefore, if we prove that every BS factor of length ≤ 7 *and BS factors of the form* $t\varphi(\varepsilon)t' \in \{241323142, 314232413\}$ *have* 4 *return words, then applying Proposition 6.1.8 with the fact that* φ *is injective, we will have shown that* $\#Ret(w) = 4$ *for every* $w \in \mathcal{L}(u)$.

For the BS factors $1, 2, 23, 2413$, *the return words are easily determined:*

$$\begin{aligned}
Ret(1) &= \{13, 1323, 1424, 142324\}, \\
Ret(2) &= \{23, 2314, 2413, 241314\}, \\
Ret(23) &= \{2314, 2314241314, 232413, 232413142413\}, \\
Ret(2413) &= \{241314, 24131423, 24132314, 2413231423\}.
\end{aligned}$$

The return words of the weak BS factor 2413142 *are factors of* $\varphi(v)$, *with a factor* v *of length* $|v| \geq 2$ *having prefix* 2 *or* 3, *suffix* 2 *or* 3 *and no other occurrence of* 2 *and* 3. *Since the only possibilities for* v *are* $23, 2413, 32, 3142$, *we obtain*

$$Ret(2413142) = \{24131423, 2413142324132314 23, 24131424132314, 241314241323142324132314\}.$$

The return words of the BS factor 241323142 *are factors of* $\varphi(v)$, *with a factor* v *of length* $|v| \geq 4$ *containing either* 1 *or* 2 *as the second letter and* 1 *or* 2 *as the last but one letter and having no other occurrences of* 1 *and* 2. *Since the only possibilities for* v *are* 41323, 32314, 31423, 31424, 42413, 32413, 41314, 42324, *we obtain*

$$Ret(241323142)=\{2413231423, 2413231423241314, 2413231424131423, 24132314241314232413242\}.$$

6.2.4 Property $\mathcal{R}_m$ for u_β associated with Parry numbers

In this section, we describe which infinite words associated with simple Parry numbers have the property $\mathcal{R}_m$. For non-simple Parry numbers (defined in Section 2.3.1), this question stays open: neither special factors nor complexity have been described if u_β is defined over an m-letter alphabet with $m \geq 3$. In the case of non-simple quadratic Parry numbers, the alphabet of u_β equals $\{0, 1\}$, thus, only the Sturmian case corresponding to parameters $p = q + 1$ satisfies $\mathcal{R}_2$.

For simple Parry numbers, all prefixes of u_β are LS factors, with all m letters being left extensions [14]. For every factor w, the tree of return words constructed by the left extensions (see Section 6.1.2) contains therefore a vertex with m children, the shortest prefix of u_β having w as a suffix. Therefore, every factor w has at least m return words. If there exists a LS factor which is not a prefix of u_β, then this factor has more than m return words. By Proposition 6.1.1, we obtain the following statement.

Proposition 6.2.16. *Let* u_β *be a fixed point of the substitution* φ *given by* (2.23). *Then* u_β *satisfies* $\mathcal{R}_m$ *if and only if* $\mathcal{C}(n) = (m-1)n + 1$ *for all* $n \in \mathbb{N}_0$.

Bernat, Masáková, and Pelantová in [14] characterize u_β associated with simple Parry numbers having an affine complexity (Theorem 3.3.6), in terms of the Rényi expansion of unity. It is readily seen that the complexity is then necessarily given by $\mathcal{C}(n) = (m-1)n + 1$ for all $n \in \mathbb{N}_0$.

Corollary 6.2.17. *Let* u_β *be an infinite word associated with a simple Parry number. Then* u_β *satisfies* $\mathcal{R}_m$ *if and only if* $t_m = 1$ *and* $t_j \dots t_{m-1} t_1 \dots t_{j-1} \preceq t_1 \dots t_{m-1}$ *for all* $j \in \{2, \dots, m-1\}$.

For the seek of completeness, let us recall that the language of u_β is closed under reversal if and only if $t_1 = t_2 = \cdots = t_{m-1}$. In this case, u_β satisfying $\mathcal{R}_m$ is an Arnoux-Rauzy word of order m.

6.3 Recurrence function of u_β associated with quadratic non-simple Parry numbers

The study of the recurrence function (vaguely defined in Section 2.2.4) was initiated by Hedlund and Morse in [66]. They revealed the following relation between the recurrence function and the complexity of any infinite word

$$R(n) \geq \mathcal{C}(n) + n - 1 \quad \text{for all } n \in \mathbb{N}.$$

For infinite words which are not periodic, they refined the relation as

$$R(n) \geq \mathcal{C}(n) + n \quad \text{for all } n \in \mathbb{N}. \tag{6.3}$$

In the other direction, a similar generally valid inequality cannot be established since it is possible to construct Sturmian words whose recurrence function grows arbitrarily fast, as shown by Cassaigne in [29].

Cassaigne in [29] determined the recurrence function for Sturmian words, taking into account continued fractions of their slope. Furthermore, the same author in [30] has given a general algorithm describing how to determine the recurrence function if we know return words. He demonstrated his result on the example of the Thue-Morse word. This algorithm constitutes the cornerstone of the new result of this section – the derivation of the recurrence function for infinite words u_β associated with quadratic non-simple Parry numbers. Let us start with a precise definition of the recurrence function.

Definition 6.3.1. *The recurrence function of an infinite word u is the map $R_u : \mathbb{N} \to \mathbb{N} \cup \{+\infty\}$ defined by*

$$R_u(n) = \min\{N \in \mathbb{N} \mid \forall v \in \mathcal{L}_N(u), \mathcal{L}_n(v) = \mathcal{L}_n(u)\},$$

and we put $R_u(n) := \infty$ if the above set is empty.

We will write $R(n)$ instead of $R_u(n)$ provided it causes no confusion. Clearly, u is uniformly recurrent if and only if $R(n)$ is finite for every $n \in \mathbb{N}$. In order to get another expression for $R(n)$, convenient to work with, let us introduce some more terms.

Definition 6.3.2. *Let u be an infinite uniformly recurrent word.*

- *Let $w \in \mathcal{L}(u)$, then $l(w) = \max\{|v| \mid v \in Ret(w)\}$ is called the maximal return time of w in u.*
- *For all $n \in \mathbb{N}$, we define $l(n) = \max\{l(w) \mid w \in \mathcal{L}_n(u)\}$.*

Once the lengths of return words of every factor determined, the following proposition from [30] allows to calculate the recurrence function $R(n)$.

Proposition 6.3.3. *For any infinite uniformly recurrent word u, and, for any $n \in \mathbb{N}$, one has*

$$R(n) = l(n) + n - 1.$$

The task to compute the recurrence function may be simplified using the notion of singular factors. A factor $w \in \mathcal{L}(u)$ is called *singular* if $|w| = 1$ or there exist a word $v \in \mathcal{L}(u)$ and letters $a, a', b, b' \in \mathcal{A}$ such that $w = avb$, $a \neq a'$, $b \neq b'$, and $\{avb', a'vb\} \subset \mathcal{L}(u)$. Obviously, v is a non-weak BS factor.

Proposition 6.3.4. *Let u be a uniformly recurrent word and $n \geq 1$. If $l(n-1) < l(n)$, then there exists a singular factor w of length n such that $l(w) = l(n)$.*

A singular factor w is said to be *essential* if $l(w) = l(|w|) > l(|w|-1)$. To calculate $l(n)$, it is sufficient to consider singular, or, even, only essential singular factors of length $\leq n$.

Theorem 6.3.5. *Let u be a uniformly recurrent word and $n \geq 1$.*

$$l(n) = \max\{l(w) \mid |w| \leq n \text{ and } w \text{ singular}\} = \max\{l(w) \mid |w| \leq n \text{ and } w \text{ essential singular}\}.$$

Now, we are able to give an **algorithm for computing the recurrence function** of an infinite uniformly recurrent word u:

1. Determine BS factors.
2. Deduce the form of singular factors and compute their lengths.
3. For every singular factor, determine the associated return words and compute their lengths.
4. Compute the function $l(n)$ to get the recurrence function $R(n)$ for every $n \in \mathbb{N}$.

Let us apply the algorithm for computing the recurrence function to the infinite word u_β associated with quadratic non-unit non-simple Parry numbers, i.e., being the fixed point of the substitution $\varphi(0) = 0^p1,\ \varphi(1) = 0^q1,\ p-1 > q$.

1. The BS factors of u_β are described in Corollary 3.4.5.
2. Combining Item *2.* of Lemma 3.4.3, Lemma 3.4.4, and Corollary 3.4.5, we deduce the form of singular factors.

   Proposition 6.3.6. *The set of all singular factors of u_β is given by the union of*

   $$\begin{array}{l} \{0,1\}, \\ \{S_r^{(n)}(0,0) \mid n \in \mathbb{N},\ 0 \leq r \leq p-2\}, \\ \{S_q^{(n)}(1,0) \mid n \in \mathbb{N}\}, \\ \{S_q^{(n)}(0,1) \mid n \in \mathbb{N}\}, \\ \{S_q^{(n)}(1,1) \mid n \in \mathbb{N}\}, \end{array}$$

   where $S_r^{(n)}(a,b) = aW_r^{(n)}b$, $n \in \mathbb{N}$, $r \neq q$, and $S_q^{(n)}(a,b) = aV^{(n)}b$.

   To compute the lengths of singular factors, it is enough to compute the lengths of BS factors. See Section 3.4 for recurrent formulae for lengths.

3. The description of return words of singular factors is simplified by the following lemma, obtained applying rules from Section 6.1.

   Lemma 6.3.7. *Let $n \geq 2$, $r \in \{0, \ldots, p-2\}$. The following sets are equal*

   $$\{|w| \mid w \in Ret(S_r^{(n)}(a,b))\} = \{|\varphi(w')| \mid w' \in Ret(S_r^{(n-1)}(a,b))\}.$$

Proof. Let us start with $S_r^{(n)}(0,0)$ for $r \neq q$

$$S_r^{(n)}(0,0) = 0W_r^{(n)}0 = 00^q1\varphi(W_r^{(n-1)})0^q0.$$

Clearly, $S_r^{(n)}(0,0)$ is not BS, and, using Section 6.1.1, return words of $S_r^{(n)}(0,0)$ have the same lengths as return words of $\varphi\big(0W_r^{(n-1)}0\big) = \varphi\big(S_r^{(n-1)}(0,0)\big)$. Since $\varphi\big(S_r^{(n-1)}(0,0)\big)$ has a unique interpretation $\big(S_r^{(n-1)}(0,0),\ 0,\ 0\big)$, as a consequence of Corollary 6.1.9, we have $Ret\big(\varphi(S_r^{(n-1)}(0,0))\big) = \varphi\big(Ret(S_r^{(n-1)}(0,0))\big)$. To summarize,

$$\{|w| \bigm| w \in Ret(S_r^{(n)}(0,0))\} = \{|\varphi(w')| \bigm| w' \in Ret(S_r^{(n-1)}(0,0))\}.$$

The case of $S_q^{(n)}(0,1)$ is analogous to the previous one.

Slightly different is the case of $S_q^{(n)}(1,1)$. We have

$$S_q^{(n)}(1,1) = 1V^{(n)}1 = 10^q1\varphi(V^{(n-1)})0^q1.$$

Again, $S_q^{(n)}(1,1)$ is not BS, and, using Section 6.1.1, return words of $S_q^{(n)}(1,1)$ has the same lengths as return words of $\varphi\big(01V^{(n-1)}1\big)$. Since $\varphi\big(01V^{(n-1)}1\big)$ has a unique interpretation $\big(01V^{(n-1)}1,\ 0,\ 0\big)$, as a consequence of Corollary 6.1.9, we get $Ret\big(\varphi(01V^{(n-1)}1)\big) = \varphi\big(Ret(01V^{(n-1)}1)\big)$. Applying again Section 6.1.1, since $1V^{(n-1)}1$ is not LS, it holds $Ret(01V^{(n-1)}1) = 0Ret(1V^{(n-1)}1)0^{-1}$. Therefore $\{|\varphi(w')| \mid w' \in \varphi\big(Ret(01V^{(n-1)}1)\big)\} = \{|\varphi(w')| \mid w' \in \varphi\big(Ret(1V^{(n-1)}1)\big)\}$. To sum up

$$\{|w| \bigm| w \in Ret\big(S_q^{(n)}(1,1)\big)\} = \{|\varphi(w')| \bigm| w' \in Ret\big(S_q^{(n-1)}(1,1)\big)\}.$$

The case of $S_q^{(n)}(1,0)$ is analogous to the precedent one. □

Now, it suffices to determine return words for the simplest singular factors $S_r^{(1)}(a,b)$. Lemma 6.3.7 implies that the lengths of return words of all the other singular factors are obtained by calculating the lengths of images of the simplest return words. Here are the return words of the simplest singular factors.

- For the trivial singular factors $0,1$,

$$Ret(0) = \{0, 01\} \text{ and } Ret(1) = \{10^p, 10^q\}. \tag{6.4}$$

- For $S_0^{(1)}(0,0) = 00$,

$$\begin{array}{ll} Ret(00) = \{0, 001\} & \text{if } q \geq 2, \\ Ret(00) = \{0, 001, 00101\} & \text{if } q = 1. \end{array} \tag{6.5}$$

- For $S_r^{(1)}(0,0) = 00^r0$,

$$Ret(00^r0) = \begin{cases} \{0^p1, 0^p10^q1\} & \text{if } r = p-2\ , \\ \{0, 0^{r+2}1, 0^{r+2}10^q1\} & \text{if } q-2 < r < p-2, \\ \{0, 0^{r+2}1\} & \text{if } 1 \leq r \leq q-2. \end{cases} \tag{6.6}$$

- For $S_q^{(1)}(1,0) = 10^q0$,

$$Ret(10^q0) = \{10^p, 10^p10^q\}. \tag{6.7}$$

- For $S_q^{(1)}(0,1) = 00^q1$,

$$Ret(00^q1) = \{0^{q+1}10^{p-(q+1)}, 0^{q+1}10^q10^{p-(q+1)}\}. \tag{6.8}$$

- For $S_q^{(1)}(1,1) = 10^q1$,

$$Ret(10^q1) = \{1\varphi(10^p)1^{-1}, 1\varphi(10^q)1^{-1}\}. \tag{6.9}$$

4. The last step is to compute $l(k)$, $k \in \mathbb{N}$. Before starting, let us exclude singular factors which are not essential. Naturally, we apply Lemma 6.3.7 to determine the maximal return times $l(w)$ of a singular factor w.

   - Obviously, 0 is not an essential singular factor.
   - Since $|S_q^{(n)}(1,0)| = |S_q^{(n)}(0,1)| = |S_q^{(n)}(1,1)|$, but from Relations (9.8), (9.9), and (9.10), it is clear that for all $n \in \mathbb{N}$, one gets $l(S_q^{(n)}(1,0)) = l(S_q^{(n)}(0,1)) < l(S_q^{(n)}(1,1))$. Thus, $S_q^{(n)}(1,0)$ and $S_q^{(n)}(0,1)$ are not essential singular factors and one does not have to consider them in calculation of $l(k)$, $k \in \mathbb{N}$.
   - Analogously, if $q \geq 2$, we have $|S_0^{(n+1)}(0,0)| > |S_q^{(n)}(1,1)|$, while $l(S_0^{(n+1)}(0,0)) < l(S_q^{(n)}(1,1))$ for all $n \in \mathbb{N}$. Hence, the singular factors $S_0^{(n+1)}(0,0)$ are not essential for $q \geq 2$, $n \in \mathbb{N}$.
   - Next, if $p - 2 \geq r \geq q$, we have $|S_r^{(n)}(0,0)| \geq |S_q^{(n)}(1,1)|$, nevertheless, $l(S_r^{(n)}(0,0)) < l(S_q^{(n)}(1,1))$ for all $n \in \mathbb{N}$. Therefore, $S_r^{(n)}(0,0)$, $r \geq q$, are not essential.
   - If $1 \leq r \leq q-2$, then we obtain $|S_r^{(n+1)}(0,0)| > |S_q^{(n)}(1,1)|$, but $l(S_r^{(n+1)}(0,0)) < l(S_q^{(n)}(1,1))$ for all $n \in \mathbb{N}$, thus, the singular factors $S_r^{(n+1)}(0,0)$, $1 \leq r \leq q-2$, are not essential.
   - The last remark is that for the trivial singular factor $w = 1$, we have $|w| < |S_r^{(1)}(0,0)|$, $1 \leq r \leq q-2$, but $l(S_r^{(1)}(0,0)) < l(w)$, hence, $S_r^{(1)}(0,0)$, $1 \leq r \leq q-2$, are not essential.

   The previous facts imply that to calculate $l(k)$, we have to take into account only the trivial singular factor 1, the non-trivial singular factors of the form $S_q^{(n)}(1,1)$, and, eventually, $S_0^{(n)}(0,0)$ and $S_{q-1}^{(n)}(0,0)$. The formulae for $l(k)$, $k \in \mathbb{N}$, split into more cases, according to the values taken by p and q.

   (a) For $q \geq 2$, combining the previous facts and the description of the simplest singular factors, we obtain the following formula for $l(k), k \in \mathbb{N}$,

   - If $2q + 1 \geq p$, then

$$\begin{aligned} l(1) = \cdots = l(q) &= p+1, \\ l(q+1) &= 2q+3, \\ l(k) &= |\varphi^n(10^p)| && \text{for } |S_q^{(n)}(1,1)| \leq k < |S_{q-1}^{(n+1)}(0,0)|,\ n \in \mathbb{N}, \\ l(k) &= |\varphi^n(0^{q+1}10^q1)| && \text{for } |S_{q-1}^{(n+1)}(0,0)| \leq k < |S_q^{(n+1)}(1,1)|,\ n \in \mathbb{N}. \end{aligned}$$

   - If $2q + 1 < p$, then

$$\begin{aligned} l(1) = \cdots = l(q+1) &= p+1, \\ l(k) &= |\varphi^n(10^p)| && \text{for } |S_q^{(n)}(1,1)| \leq k < |S_q^{(n+1)}(1,1)|,\ n \in \mathbb{N}. \end{aligned}$$

(b) For $q = 1$ and $p = 3$, then it holds for $l(k)$, $k \in \mathbb{N}$,

$$\begin{aligned} l(1) &= 4, \\ l(k) &= |\varphi^{n-1}(00101)| \quad \text{for } |S_0^{(n)}(0,0)| \le k < |S_1^{(n)}(1,1)|,\ n \in \mathbb{N}, \\ l(k) &= |\varphi^{n}(10^3)| \qquad \text{for } |S_1^{(n)}(1,1)| \le k < |S_0^{(n+1)}(0,0)|,\ n \in \mathbb{N}. \end{aligned}$$

(c) For $q = 1$ and $p > 3$, we get

$$\begin{aligned} l(1) = l(2) &= p + 1, \\ l(k) &= |\varphi^{n}(10^p)| \qquad \text{for } |S_1^{(n)}(1,1)| \le k < |S_1^{(n+1)}(1,1)|,\ n \in \mathbb{N}. \end{aligned}$$

Having calculated the formula for $l(k)$, $k \in \mathbb{N}$, we have also the recurrence function computed since $R(k) = l(k) + k - 1$.

Remark 6.3.8. *Let us discuss the Sturmian case of u_β, i.e., given by parameters $p - 1 = q$. BS factors have been described in Remark 3.4.9. As a straightforward consequence, the set of singular factors is deduced:*

$$\{S_r^{(n)}(0,0) \mid 0 \le r \le p-2,\ n \in \mathbb{N}\} \cup \{S_{p-1}^{(n)}(1,1)\},$$

where $S_r^{(n)}(a,b) = aW_r^{(n)}b$. It is not difficult to show that

$$\{|w| \bigm| w \in Ret(S_r^{(n)}(a,b))\} = \{|\varphi(w')| \bigm| w' \in Ret(S_r^{(n-1)}(a,b))\}$$

for all $n \ge 2$ and $0 \le r \le p-1$. Thus, to determine lengths of return words, it is sufficient to restrict the considerations to the return words of the shortest singular factors. Here are their return words.

$$Ret(0^r) = \{0, 0^r1\} \quad 1 \le r \le p-1.$$

This time, all singular factors are essential and $l(k), k \in \mathbb{N}$, is easy to determine.

$$\begin{aligned} l(k) &= k + 1 \qquad \textit{for } 1 \le k \le p-1, \\ l(k) &= |\varphi^n(0^{p-1}1)| \quad \textit{for } |S_{p-1}^{(n+1)}| \le k < |S_1^{(n+2)}|,\ n \in \mathbb{N}_0, \\ l(k) &= |\varphi^n(0^r1)| \quad \textit{for } |S_r^{(n+1)}| \le k < |S_{r+1}^{(n+1)}|,\ 1 \le r \le p-2,\ n \in \mathbb{N}. \end{aligned}$$

In conclusion, let us provide a table of the first 18 values of $l(k)$ and $R(k)$ for the simplest Sturmian case $p = 2$ and $q = 1$.

$l(k)$	3	5	8	8	13	13	13	21	21	21	21	21	34	34	34	34	34	34
$R(k)$	3	6	10	11	17	18	19	28	29	30	31	32	46	47	48	49	50	51

Chapter 7

Frequencies

This chapter studies the problematics of factor frequencies in an infinite word. To be specific, we tackle two tasks. The first one is to improve the so-far known upper bound on the number of factor frequencies. We improve this upper bound in the case of the infinite words whose language has a symmetry. The second task is to determine the actual values of factor frequencies in two infinite words – u_β associated with quadratic non-simple Parry numbers (representing fixed points of substitutions) and the palindromeless reversal closed word (representing words with a finite number of palindromes). Throughout this chapter, a central role is played by (reduced) Rauzy graphs.

7.1 Rauzy graphs and factor frequencies

Rauzy graphs, despite of their simplicity, have turned out to be a powerful tool in the study of various combinatorial properties of words. The first one to use the idea to label the edges of Rauzy graphs with frequencies was Dekking [41] in order to show that for every length, there exist at most three different factor frequencies in the Fibonacci word. Moreover, he has described, for every n, the set of frequencies of factors of length n and the number of factors of length n having the same frequency.

It is not difficult to explain why the factor frequencies of Sturmian words attain at most three values for every length. The reduced Rauzy graphs of every Sturmian word take only the forms depicted in Figure 2.4; that is, the graph consists either of one vertex (corresponding to a BS factor) and two edges, or two vertices (corresponding to a LS and a RS factor) and three edges. As a consequence, there are at most three edge labels in the Rauzy graph Γ_n for any length n.

Berthé in [17], observing also the evolution of Rauzy graphs for growing factor lengths, generalized Dekking's result for all Sturmian words.[1] More precisely, for every Sturmian word with the slope α, knowing the consecutive n-Farey fractions $\frac{p_1}{q_1}, \frac{p_2}{q_2}$ such that $\frac{p_1}{q_1} < \alpha < \frac{p_2}{q_2}$, the exact values of frequencies of factors of length n and also the number of factors of length n having the same frequency have been derived in [17].

With the help of Rauzy graphs, Boshernitzan in [21] has deduced an upper bound on the number of different frequencies in an aperiodic recurrent infinite word. According to his result, the number of frequencies of factors of length $n+1$ does not exceed $3\Delta\mathcal{C}(n)$.

Since $\Delta\mathcal{C}(n)$ is known to be bounded for infinite words with sublinear complexity, it follows for Arnoux-Rauzy words, m-interval exchange words, and fixed points of primitive substitutions that the number of different frequencies of factors of the same length is bounded.

[1] Note that this result follows also from the 3 gap theorem by Sós [104].

Let us present the estimates leading to the result of Boshernitzan since their improvement for infinite words with symmetries is our first important goal. Let u be an aperiodic recurrent infinite word and assume that its factor frequencies exist. The idea is simple. We calculate the number of edges in the reduced Rauzy graph $\tilde{\Gamma}_n$ of u (defined in Section 2.2.12) in order to get an upper bound on the number of edge labels in $\tilde{\Gamma}_n$. As the sets of edge labels of $\tilde{\Gamma}_n$ and Γ_n coincide, we get in fact an upper bound on the number of frequencies of factors in $\mathcal{L}_{n+1}(u)$.

For every RS factor $w \in \mathcal{L}_n(u)$, it holds that $\#Rext(w)$ edges begin in w, and, for every LS factor $v \in \mathcal{L}_n(u)$ which is not RS, only one edge begins in v, thus we get the following relation

$$\#\{e|\ e \text{ edge in } \tilde{\Gamma}_n\} = \sum_{w \text{ RS in } \mathcal{L}_n} \#Rext(w) + \sum_{v \text{ LS not RS in } \mathcal{L}_n} 1. \tag{7.1}$$

Using Proposition 2.2.1, we deduce that

$$\#\{e|\ e \text{ edge in } \tilde{\Gamma}_n\} = \Delta\mathcal{C}(n) + \sum_{w \text{ RS in } \mathcal{L}_n} 1 + \sum_{v \text{ LS not RS in } \mathcal{L}_n} 1. \tag{7.2}$$

Since $\#Rext(w) - 1 \geq 1$ for any RS factor w, and, similarly, $\#Lext(w) - 1 \geq 1$ for any LS factor, we have

$$\#\{w \in \mathcal{L}_n(u)|\ w\ RS\} \ \leq\ \Delta\mathcal{C}(n) \quad \text{and} \quad \#\{w \in \mathcal{L}_n(u)|\ w\ LS\} \ \leq\ \Delta\mathcal{C}(n). \tag{7.3}$$

The following result, initially proved in [21], follows immediately combining (7.2) and (7.3).

Theorem 7.1.1. *Let u be an aperiodic recurrent infinite word such that for every factor $w \in \mathcal{L}(u)$, the frequency $\rho(w)$ exists. Then, for every $n \in \mathbb{N}$, it holds*

$$\#\{\rho(e) \bigm| e \in \mathcal{L}_{n+1}(u)\} \quad \leq \quad 3\Delta\mathcal{C}(n).$$

7.2 Symmetries in Rauzy graphs and factor frequencies

The aim of this section is to show that Boshernitzan's upper bound $3\Delta\mathcal{C}(n)$ can be further diminished if the labeled Rauzy graphs of the infinite word in question have a nontrivial group of automorphisms. Examples of such automorphisms are symmetries defined in Section 6.1.3 (mirror symmetry and letter permutations). Let us mention that the idea to exploit the mirror symmetry of the Rauzy graph was already used by Baláži, Masáková, and Pelantová in [10] and it has led to the estimate (4.2) on the palindromic complexity in terms of the first difference of factor complexity.

Let us improve the estimate from Theorem 7.1.1 for aperiodic infinite words u whose language is closed under reversal and such that the frequency of every factor exists. The following two properties may be easily checked.

1. Such words are recurrent.
2. For any pair of factors $w, v \in \mathcal{L}(u)$, it holds

$$\frac{\#\{\text{occurrences of } w \text{ in } v\}}{|v|} = \frac{\#\{\text{occurrences of } \overline{w} \text{ in } \overline{v}\}}{|\overline{v}|}.$$

The definition of factor frequency in (2.11) implies $\rho(w) = \rho(\overline{w})$ for all factors w of u.

With the above two ingredients in hand, we are able to prove a lemma, essential for determining of an improved upper bound on the number of factor frequencies.

Lemma 7.2.1. *Let u be an aperiodic infinite word whose language $\mathcal{L}(u)$ is closed under reversal and such that for every factor $w \in \mathcal{L}(u)$, the frequency $\rho(w)$ exists. Then, for every $n \in \mathbb{N}$, we have*

$$\#\{\rho(e) | e \in \mathcal{L}_{n+1}(u)\} \quad \leq \quad \frac{1}{2}\Big(\mathcal{P}(n) + \mathcal{P}(n+1) + \Delta\mathcal{C}(n) - X - Y\Big) + Z,$$

where X *is the number of BS factors of length* n*,*
Y *is the number of BS palindromic factors of length* n*,*
Z *is the number of RS factors of length* n*.*

Proof. Let Γ_n be the labeled Rauzy graph of u of order n. Then the mirror map μ maps Γ_n onto itself (since $\mathcal{L}(u)$ is closed under reversal). Thanks to the relation $\rho(w) = \rho(\overline{w})$ for all $w \in \mathcal{L}(u)$, the map μ is even an automorphism of the labeled Rauzy graph Γ_n. Clearly, every simple path f in Γ_n is mapped by μ to the simple path $\overline{f}$ having the same label. Hence, μ induces an automorphism on the reduced Rauzy graph $\tilde{\Gamma}_n$, too.

We know already that the set of edge labels of $\tilde{\Gamma}_n$ is equal to the set of edge labels of Γ_n. Let us denote by A the number of edges f in $\tilde{\Gamma}_n$ (the number of simple paths in Γ_n) such that f is mapped by μ onto itself and by B the number of edges f in $\tilde{\Gamma}_n$ such that f is not mapped by μ onto itself. Then, obviously,

$$\#\{f | \ f \text{ edge in } \tilde{\Gamma}_n\} = A + B.$$

If a simple path $f = f_1 f_2 \dots f_m$ is mapped by μ onto itself, then f is a palindrome. Consequently, if m and n have the same parity, then the central factor of f of length n is a palindromic vertex in Γ_n, and if m and $n+1$ have the same parity, then the central factor of f of length $n+1$ is a palindromic edge in Γ_n. On the other hand, every palindrome of length $n+1$ is a central factor of a simple path mapped by μ onto itself and every palindrome of length n is either a central factor of a simple path mapped by μ onto itself or it is a vertex in $\tilde{\Gamma}_n$. Therefore,

$$A = \mathcal{P}(n) + \mathcal{P}(n+1) - \#\{w \in \mathcal{L}_n(u) | \ w \text{ BS in } \mathcal{P}al_n\}. \tag{7.4}$$

We subtract the number of palindromic BS factors of $\mathcal{L}_n(u)$, in the statement denoted by Y, since they are not factors of any simple path – they are vertices in $\tilde{\Gamma}_n$.

Now, let us turn our attention to the edges of $\tilde{\Gamma}_n$ that are not mapped by μ onto themselves. For every such edge f, at least one distinct edge, namely $\overline{f}$, has the same label $\rho(f)$. These considerations lead to the following estimate

$$\#\{\rho(e) | \ e \in \mathcal{L}_{n+1}(u)\} \leq A + \tfrac{1}{2}B = \tfrac{1}{2}A + \tfrac{1}{2}(A + B). \tag{7.5}$$

Rewriting Equation (7.2), we obtain

$$A + B = \Delta\mathcal{C}(n) + 2Z - X. \tag{7.6}$$

This fact together with (7.4) and (7.5) proves the statement. □

If we apply on $\mathcal{P}(n) + \mathcal{P}(n+1)$ and Z from Lemma 7.2.1 the estimates (4.2) and (7.3), respectively, we obtain immediately the main theorem.

Theorem 7.2.2. *Let u be an aperiodic infinite word whose language $\mathcal{L}(u)$ is closed under reversal and such that for every factor $w \in \mathcal{L}(u)$, the frequency $\rho(w)$ exists. Then, for every $n \in \mathbb{N}$, we have*

$$\#\{\rho(e) | e \in \mathcal{L}_{n+1}(u)\} \quad \leq \quad 2\Delta\mathcal{C}(n) + 1 - \tfrac{1}{2}X - \tfrac{1}{2}Y, \tag{7.7}$$

where X is the number of BS factors of length n and Y is the number of BS palindromic factors of length n.

Corollary 7.2.3. *Let u be an infinite word whose language $\mathcal{L}(u)$ is closed under reversal and such that for every factor $w \in \mathcal{L}(u)$, the frequency $\rho(w)$ exists. Then the number of distinct factor frequencies obeys, for all $n \in \mathbb{N}$,*

$$\#\{\rho(e) | e \in \mathcal{L}_{n+1}(u)\} \quad \leq \quad 2\Delta\mathcal{C}(n) + 1, \tag{7.8}$$

where the equality is reached if and only if u is purely periodic.

Proof. The validity for aperiodic words follows from Theorem 7.2.2. Moreover, aperiodic words contain infinitely many BS factors. Hence, according to (7.7), the strict inequality $\#\{\rho(e)|e \in \mathcal{L}_{n+1}(u)\} < 2\Delta\mathcal{C}(n) + 1$ holds for infinitely many n.

Infinite words whose languages are closed under reversal are readily seen to be either aperiodic or purely periodic. Hence, it remains to explain that the statement holds for purely periodic words.

In case of purely periodic words, for sufficiently large n, the first difference of complexity satisfies $\Delta\mathcal{C}(n) = 0$ and all factors of length n have the same frequency (see Section 2.2.6). Thus, the equality in (7.8) is realized. $\square$

Remark 7.2.4. *If we seek for infinite words reaching the upper bound from Theorem 7.2.2, the only candidates are the aperiodic recurrent infinite words*

- *satisfying $\#Rext(w) \leq 2$ for all $w \in \mathcal{L}(u)$ (since the upper bounds in (7.3) are reached),*
- *opulent in palindromes (since the upper bound in (4.2) is realized).*

Let us mention examples of infinite words which demonstrate the accuracy of the upper bound from Theorem 7.2.2.

Example 7.2.5. *Berthé in [17] has shown that for every Sturmian word u, the number of frequencies of factors of length n equals 2 if $\mathcal{L}_n(u)$ contains a BS factor, and is equal to 3 otherwise. Since any BS factor of a Sturmian word is a palindrome, the upper bound in (7.7) is realized for all $n \in \mathbb{N}$.*

Example 7.2.6. *Ferenczi and Zamboni [53] have proved that m-iet words attain the upper bound in (7.7) for all $n \in \mathbb{N}$. Their result shows that the equality in (7.7) may be reached even for words over multilateral alphabets. As Sturmian words are 2-iet words, Example 7.2.5 is a particular case of their result.*

The above examples illustrate that the upper bound (7.7) is optimal and cannot be improved, preserving the general assumptions. However, under some additional conditions, one can obtain an improved analogy of the estimate (7.7). For instance, Lemma 7.2.1 gives us the following statement.

Proposition 7.2.7. *Let u be an aperiodic infinite word having language closed under reversal, however, containing only a finite number of palindromes. Then*

$$\#\{\rho(e)|e \in \mathcal{L}_{n+1}(u)\} \quad \leq \quad \tfrac{3}{2}\Delta\mathcal{C}(n) - \tfrac{1}{2}X \quad \textit{for all but finitely many } n \in \mathbb{N},$$

where X is the number of BS factors of length n.

An example of an infinite word satisfying the assumptions of Proposition 7.2.7 can be found in Section 3.3.5. We shell determine the values of factor frequencies of this word in a forthcoming section.

The essential idea of our approach relies in the fact that the closeness of the language under reversal implies the existence of a non-trivial automorphism of the labeled Rauzy graph. More generally, our method can be applied on any infinite word u whose language $\mathcal{L}(u)$ has a symmetry $S : \mathcal{L}(u) \to \mathcal{L}(u)$ (defined in Section 6.1.3). Let us recall that the group of all such symmetries S is generated by the mirror image map and permutations of letters (extended to $\mathcal{L}(u)$ as morphisms).

If the language of a binary word is closed under an exchange S of letters, no simple path is mapped by S onto itself, and, thus, each frequency is assigned to at least two edges in the reduced Rauzy graph $\tilde{\Gamma}_n$. As the number of edges is at most $3\Delta\mathcal{C}(n)$, we obtain for frequencies the following upper bound

$$\#\{\rho(e) | e \in \mathcal{L}_{n+1}(u)\} \quad \leq \quad \tfrac{3}{2}\Delta\mathcal{C}(n).$$

Example 7.2.8. *The Thue-Morse word u_{TM} has the most symmetrical language among binary words in the sense that $\mathcal{L}(u_{TM})$ is both closed under reversal and also under exchange of letters. It explains why the upper bound from Theorem 7.2.2 overestimates the actual number of factor frequencies of u_{TM}. For concrete values of factor frequencies consult [54].* [2]

7.3 Frequencies of fixed points of substitutions

In this section, we intend to derive the values of factor frequencies of the infinite word u_β associated with a quadratic non-simple Parry number β. The following method enables to get the factor frequencies recurrently.

7.3.1 Recurrent formula for factor frequencies

Let us recall a recurrent formula established by Frid in [54] for the derivation of factor frequencies in fixed points $u = u_0 u_1 u_2 \ldots$ of substitutions φ satisfying:

1. φ is non-erasing,
2. $\rho(v)$ exists for every $v \in \mathcal{L}(u)$,
3. $\lim_{k\to\infty} \frac{|\varphi^{k+1}(u_0)|}{|\varphi^k(u_0)|} = \theta > 1$.

Under the above conditions, it is possible to calculate recurrently the frequency of each factor $v \in \mathcal{L}(u)$ knowing letter frequencies. Notice that the conditions exact neither the primitivity from the substitution φ nor the positivity from the frequencies of factors of u.

Theorem 7.3.1. *Let $v, w \in \mathcal{L}(u)$, then*

$$\#\{\textit{occurences of } v \textit{ in } \varphi(w)\} = \sum_{s \in I(v)} \#\{\textit{occurrences of } a(s) \textit{ in } w\},$$

where $I(v)$ denotes the set of interpretations of v and $a(s)$ is the ancestor of an interpretation s.

[2] The first one to derive factor frequencies in the Thue-Morse word was Dekking [41].

Corollary 7.3.2. *For every $v \in \mathcal{L}(u)$, we have*

$$\rho(v) = \frac{1}{\theta} \sum_{s \in I(v)} \rho(a(s)). \tag{7.9}$$

If φ is a strictly growing substitution, i.e., $|\varphi(a)| \geq 2$ for all $a \in \mathcal{A}$, then ancestors of any word v of length greater than 2 cannot be as long as the word v itself. Thus, in such a case, we have to solve a system of linear equations for frequencies of factors of length 2; the frequencies of factors of larger lengths can be computed recurrently using Corollary 7.3.2.

7.3.2 Frequencies of u_β associated with quadratic non-simple Parry numbers

Let us recall that the substitution matrix of the infinite word u_β associated with a quadratic non-simple Parry number β, defined in Section 2.3.4, is of the form $M = \begin{pmatrix} p & 1 \\ q & 1 \end{pmatrix}$. The left eigenvector (l_1, l_2) corresponding to the larger eigenvalue β and satisfying $l_1 + l_2 = 1$ is equal to $(1 - \frac{1}{\beta}, \frac{1}{\beta})$. Consequently, according to the result of Durand [45], the frequencies of all factors of u_β exist and we have $\rho(0) = 1 - \frac{1}{\beta}$ and $\rho(1) = \frac{1}{\beta}$. In addition, using Equation (2.19), we obtain

$$\lim_{k \to \infty} \frac{|\varphi^{k+1}(u_0)|}{|\varphi^k(u_0)|} = \beta.$$

Remark that for $p - 1 = q$, the word u_β is Sturmian, and, thus, factor frequencies may be calculated using the method of Berthé [17] and the upper bound given in Theorem 7.2.2 is attained. Therefore, in the sequel, we limit our considerations to the case $p - 1 > q$.

First, we compute the values of frequencies of BS factors (described in Section 3.4) using the recurrent formula from Corollary 7.3.2. Second, we introduce some necessaries for the construction of reduced Rauzy graphs $\tilde{\Gamma}_l$ for growing l. It is not difficult to see that these necessaries are also sufficient for the construction of $\tilde{\Gamma}_{l+1}$ from $\tilde{\Gamma}_l$ and that they allow us to determine, using Kirchhoff's law, for every $n \in \mathbb{N}$, the set of frequencies of $\mathcal{L}_l(u_\beta)$ for $l \in \{|W_1^{(n)}| + 1, \ldots, |W_1^{(n+1)}|\}$, knowing just frequencies of BS factors, even only of two BS factors $W_0^{(n+1)}$ and $W_1^{(n)}$. However, since the construction of reduced Rauzy graphs is rather technical, we give instead only a list of explicit values of factor frequencies. Finally, observing the results on factor frequencies, we deduce for which lengths $l \in \mathbb{N}$, the upper bound from Theorem 7.2.2 is reached.

Frequencies of BS factors of u_β

Applying Corollary 7.3.2, we can derive a recurrent relation for frequencies of BS factors.

Lemma 7.3.3. *Let u_β be the fixed point of the substitution φ defined by $\varphi(0) = 0^p1$, $\varphi(1) = 0^q1$, where $p - 1 > q \geq 1$. Let $n \geq 1$, then*

$$\begin{aligned} \rho(W_k^{(n+1)}) &= \tfrac{1}{\beta}\rho(W_k^{(n)}), \quad k \in \{0, \ldots, p-2\},\ k \neq q, \\ \rho(V^{(n+1)}) &= \tfrac{1}{\beta}\rho(V^{(n)}), \\ \rho(U^{(n+1)}) &= \tfrac{1}{\beta}\rho(U^{(n)}). \end{aligned} \tag{7.10}$$

Proof. Observation 3.4.2 implies that any factor of the form $v = 0^q1\varphi(w)0^q$ has the following set of interpretations

$$I(v) = \{(0w0, p-q, p-q+1),\ (0w1, p-q, 1),\ (1w0, 0, p-q+1),\ (1w1, 0, 1)\}.$$

Of course, if $awb \notin \mathcal{L}(u_\beta)$, then $\rho(awb) = 0$. Corollary 7.3.2 together with Lemma 2.2.5 states that

$$\rho(v) = \frac{1}{\beta}\big(\rho(0w0) + \rho(0w1) + \rho(1w0) + \rho(1w1)\big) = \frac{1}{\beta}\rho(w).$$

$\square$

Thanks to the simple form of the recurrent relation for frequencies of BS factors and thanks to the knowledge of letter frequencies, we can even calculate the explicit values of frequencies of BS factors.

Corollary 7.3.4. *Let $n \geq 1$, then*

$$\begin{array}{rcl} \rho(W_k^{(n+1)}) & = & \frac{1}{\beta^n}\rho(W_k^{(1)}), \quad k \in \{0,\ldots,p-2\},\ k \neq q, \\ \rho(V^{(n+1)}) & = & \frac{1}{\beta^n}\rho(V^{(1)}), \\ \rho(U^{(n+1)}) & = & \frac{1}{\beta^n}\rho(U^{(1)}). \end{array} \tag{7.11}$$

For the shortest BS factors, we have

$$\begin{array}{rcll} \rho(W_0^{(1)}) & = & \rho(\varepsilon) = 1, & \\ \rho(W_k^{(1)}) & = & \rho(0^k) = \frac{p-k+1}{\beta}\rho(0) + \frac{q-k+1}{\beta}\rho(1), & \textit{for } 1 \leq k < q, \\ \rho(V^{(1)}) & = & \rho(0^q) = \frac{p-q+1}{\beta}\rho(0) + \frac{1}{\beta}\rho(1), & \\ \rho(W_k^{(1)}) & = & \rho(0^k) = \frac{p-k+1}{\beta}\rho(0), & \textit{for } q+1 \leq k < p-1, \\ \rho(U^{(1)}) & = & \rho(0^{p-1}) = \frac{2}{\beta}\rho(0). & \end{array} \tag{7.12}$$

Proof. In order to keep the relation $\rho(W_0^{(2)}) = \frac{1}{\beta}\rho(W_0^{(1)})$ valid, and, since $\rho(W_0^{(2)}) = \rho(1) = \frac{1}{\beta}$, it is natural to put $\rho(\varepsilon) := 1$. For $k = 1$, we have $\rho(W_k^{(1)}) = \rho(0)$, which is in correspondence with the second formula in the above list. To calculate frequencies of the other shortest BS factors, we use again Corollary 7.3.2. Hence, we have to describe interpretations of the shortest BS factors. This task is easy to solve considering the form of the substitution φ. For $2 \leq k \leq q$, we obtain $I(0^k) = \{(0,0,p-k+1),\ldots,(0,p-k,1),(1,0,q-k+1),\ldots,(1,q-k,1)\}$, hence $\rho(0^k) = \frac{p-k+1}{\beta}\rho(0) + \frac{q-k+1}{\beta}\rho(1)$, and, for $q+1 \leq k \leq p-1$, the set of interpretations is $I(0^k) = \{(0,0,p-k+1),\ldots,(0,p-k,1)\}$, thus $\rho(0^k) = \frac{p-k+1}{\beta}\rho(0)$. $\square$

Necessaries for construction of reduced Rauzy graphs of u_β

In order to construct reduced Rauzy graphs, it is necessary to know more details on BS factors of u_β:

- If w is a BS factor, we need to find, for every $a \in \mathit{Rext}(w)$ such that wa is LS, the shortest BS factor v containing wa as a prefix. As every BS factor is a palindrome (see Section 4.3), aw is then a suffix of v and the factor starting in wa and ending in aw is a simple path. Applying Item *4.* of Lemma 3.4.3, we reveal the following relations for BS factors with lengths in $\{|W_1^{(n)}|,\ldots,|W_1^{(n+1)}|\}$ (words on the right-hand side are the shortest BS factors containing words on the left-hand side as prefixes):

$$
\begin{array}{rll}
W_k^{(n)}0 & \text{is a prefix of} \quad W_{k+1}^{(n)}, & 1 \le k < q-1, \\
W_{q-1}^{(n)}0 & \text{is a prefix of} \quad V^{(n)}, & \\
V^{(n)}0 & \text{is a prefix of} \quad W_{q+1}^{(n)}, & \\
V^{(n)}1 & \text{is a prefix of} \quad W_0^{(n+1)}, & \\
W_k^{(n)}0 & \text{is a prefix of} \quad W_{k+1}^{(n)}, & q+1 \le k < p-2, \\
W_{p-2}^{(n)}0 & \text{is a prefix of} \quad U^{(n)}, & \\
W_0^{(n+1)}0 & \text{is a prefix of} \quad W_1^{(n+1)}. &
\end{array}
$$

- It is also indispensable to know the ordering of BS factors according to their lengths. The ordering is obvious for pairs of BS factors such that one is a prefix of the other, therefore, the only question left is the position of $|W_0^{(n+1)}|$ in $\{|W_1^{(n)}|, \dots, |W_1^{(n+1)}|\}$. In order to compare lengths, the same recurrent formula for computing lengths as the one from Section 3.4 is used. Two cases are to be considered, according to the relation of lengths $|U^{(n)}| \lesseqgtr |W_0^{(n+1)}|$:

  1. If $p-1 < 2q+1$, then $|W_1^{(n)}| < \cdots < |W_{q-1}^{(n)}| < |V^{(n)}| < |W_{q+1}^{(n)}| < \cdots < |W_{p-2}^{(n)}| < |U^{(n)}| < |W_0^{(n+1)}| < |W_1^{(n+1)}|$ for all $n \in \mathbb{N}$, thus there is at most one BS factor for every length. BS factors are illustrated in Figure 7.1.

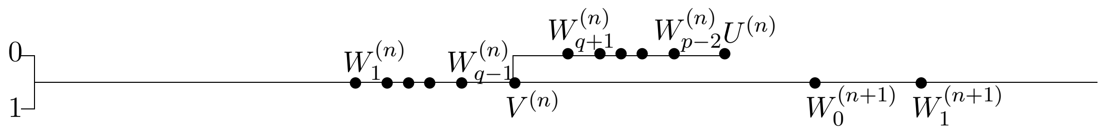


Fig. 7.1: Illustration of a sector of the infinite LS branch of u_β for $p-1 < 2q+1$. The sector shows BS factors of lengths between $|W_1^{(n)}|$ and $|W_1^{(n+1)}|$.

  2. If $p-1 \ge 2q+1$, then $|W_1^{(n)}| < \cdots < |W_{q-1}^{(n)}| < |V^{(n)}| < |W_{q+1}^{(n)}| < \cdots < |W_{2q}^{(n)}| < |W_0^{(n+1)}| < |W_{2q+1}^{(n)}| < |U^{(n)}| < |W_1^{(n+1)}|$ for all $n \ge 2$ and $|W_{2q+1}^{(1)}| = |W_0^{(2)}|$ since $W_{2q+1}^{(1)} = 0^{2q+1}$ and $W_0^{(2)} = 0^q10^q$. There occurs at most one BS factor for every length $l \ne 2q+1$. BS factors are illustrated in Figure 7.2.

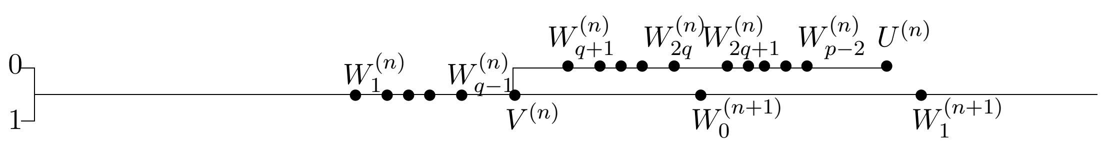


Fig. 7.2: Illustration of a sector of the infinite LS branch of u_β for $p-1 \ge 2q+1$. The sector shows BS factors of lengths between $|W_1^{(n)}|$ and $|W_1^{(n+1)}|$, $n \ge 2$.

Explicit values of factor frequencies of u_β

We have seen in the previous section that the evolution of reduced Rauzy graphs depends on the position of $|W_0^{(n+1)}|$ in $\{|W_1^{(n)}|, \dots, |W_1^{(n+1)}|\}$. In consequence, there appear two distinct situations, for $p-1 < 2q+1$ and $p-1 \ge 2q+1$. Nevertheless, both of them are quite similar, in particular, the conditions on factor lengths guaranteeing the equality in (7.7) are the same. Therefore, we present results only for the case of $p-1 \geq 2q+1$.

In addition, it is necessary to treat separately the case of $n=1$ and $n>1$ for the construction of reduced Rauzy graphs $\tilde{\Gamma}_l$ with $l \in \{|W_1^{(n)}|, \ldots, |W_1^{(n+1)}|-1\}$. In the first case, not only there are two BS factors of the same length for $2q+1=p-1$, but the difference between the lengths of consecutive BS factors may be equal to 1, while in the second case, the difference is always greater than 1. The sets of factor frequencies of $\mathcal{L}_{n+1}(u_\beta)$ for $l \in \{|W_1^{(1)}|, \ldots, |W_1^{(2)}|-1\}$ are as follows:

$$\begin{aligned}
\{f-lg, g\} \quad &\text{for} \quad l \in \{|W_1^{(1)}|, \ldots, |V^{(1)}|\},\\
\{f-qg-(l-q)h, g, h, g-h\} \quad &\text{for} \quad l \in \{|W_{q+1}^{(1)}|, \ldots, |W_{2q}^{(1)}|\},\\
\{f-qg-(q+1)h, h, g-h\} \quad &\text{for} \quad l = |W_{2q+1}^{(1)}|,\\
\{f-qg-(l-q)h, h, g-h, 2h-g\} \quad &\text{for} \quad l \in \{|W_{2q+1}^{(1)}|+1, \ldots, |U^{(1)}|-1\},\\
\{h, g-h, 2h-g\} \quad &\text{for} \quad l \in \{|U^{(1)}|, \ldots, |W_1^{(2)}|-1\},
\end{aligned}$$

where the frequencies are expressed as linear combinations of f, g, and h, with $f=\rho(0)=\rho(W_1^{(1)})$, $g=\rho(1)=\rho(W_0^{(2)})$, and $h=\frac{f-qg}{p-q}$.

The sets of factor frequencies of $\mathcal{L}_{n+1}(u_\beta)$ for $l \in \{|W_1^{(n)}|, \ldots, |W_1^{(n+1)}|-1\}$, $n \geq 2$, reads:

$$\begin{aligned}
\{f-kg, g\} \quad &\text{for} \quad l = |W_k^{(n)}|,\\
&\qquad\ \ k \in \{1, \ldots, q-1\},\\
\{f-kg, g, f-(k+1)g\} \quad &\text{for} \quad |W_k^{(n)}| < l < |W_{k+1}^{(n)}|,\\
&\qquad\ \ k \in \{1, \ldots, q-1\},\\
\{f-qg, g\} \quad &\text{for} \quad l = |V^{(n)}|,\\
\{f-qg, g, h, f-qg-h, g-h\} \quad &\text{for} \quad |V^{(n)}| < l < |W_{q+1}^{(n)}|,\\
\{f-qg-(k-q)h, g, h, g-h\} \quad &\text{for} \quad l = |W_k^{(n)}|,\\
&\qquad\ \ k \in \{q+1, \ldots, 2q\},\\
\{f-qg-(k-q)h, g, f-qg-(k+1-q)h,\ h, g-h\} \quad &\text{for} \quad |W_k^{(n)}| < l < |W_{k+1}^{(n)}|,\\
&\qquad\ \ k \in \{q+1, \ldots, 2q-1\},\\
\{f-qg-qh, g, f-qg-(q+1)h, h, g-h\} \quad &\text{for} \quad |W_{2q}^{(n)}| < l < |W_0^{(n)}|,\\
\{f-qg-qh, f-qg-(q+1)h, h, g-h\} \quad &\text{for} \quad l = |W_0^{(n)}|,\\
\{f-qg-qh, f-qg-(q+1)h, h, g-h, 2h-g\} \quad &\text{for} \quad |W_0^{(n)}| < l < |W_{2q+1}^{(n)}|,\\
\{f-qg-(k-q)h, h, g-h, 2h-g\} \quad &\text{for} \quad l = |W_k^{(n)}|,\\
&\qquad\ \ k \in \{2q+1, \ldots, p-2\},\\
\{f-qg-(k-q)h,\ f-qg-(k+1-q)h, h, g-h, 2h-g\} \quad &\text{for} \quad |W_k^{(n)}| < l < |W_{k+1}^{(n)}|,\\
&\qquad\ \ k \in \{2q+1, \ldots, p-3\},\\
\{f-qg-(p-2-q)h, h, g-h, 2h-g\} \quad &\text{for} \quad |W_{p-2}^{(n)}| < l < |U^{(n)}|,\\
\{h,\ g-h,\ 2h-g\} \quad &\text{for} \quad |U^{(n)}| \leq l < |W_1^{(n+1)}|,
\end{aligned}$$

where the frequencies are functions of f, g, and h, with $f=\rho(W_1^{(n)}), g=\rho(W_0^{(n)})$, and $h=\frac{f-qg}{p-q}$.

Reaching the upper bound from Theorem 7.2.2

As we know, the infinite word u_β is aperiodic and recurrent, its language $\mathcal{L}(u_\beta)$ is closed under reversal, and its factor frequencies exist. In consequence, Theorem 7.2.2 holds for u_β. Moreover, u_β is defined over a binary alphabet and is opulent in palindromes (see Corollary 4.3.4); hence, in reference to Remark 7.2.4, u_β satisfies the two necessary conditions for reaching the equality in (7.7). It is therefore reasonable to ask for which lengths $l \in \mathbb{N}$, the equality in

$$\#\{\rho(e)|e \in \mathcal{L}_{l+1}(u_\beta)\} \quad \leq \quad 2\Delta\mathcal{C}(l) + 1 - \tfrac{1}{2}X - \tfrac{1}{2}Y,$$

where X is the number of BS factors of length l and Y is the number of BS palindromic factors of length l, is attained.

Thanks to Section 3.4, we know that all BS factors of u_β are palindromes and we have the following formula for the first difference of complexity:

$$\Delta\mathcal{C}(l) = \begin{cases} 2 & \text{if } |V^{(n)}| < l \leq |U^{(n)}| \text{ for some } n \in \mathbb{N}, \\ 1 & \text{otherwise.} \end{cases}$$

The question may be thus simplified as follows: For which lengths $l \in \mathbb{N}$, the following formula holds:

$$\#\{\rho(e)|e \in \mathcal{L}_{l+1}(u_\beta)\} \quad = \quad \begin{cases} 5 - \#\{w \in \mathcal{L}_l(u_\beta) \mid w \text{ BS}\} & \text{if } |V^{(n)}| < l \leq |U^{(n)}|,\ n \in \mathbb{N}, \\ 3 - \#\{w \in \mathcal{L}_l(u_\beta) \mid w \text{ BS}\} & \text{otherwise ?} \end{cases}$$

In the case of parameters p, q satisfying $p - 1 \geq 2q + 1$, the answer may be provided looking at the explicit values of factor frequencies given in the previous section. The upper bound from Theorem 7.2.2 is realized for all lengths l satisfying $l \notin \{|W_{p-2}^{(n)}|, \dots, |U^{(n)}|\},\ n \geq 2$. For lengths $l \in \{|W_{p-2}^{(n)}|, \dots, |U^{(n)}|\},\ n \geq 2$, the upper bound from Theorem 7.2.2 is by one greater than the actual number of frequencies; that is, $\#\{\rho(e)|e \in \mathcal{L}_{l+1}(u_\beta)\} = 2\Delta C(l) - \#\{w \in \mathcal{L}_l(u_\beta) \mid w \text{ BS}\}$. We add without proof that the result is exactly the same for the case $p - 1 < 2q + 1$.

7.4 Frequencies of a palindromeless reversal closed word

The infinite word z whose language contains only a finite number of palindromes has been defined in (3.23). According to Section 3.3.5, z is linearly recurrent. In reference to Section 2.2.6, linear recurrence guarantees the existence of factor frequencies. The word z is aperiodic, therefore every factor w which is not BS may be uniquely extended to the shortest BS factor v containing w. Then, Corollary 2.2.6 implies that $\rho(w) = \rho(v)$.

As the sets of special factors in $\mathcal{L}_l(z)$ become regular for $l \geq 14$, we restrict our considerations to the factors of length ≥ 14. First, we compute explicitly the frequencies of BS factors. Second, observing the evolution of reduced Rauzy graphs $\tilde{\Gamma}_l$ for growing $l \geq 14$, we are capable to determine the set of frequencies of $\mathcal{L}_l(u_\beta)$ for $l \in \{|z_n| + 1, \dots, |z_{n+1}|\},\ n \geq 2$, knowing just the frequencies of BS factors.

Proposition 7.4.1. *For every $n \geq 2$, the frequencies of BS factors of z satisfy*

$$\rho(z_n) = \rho(\overline{z_n}) = \tfrac{1}{2^{n+3}} \quad \text{and} \quad \rho(\overline{z_n}01z_n) = \rho(\overline{z_n}10z_n) = \tfrac{1}{2^{n+4}}.$$

Proof. Since the formula (3.25) determines all occurrences of z_n in z for $n \geq 2$, we deduce that the set of occurrences of $z_n,\ n \geq 2$, equals $\{0\} \cup \{k \cdot 2^{n+3} - 1 \mid k \in \mathbb{N}\}$. It follows then directly from the definition of factor frequency that $\rho(z_n) = \frac{1}{2^{n+3}}$. Since the language of z is closed under reversal, we have $\rho(\overline{z_n}) = \rho(z_n)$.

Similarly, since $\overline{z_n}01z_n$ is reversal of $\overline{z_n}10z_n$, both factors have the same frequency. Moreover, thanks to Corollary 2.2.6 and the formula (3.25), we deduce $\rho(\overline{z_n}01z_n) = \rho(\overline{z_n}0)$ and $\rho(\overline{z_n}10z_n) = \rho(\overline{z_n}1)$. Finally, applying Kirchhoff's law, we get $\rho(\overline{z_n}0) + \rho(\overline{z_n}1) = \rho(\overline{z_n})$. Therefore, using the previous result for frequency of $\overline{z_n}$, we obtain $\rho(\overline{z_n}01z_n) = \rho(\overline{z_n}10z_n) = \frac{1}{2^{n+4}}$.

□

In order to construct the reduced Rauzy graphs $\tilde{\Gamma}_l,\ l \in \{|z_n|, \dots, |z_{n+1}|\},\ n \geq 2$, the following ingredients are needed.

1. The list of special factors of length ≥ 14: BS and LS factors have been described in Section 3.3.5. RS factors are reversals of LS factors.

2. For every BS factor w and for every $a \in Rext(w)$ such that wa is LS, we need to determine the shortest BS factor containing wa as a prefix. This is easy observing Figure 3.3.

Let us comment Figure 7.3, which illustrates the derivation of explicit values of edge labels of reduced Rauzy graphs $\tilde{\Gamma}_l,\ l \in \{|z_n|, \dots, |z_{n+1}|\},\ n \geq 2$.

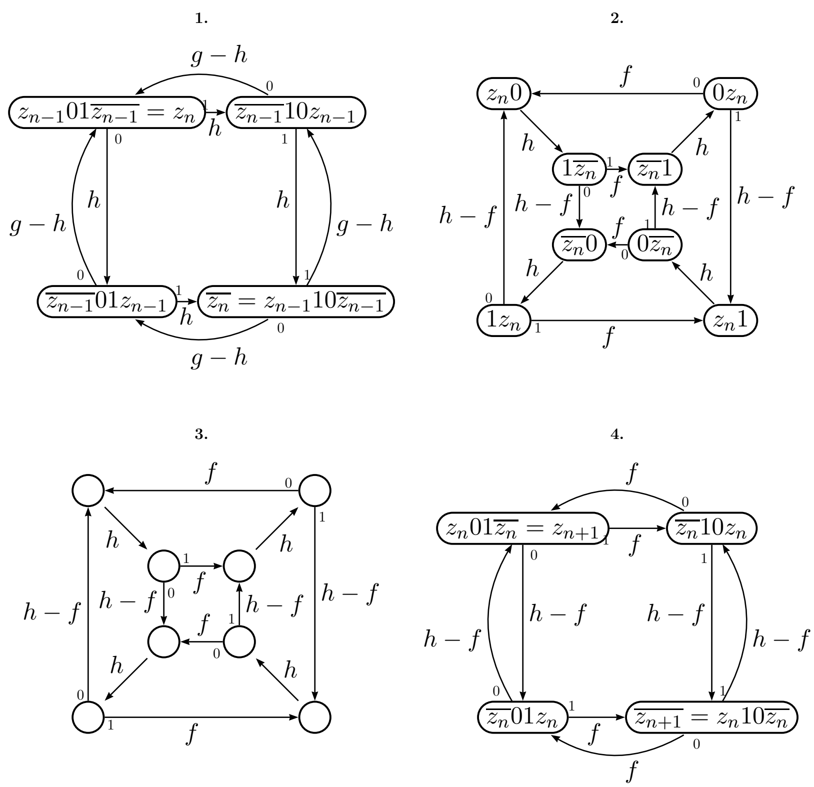


Fig. 7.3: Reduced Rauzy graphs $\tilde{\Gamma}_l$ of z for $l \in \{|z_n|, \dots, |z_{n+1}|\},\ n \geq 2$.

1. For $l = |z_n|$, denote by $g := \rho(z_n)$. There are four vertices in the reduced Rauzy graph- BS factors z_n, $\overline{z_n}$, $\overline{z_{n-1}}01z_{n-1}$, and $\overline{z_{n-1}}10z_{n-1}$. Observing the factorization of z in (3.25), it is straightforward to set the edges in the graph. Let us denote by h the label of the edge $z_n \to \overline{z_{n-1}}10z_{n-1}$. Since $\overline{z_{n-1}}10z_{n-1}$ is a weak BS factor, each time we arrive in $\overline{z_{n-1}}10z_{n-1}$ taking the edge $z_n \to \overline{z_{n-1}}10z_{n-1}$, we have no choice (since $1\overline{z_{n-1}}10z_{n-1}$ can only be followed by 1) and we have to take the edge $\overline{z_{n-1}}10z_{n-1} \to \overline{z_n}$. Consequently, the label of the edge $\overline{z_{n-1}}10z_{n-1} \to \overline{z_n}$ is h. As $\mathcal{L}(z)$ is closed under reversal, we deduce that the labels of $\overline{z_{n-1}}01z_{n-1} \to \overline{z_n}$ and $z_n \to \overline{z_{n-1}}01z_{n-1}$ are also equal to h. Using Proposition 7.4.1, we learn that frequencies of all vertices are equal to g. Kirchhoff's law says that the sum of the labels of edges ending, respectively starting in any vertex equals g. Thus, summing the labels of edges ending, respectively starting in $\overline{z_{n-1}}01z_{n-1}$ and $\overline{z_{n-1}}10z_{n-1}$, we learn that the labels of remaining edges are equal to $g-h$. By Kirchhoff's law applied on the edges starting in z_n, we learn that $h = \frac{1}{2}g$. Consequently, there is only one edge label $\frac{1}{2}g$ in the reduced Rauzy graph.

2. For $l = |z_n| + 1$, since z_n and $\overline{z_n}$ are strong BS factors, there are eight vertices. Edges are again easy to derive observing factorization of z in (3.25). Let us denote by $f := \rho(0z_n0)$, then we obtain, by Kirchhoff's law, the edge labels of $\tilde{\Gamma}_l$: $h,\ f,\ h - f$.

3. For $|z_n| + 1 < l < |z_{n+1}|$, by Corollary 2.2.6, the edge labels do not change.

4. For $l = |z_{n+1}|$, observing Figure 3.3, we see that the edges labeled by h become vertices. By the weakness of $\overline{z_n}01z_n$, we learn that $f = \frac{1}{2}h$.

Let us resume the obtained result on the factor frequencies in the following theorem.

Theorem 7.4.2. *Let z be the infinite word defined in* (3.23)*. Then, for every $n \geq 2$, we have*

$$\{\rho(e) \mid e \in \mathcal{L}_{l+1}(z)\} = \begin{array}{ll} \{\frac{1}{2}g\} & \textit{for } l = |z_n|, \\ \{\frac{1}{2}g,\ \frac{1}{4}g\} & \textit{for } |z_n| < l < |z_{n+1}|, \end{array}$$

where $g = \rho(z_n) = \frac{1}{2^{n+3}}$.

Chapter 8

Balance property

In general, it is a difficult task to determine the minimal constant c for which an infinite word is c-balanced (for a definition see Section 2.2.7). The pioneers in the study of balances were Hedlund and Morse – they proved in particular that aperiodic balanced words coincide with Sturmian words (Theorem 2.4.1). Linearly recurrent AR words are known to be c-balanced for some c. However, this statement cannot be generalized for all AR words since the authors of [31] have proved that for every $c \in \mathbb{N}$, one can construct an AR word which is not c-balanced. Adamczewski [1] has studied c-balanced fixed points of primitive substitutions. He has shown that if u is a fixed point of a primitive substitution, then u is c-balanced for some constant c if all eigenvalues of the substitution matrix different from the Perron-Frobenius eigenvalue λ are in modulus < 1.

In case of infinite words u_β associated with quadratic Parry numbers β, thanks to the above mentioned result of Adamczewski, we know that every u_β is c-balanced for some c. The evaluation of the constant c is so far the least studied among combinatorial problems considered for infinite words u_β. According to Remark 2.3.4, u_β is balanced if and only if β is a quadratic unit. For infinite words u_β associated with quadratic simple Parry numbers β, i.e., having the Rényi expansion of unity of the form $d_\beta(1) = pq,\ p \geq q \geq 1$, Turek in [106] has found the smallest possible c such that u_β is c-balanced; this value is $c = 1 + \lfloor \frac{p-1}{p-q+1} \rfloor$. For other types of irrational algebraic numbers β, the balance property has not been described yet.

In this chapter, we prove that u_β is $\lceil \frac{p-1}{q} \rceil$-balanced for β being a quadratic non-simple Parry number. We show that this is optimal – it cannot be lowered. Our method might be applied also for the study of balances of infinite words associated with Parry numbers of a higher degree.

8.1 u_β associated with quadratic non-simple Parry numbers

We restrict ourselves to infinite words u_β associated with non-unit quadratic non-simple Parry numbers, i.e., fixed points of substitutions $\varphi : 0 \to 0^p1,\ 1 \to 0^q1,\ 1 \leq q < p-1$.

As the first step, we find two infinite words whose prefixes of length n are factors of u_β and contain the maximal number of letters 0 (u_β turns out to have this property), respectively the maximal number of letters 1 (we denote w_β the corresponding infinite word), among all factors of u_β of length n.

Secondly, we choose suitable subsequences of prefixes of u_β and w_β so that these two subsequences $\left(u_\beta^{(n)}\right)_{n=1}^{\infty}$ and $\left(w_\beta^{(n)}\right)_{n=1}^{\infty}$ fully determine the balance property of u_β.

Finally, the study of the behavior of the sequence $\left(|w_\beta^{(n)}|_1 - |u_\beta^{(n)}|_1\right)_{n=1}^{\infty}$ results in the determination of the minimal constant c such that u_β is c-balanced.

Proposition 8.1.1. *Any prefix of u_β contains at least the same number of letters 0 as any other factor of the same length.*

Proof. We prove the statement by contradiction. Let us assume that there exist some $k \in \mathbb{N}$ and a factor $v = v_0 v_1 v_2 \cdots v_{k-1}$ of u_β such that $|u|_0 < |v|_0$, where $u = u_0 u_1 u_2 \cdots u_{k-1}$ is the prefix of u_β of length k. We choose the minimal k with this property. Then

$$|u|_0 + 1 = |v|_0. \tag{8.1}$$

Obviously, u contains some letter 1, therefore, it has the whole factor 0^p1 as its prefix. Since k is minimal, $u_{k-1} = 1$ and $v_0 = v_{k-1} = 0$. Observation 3.4.1 together with $u_{k-1} = 1$ imply that 0^q1 is a suffix of u. Then 0^{q+1} is both a prefix and a suffix of v due to the minimality of k. We again apply Observation 3.4.1 to deduce that there are uniquely determined integers j and ℓ satisfying $0 \le j \le p-q-1$, $0 \le \ell \le p-q-1$ such that $10^j v 0^\ell 1$ is a factor of u_β.

According to Observation 3.4.2, there exists a unique interpretation $(u', 0, 0)$ of u and two interpretations $(0v', p, 0)$ and $(1v', q, 0)$ of $10^j v 0^\ell 1$. In other words, there exists a factor u' of u_β such that $u = \varphi(u')$ and a factor v' of u_β such that $10^j v 0^\ell 1 = 1\varphi(v')$. As $\{\varphi(0), \varphi(1)\}$ is a prefix code, u' is a prefix of u_β.

If we rewrite Equation (8.1) equivalently as $|u|_1 = |v|_1 + 1$, we obtain $|\varphi(v')|_1 = |\varphi(u')|_1$, and, therefore, $|u'| = |v'|$. However, as the word $\varphi(v')$ is longer than $\varphi(u')$, already v', a shorter factor than v, satisfies $|v'|_0 > |u'|_0$, which contradicts the minimality of k. $\square$

Next, we want to find an infinite word w_β whose prefixes contain the maximal number of letters 1. For this purpose, let us introduce a sequence of factors of u_β and let us observe some of its properties. We define the sequence $\left(w_\beta^{(n)}\right)_{n=1}^{\infty}$ by

$$\begin{aligned} w_\beta^{(1)} &= 1 \\ w_\beta^{(n)} &= 1\varphi(w_\beta^{(n-1)}) \quad \text{for } n \ge 2. \end{aligned} \tag{8.2}$$

According to Item *1.* of Lemma 3.4.3, the words $w_\beta^{(n)}$ are factors of u_β.

Lemma 8.1.2. *For all $n \in \mathbb{N}$,*

$$w_\beta^{(n+1)} = w_\beta^{(n)} u^{(n)} 1,$$

where $u^{(n)}$ is a prefix of u_β.

Proof. Let us proceed by induction on n. For $n = 1$, we have $w_\beta^{(2)} = 1\varphi(w_\beta^{(1)}) = 10^q1 = w_\beta^{(1)} 0^q 1$, i.e., $u^{(1)} = 0^q$. Assume for some $n \ge 2$ that $w_\beta^{(n)} = w_\beta^{(n-1)} u^{(n-1)} 1$, where $u^{(n-1)}$ is a prefix of u_β. Then

$$w_\beta^{(n+1)} = 1\varphi(w_\beta^{(n)}) = w_\beta^{(n)} u^{(n)} 1\,,$$

where $u^{(n)} = \varphi(u^{(n-1)})0^q$ is a prefix of u_β according to Observation 3.4.1. $\square$

Lemma 8.1.2 guarantees that $w_\beta^{(n)}$ is a prefix of $w_\beta^{(n+1)}$ and the sequence $\left(|w_\beta^{(n)}|\right)_{n=1}^{\infty}$ is strictly increasing, thus

$$w_\beta = \lim_{n\to\infty} w_\beta^{(n)} \tag{8.3}$$

is a well defined infinite word on $\{0, 1\}$.

It follows from the definition of $w_\beta^{(n)}$ that this infinite word fulfils

$$w_\beta = 1\varphi(w_\beta). \tag{8.4}$$

Proposition 8.1.3. *Any prefix of w_β contains at least the same number of letters 1 as any other factor of the same length.*

Proof. We prove the statement by contradiction. The ideas are analogous to those ones from the proof of Proposition 8.1.1. Let us assume that there exist some $k \in \mathbb{N}$ and a factor $v = v_0 v_1 v_2 \cdots v_{k-1}$ of u_β such that $|w|_1 < |v|_1$, where $w = w_0 w_1 w_2 \cdots w_{k-1}$ is the prefix of w_β of length k. We choose the minimal k with this property. Then

$$|v|_1 = |w|_1 + 1. \tag{8.5}$$

The minimality of k implies that $v_0 = v_{k-1} = 1$, and $w_{k-1} = 0$. The fact that w is a prefix of w_β, which satisfies (8.4), implies $w_0 = 1$.

Observation 3.4.1 together with $v_{k-1} = 1$ implies that $0^q 1$ is a suffix of v. Due to the minimality of k, the factor w has 0^{q+1} as a suffix.

Applying again Observation 3.4.1, there is a uniquely determined integer j satisfying $0 \leq j \leq p - q - 1$ such that $w0^j 1$ is a factor of u_β.

Observation 3.4.2 guarantees that there exist two interpretations $(0w', p, 0)$ and $(1w', q, 0)$ of $w0^j1$. In other words, $w0^j1 = 1\varphi(w')$ for a unique factor w' of u_β. Moreover, since $\{\varphi(0), \varphi(1)\}$ is a prefix code, the factor w' is a prefix of w_β. Similarly, v has two interpretations $(0v', p, 0)$ and $(1v', q, 0)$. Hence, $v = 1\varphi(v')$ for a factor v' of u_β.

Taking into account Equation (8.5), it follows that $\varphi(v')$ and $\varphi(w')$ contain the same number of letters 1, hence, $|v'| = |w'|$. As $\varphi(v')$ is shorter than $\varphi(w')$, the word v', a shorter factor than v, contains more letters 1 than w', which is a contradiction with the minimality of k. □

We have already defined in (8.2) the sequence $\left(w_\beta^{(n)}\right)_{n=1}^{\infty}$. Furthermore, we define $\left(u_\beta^{(n)}\right)_{n=1}^{\infty}$ by

$$u_\beta^{(n)} = \text{prefix of } u_\beta \text{ of length } |w_\beta^{(n)}|.$$

Let us show that these sequences fully determine the minimal constant c such that u_β is c-balanced.

Lemma 8.1.4. *Let v, v' be factors of u_β of the same length k, let n be a positive integer such that $|w_\beta^{(n)}| \leq k < |w_\beta^{(n+1)}|$. Then*

$$\big||v|_1 - |v'|_1\big| \leq |w_\beta^{(n)}|_1 - |u_\beta^{(n)}|_1.$$

Proof. Propositions 8.1.1 and 8.1.3 imply

$$\big||v|_1 - |v'|_1\big| \leq |w|_1 - |u|_1,$$

where u and w are prefixes of u_β and w_β, respectively, of length k.

Lemma 8.1.2 together with the assumption $k < |w_\beta^{(n+1)}|$ implies that $w = w_\beta^{(n)}\hat{u}$ for some prefix $\hat{u}$ of u_β. Let us write the factor u in the form $u = u_\beta^{(n)}\hat{v}$. Using Proposition 8.1.1, we get

$$|w|_1 - |u|_1 = |w_\beta^{(n)}|_1 - |u_\beta^{(n)}|_1 + |\hat{u}|_1 - |\hat{v}|_1 \leq |w_\beta^{(n)}|_1 - |u_\beta^{(n)}|_1\,,$$

which concludes the proof of the statement. □

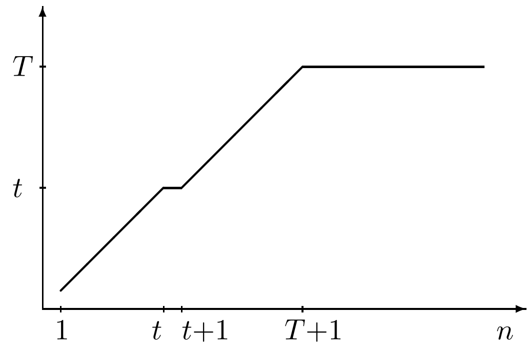


Fig. 8.1: Illustration of the sequence $(D_n)_{n=1}^{\infty}$, where $D_n = |w_\beta^{(n)}|_1 - |u_\beta^{(n)}|_1$. The consecutive values are connected with a line and $t := \lfloor \frac{p+q}{q+1} \rfloor$ and $T = \lceil \frac{p-1}{q} \rceil$.

Lemma 8.1.4 enables us to deduce the optimal balance bound of u_β by investigation of the sequence $(D_n)_{n=1}^{\infty}$, where

$$D_n := |w_\beta^{(n)}|_1 - |u_\beta^{(n)}|_1.$$

The optimal balance bound c is then equal

$$c = \max\{D_n \mid n \in \mathbb{N}\}. \tag{8.6}$$

In the sequel, we show that the sequence $(D_n)_{n=1}^{\infty}$ has the form depicted in Figure 8.1, which proves that u_β is $\lceil \frac{p-1}{q} \rceil$-balanced and that this bound cannot be diminished.

To determine the value of D_{n+1} using the value of $D_n = |w_\beta^{(n)}|_1 - |u_\beta^{(n)}|_1$, it is important to take into account the following obvious facts.

1. Since the number of letters 0 in the word $u_\beta^{(n)}$ is by D_n greater than in $w_\beta^{(n)}$, the length of $\varphi(u_\beta^{(n)})$ is by $(p-q)D_n$ letters greater than the length of $\varphi(w_\beta^{(n)})$.
2. $w_\beta^{(n+1)} = 1\varphi(w_\beta^{(n)})$.
3. $u_\beta^{(n+1)}$ is a prefix of u_β chosen so that $|u_\beta^{(n+1)}| = |w_\beta^{(n+1)}|$.
4. Since u_β is the fixed point of the substitution, $\varphi(u_\beta^{(n)})$ is a prefix of u_β as well.
5. $u_\beta^{(n+1)}$ can be obtained from $\varphi(u_\beta^{(n)})$ by erasing its suffix of length $(p-q)D_n - 1$.
6. As the lengths of $w_\beta^{(n)}$ and $u_\beta^{(n)}$ are the same, $\varphi(w_\beta^{(n)})$ and $\varphi(u_\beta^{(n)})$ contain the same number of letters 1.

These six simple facts imply the following recurrence relation for the sequence $(D_n)_{n=1}^{\infty}$:

$$D_{n+1} = 1 + |v|_1\,, \quad \text{where } v \text{ is a suffix of } \ \varphi(u_\beta^{(n)}) \ \text{ and } \ |v| = (p-q)D_n - 1. \tag{8.7}$$

Consequently, to determine the value of D_{n+1}, one needs to know the form of the suffix of $\varphi(u_\beta^{(n)})$, hence the form of the suffix of $u_\beta^{(n)}$.

Proposition 8.1.5. *Let u_β be the fixed point of the substitution φ defined by $\varphi(0) = 0^p1$, $\varphi(1) = 0^q1$, where $p - 1 > q \geq 1$, and let $t = \lfloor \frac{p+q}{q+1} \rfloor$ and $T = \lceil \frac{p-1}{q} \rceil$.*

1. *If $n \leq t$, then $D_n = n$ and $u_\beta^{(n)}$ has the suffix 0^n.*
2. *If $t+1 \leq n \leq T+1$, then $D_n = n-1$ and $u_\beta^{(n)}$ has the suffix $0^p10^{(n-1)(q+1)-p}$.*
3. *If $T+1 \leq n$, then $D_n = T$ and $u_\beta^{(n)}$ has the suffix 0^{T-1}.*

Proof. Let us show the statement by induction on $n \in \mathbb{N}$. Let $n = 1$, then $w_\beta^{(1)} = 1, u_\beta^{(1)} = 0$, hence, we have $D_1 = |w_\beta^{(1)}|_1 - |u_\beta^{(1)}|_1 = 1$.

Let us suppose that for some n, $1 < n \leq t-1$, it holds

$$D_n = n \text{ and } u_\beta^{(n)} \text{ has the suffix } 0^n.$$

We apply the rule (8.7) to calculate D_{n+1}. The word $\varphi(u_\beta^{(n)})$ has the suffix

$$\varphi(0^n) = \underbrace{(0^p1)\dots(0^p1)}_{n \text{ times}}.$$

We erase from this word of length $(p+1)n$ the suffix v of length $(p-q)n-1$. Let us show that in this procedure, we have erased all n letters 1, i.e., $|v|_1 = n$, and, consequently, $D_{n+1} = 1+n$. To verify this statement, it suffices to prove the inequality

$$(p+1)(n-1)+1 \leq (p-q)n-1, \tag{8.8}$$

which is equivalent with $n \leq \frac{p+q}{q+1} - 1$. Since n is an integer, the inequality means $n \leq \lfloor \frac{p+q}{q+1} \rfloor - 1 = t-1$, which is in accordance with the induction hypothesis. Now, we have to show that at least $n+1$ letters remain in the word $\varphi(0^n)$ after removing the suffix v of length $(p-q)n-1$, i.e., we have to verify $(p+1)n - (p-q)n + 1 \geq n+1$. This inequality is easy to check.

Let us show how *2.* follows from *1.* For $n = t$, *1.* implies that

$$D_t = t \;\text{ and } u_\beta^{(t)} \;\text{ has the suffix } 0^t.$$

Clearly,

$$\varphi(0^t) = \underbrace{(0^p1)\dots(0^p1)}_{t \text{ times}}$$

is a suffix of $\varphi(u_\beta^{(t)})$.

In order to prove $D_{t+1} = t$, we have to show that the suffix of length $(p-q)D_t - 1 = (p-q)t-1$ of the word $\varphi(0^t)$ contains exactly $t-1$ letters 1. So we have to prove

$$(p+1)(t-2)+1 \leq (p-q)t-1 \leq (p+1)(t-1),$$

or, equivalently, $\frac{p}{q+1} \leq t \leq \frac{2p}{q+1}$, which is a consequence of the definition of t.

By erasing the suffix v, we have removed $t-1$ letters 1 from the word $\varphi(0^t)$ which has t letters 1. The remaining part of this word (and therefore the suffix of $u_\beta^{(t+1)}$) is 0^p10^r, where $r = (p+1)(t-1) - |v| = (q+1)t - p$.

Now, suppose that for some $t+1 < n \leq T$, it holds

$$D_n = n-1 \text{ and } u_\beta^{(n)} \;\text{ has the suffix } 0^p10^{(n-1)(q+1)-p}.$$

Then $\varphi(u_\beta^{(n)})$ has the suffix

$$\varphi(0^p 1 0^{(n-1)(q+1)-p}) = \underbrace{(0^p1)\dots(0^p1)}_{p \text{ times}}\, 0^q 1 \underbrace{(0^p1)\dots(0^p1)}_{(n-1)(q+1)-p \text{ times}}.$$

We want to prove that the suffix v of $\varphi(u_\beta^{(n)})$ of length $(p-q)(n-1)-1$ satisfies $|v|_1 = n-1$ and that $u_\beta^{(n+1)}$ has the suffix $0^p 1 0^{n(q+1)-p}$. Before writing down the inequalities to be shown, notice the following two facts. If we erase v from the end of $\varphi(u_\beta^{(n)})$, we erase necessarily $0^q 1 \underbrace{(0^p1)\dots(0^p1)}_{(n-1)(q+1)-p \text{ times}}$. To see this, it suffices to prove the inequality (easily feasible using (8.12))

$$(q+1) + (p+1)\big((n-1)(q+1)-p\big) \le (p-q)(n-1)-1. \tag{8.9}$$

At the same time, if we erase v from the end of $\underbrace{(0^p1)\dots(0^p1)}_{p \text{ times}}\, 0^q 1 \underbrace{(0^p1)\dots(0^p1)}_{(n-1)(q+1)-p \text{ times}}$, it still keeps a prefix longer than $p+1$. This follows from the following inequality (easy to check)

$$(p-q)(n-1)-1 < (p+1)(p-1) + (q+1) + (p+1)\big((n-1)(q+1)-p\big). \tag{8.10}$$

Knowing the relations (8.9) and (8.10), what we have to show are the following two inequalities

$$(q+1)+(n-3)(p+1)+1 \le (p-q)(n-1)-1 \le (q+1)+(n-2)(p+1)-\big(n(q+1)-p\big). \tag{8.11}$$

The first one shows that $|v|_1 \ge n-1$, while the second one shows that $|v|_1 \le n-1$ and that $u_\beta^{(n+1)}$ has the suffix $0^p 1 0^{n(q+1)-p}$. As it is easily verified for positive integers a, b

$$\left\lceil \frac{a}{b} \right\rceil \le \frac{a}{b} + \frac{b-1}{b}\,,$$

we get

$$T = \left\lceil \frac{p-1}{q} \right\rceil \le \frac{p-1}{q} + \frac{q-1}{q} = \frac{p+q-2}{q}\,. \tag{8.12}$$

The first inequality in (8.11) is equivalent with $n \le \frac{2p}{q+1}$. Since $n \le T \le \frac{p+q-2}{q}$ it is enough to verify that $\frac{p+q-2}{q} \le \frac{2p}{q+1}$, which is equivalent with $(q+1)(q-2) \le p(q-1)$. This equation holds because in our substitution $p > q+1$. The second inequality in (8.11) is trivial.

Finally, let us show how *3.* follows from *2.* For $n = T+1$, *2.* implies that

$$u_\beta^{(n)} \text{ has the suffix } 0^{T-1} \text{ and } D_n = T. \tag{8.13}$$

Consequently, the word $\varphi(u_\beta^{(n)})$ has the suffix

$$\varphi(0^{T-1}) = \underbrace{(0^p1)(0^p1)\dots(0^p1)}_{(T-1) \text{ times}}.$$

We erase from this word the suffix v of length $(p-q)T-1$. Performing this procedure, we have erased all the letters 1, i.e., $T-1$ letters 1. To verify this statement, it suffices to prove the inequality

$$(p+1)(T-2)+1 \le (p-q)T-1. \tag{8.14}$$

In order to prove that, by erasing v, there are still at least $T-1$ letters left in the word $\varphi(0^{T-1})$, one has to show

$$T - 1 \leq (p+1)(T-1) - (p-q)T + 1. \tag{8.15}$$

Consequently, if we verify the inequalities (8.14) and (8.15), it will be proved that $D_{n+1} = T$ and $u_\beta^{(n+1)}$ has the suffix 0^{T-1}. It means, by virtue of (8.13), for an index $n \geq T+1$, we have shown the virtue for the index $n+1$, thus, using induction, for all $n \geq T+1$.

The inequality (8.14) holds because it is equivalent with $T \leq \frac{2p}{q+1}$. The inequality (8.15) is equivalent with $T \geq \frac{p-1}{q}$, which is evidently satisfied as $T = \lceil \frac{p-1}{q} \rceil$.

□

As an immediate consequence of Proposition 8.1.5 and the relation (9.8), we have the following essential theorem.

Theorem 8.1.6. *Let u_β be the fixed point of the substitution φ defined by $\varphi(0) = 0^p1$, $\varphi(1) = 0^q1$, where $p-1 > q \geq 1$. Then the infinite word u_β is c-balanced, where $c = \lceil \frac{p-1}{q} \rceil$. This value c is the smallest possible.*

Chapter 9

Arithmetics of $\mathbb{Z}_\beta$

In this chapter, we come back to the study of arithmetical properties of β-integers as introduced in Section 2.1.6. We pursue two objectives. The first one is to determine the maximal number $L_\oplus(\beta)$ of β-fractional positions, which may arise as a result of addition of two β-integers, provided the β-expansion of the sum is finite. The second aim is to point out how arithmetics can be in service of combinatorics and vice versa. In particular, we stress the closeness of balances of u_β and the upper and lower bound on $L_\oplus(\beta)$, for β being a quadratic non-simple Parry number.

9.1 Arithmetics of $\mathbb{Z}_\beta$ for quadratic non-simple Parry numbers

The aim of this section is to improve the upper bound on $L_\oplus(\beta)$ for a quadratic non-simple Parry number β having the Rényi expansion of unity equal to $d_\beta(1) = pq^\omega$ for $q \leq p-1$. In the case of $q = p-1$, β is a quadratic unit, as explained in Section 2.3.4. For quadratic units, it is shown in [26] that $L_\oplus(\beta) = L_\otimes(\beta) = 1$. We will therefore restrict ourselves to the case of $q < p-1$. In [65], one can find the following estimates

$$L_\oplus(\beta) \leq 3(p+1)\ln(p+1) \quad \text{and} \quad L_\otimes(\beta) \leq 4(p+1)\ln(p+1).$$

We derive an improved upper bound

$$L_\oplus(\beta) \leq \lceil \tfrac{p}{q} \rceil.$$

The shortest and lexicographically smallest sequences of coefficients of β-representations that do not fulfill the Parry condition (2.6), in the case of β being a quadratic non-unit non-simple Parry number, are the words

$$(p+1) \text{ and } pq^s(q+1), \text{ where } s \geq 0.$$

Using the equation $\beta^2 = (p+1)\beta - (p-q)$, one can easily obtain:

$$(p+1)\bullet = 10\bullet(p-q) \tag{9.1}$$

$$pq^s(q+1)\bullet = 10^{s+2}\bullet(p-q) \tag{9.2}$$

Note that the β-representations on the right-hand side of the equations are the β-expansions.

For a given finite β-representation of a number x, we apply these rules in such a way that the left side of (9.1) and (9.2) is replaced by the right side of (9.1) and (9.2), respectively. Applying these rules, we obtain a β-representation of x which is greater with respect to the radix order, and, at the same time, the sum of coefficients in the new β-representation is reduced. It follows that repeating rules (9.1) and (9.2) finitely many times, it is possible to transform any finite β-representation of x into the β-expansion of x (which is the greatest β-representation of x with respect to the radix order, as shown in Section 2.1.2).

Example: $(p+2)q(q+1)\bullet \;=\; (p+1)00\bullet \;+\; 1q(q+1)\bullet \;=\; 10(p-q)0\bullet \;+\; 1q(q+1)\bullet \;=\; 11p(q+1)\bullet \;=\; 1200\bullet(p-q)$

On the other hand, rules (9.1) and (9.2) raise the number of positions on the right-hand side of the fractional point $\bullet$. It means that the number of fractional positions in the β-expansion of x is greater than or equal to the number of fractional positions in any β-representation of x.

Observation 9.1.1. *If $x, y \geq 0$ and $x, y \in Fin(\beta)$, then $fp_\beta(x+y) \geq fp_\beta(x)$.*

The following lemma is the most important tool to estimate $L_\oplus(\beta)$.

Lemma 9.1.2. *Let $x_k x_{k-1} \cdots x_0\bullet$ be the β-expansion of a positive β-integer x and let $l \in \mathbb{N}_0$. Then either $x + \beta^l \in \mathbb{Z}_\beta$ or there exists $s \geq l$ such that*

$$\langle x+\beta^l\rangle_\beta = \begin{cases} x_k \cdots (x_{s+1}+1)0^{s+1}\bullet(p-q) & \text{for } l=0,\\ x_k \cdots (x_{s+1}+1)0^{s-l+1}(x_{l-1}-q)\cdots(x_1-q)(x_0-q-1)\bullet(p-q) & \text{for } l \geq 1.\end{cases}$$

Proof. Let $l = 0$. Suppose that $x + \beta^0 = x + 1 \notin \mathbb{Z}_\beta$. Then $x_k x_{k-1} \cdots (x_0+1)\bullet$ is not a β-expansion of $x+1$. Therefore, it has a suffix of the form $(p+1)$ or $pq^{s-1}(q+1)$, where $s \geq 1$. Applying (9.1), resp. (9.2), the β-representation of $x+1$ can be rewritten as

$$x_k x_{k-1} \cdots x_1(p+1)\bullet \;=\; x_k \cdots x_2(x_1+1)0\bullet(p-q)$$

or

$$x_k x_{k-1} \cdots x_{s+1} p q^{s-1}(q+1)\bullet \;=\; x_k \cdots (x_{s+1}+1)0^{s+1}\bullet(p-q).$$

Now, since $x_k \cdots x_1 p$, respectively $x_k \cdots x_{s+1} p q^s$, fulfills the Parry condition, we have $x_1 < p$, respectively $x_{s+1} < p$. It is thus readily seen that the expressions on the right-hand side fulfill the Parry condition (2.6), i.e., they are already the β-expansions.

Let now $l \geq 1$. Suppose that $x + \beta^l \notin \mathbb{Z}_\beta$. Clearly $l \leq k$. Then

$$x_k \cdots x_{l+1}(x_l+1)x_{l-1}\cdots x_0 \tag{9.3}$$

does not fulfill the Parry condition (2.6). This implies that x_l takes one of three values:

(a) $x_l = q-1$, (b) $x_l = p$, (c) $x_l = q$.

(a) Let $x_l = q-1$. Denote $s = \min\{i > l \mid x_i = p\}$. Obviously, $x_i = q$ for all i such that $s > i > l$. Necessarily, $x_{s+1} < p$. Suppose that for all $i < l$, it holds $x_i \geq q$ and $x_0 \geq q+1$. Then we can apply (9.2) for rearranging the β-representation of $x + \beta^l$ in the following way:

$$\begin{gathered} x_k \cdots x_{s+1} p q^{s-l} x_{l-1} \cdots x_0\bullet \;=\\ (x_{l-1}-q)\cdots(x_1-q)(x_0-q-1)\bullet \;+\; x_k \cdots x_{s+1} p q^{s-1}(q+1)\bullet \;=\\ (x_{l-1}-q)\cdots(x_1-q)(x_0-q-1)\bullet \;+\; x_k \cdots (x_{s+1}+1)0^{s+1}\bullet(p-q) \;=\\ x_k \cdots (x_{s+1}+1)0^{s-l+1}(x_{l-1}-q)\cdots(x_1-q)(x_0-q-1)\bullet(p-q)\end{gathered}$$

Since the latter expression fulfills the Parry condition (2.6), we have obtained the β-expansion of $x + \beta^l$. It remains to show that the conditions $x_0 \geq q+1$ and $x_i \geq q$ for all

$i < l$ are satisfied, in other words, that we had a right to the above rearranging. Firstly, we prove by contradiction that $x_i \geq q$ for all $i < l$. Denote by i_0 the maximal index smaller than l such that $x_{i_0} \leq q - 1$. Then, denote by j_0 the minimal index greater than i_0 such that $x_{j_0} \geq q + 1$. Such an index exists because (9.3) does not fulfill the Parry condition (2.6). Hence, the string (9.3) has the following form:

$$x_k \cdots x_{s+1} p q^{s-l} x_{l-1} \cdots x_{j_0+1} x_{j_0} q^{j_0-i_0-1} x_{i_0} x_{i_0-1} \cdots x_0,$$

where $x_{l-1}, \ldots, x_{j_0} \geq q$. Using (9.2), we get the β-representation of $x + \beta^l$ in the form:

$$x_k \cdots (x_{s+1}+1) 0^{s-l+1} (x_{l-1}-q) \cdots (x_{j_0+1}-q)(x_{j_0}-q-1) p q^{j_0-i_0-2} x_{i_0} x_{i_0-1} \cdots x_0 \bullet$$

if $j_0 > i_0 + 1$, and

$$x_k \cdots (x_{s+1}+1) 0^{s-l+1} (x_{l-1}-q) \cdots (x_{j_0+1}-q)(x_{j_0}-q-1)(x_{i_0}+p-q) x_{i_0-1} \cdots x_0 \bullet$$

if $j_0 = i_0 + 1$. In both cases, these β-representations are already the β-expansions, thus we get a contradiction with the fact that $x + \beta^l \notin \mathbb{Z}_\beta$.

Secondly, we show that $x_0 \geq q + 1$. We prove it again by contradiction. Suppose that $x_0 = q$. Then there exists $t \geq 1$ such that q^t is a suffix of the string $x_k \cdots x_0$. Consider the maximal t with this property. Then the β-representation of $x + \beta^l$ has the following form:

$$x_k \cdots x_{s+1} p q^{s-l} x_{l-1} \cdots x_{t+1} x_t q^t \bullet$$

where $x_i \geq q$ for all $i \in \{t+1, \ldots, l-1\}$ and $x_t \geq q + 1$. Applying (9.2), we can rewrite the β-representation as

$$x_k \cdots (x_{s+1}+1) 0^{s-l+1} (x_{l-1}-q) \cdots (x_{t+1}-q)(x_t-q-1) p q^{t-1} \bullet$$

This β-representation is the β-expansion, which is a contradiction with $x + \beta^l \notin \mathbb{Z}_\beta$.

(b) Let $x_l = p$. Then $x_{l+1} < p$ and $x_{l-1} \leq q$. Using (9.1), we obtain

$$x_k \cdots x_{l+1}(p+1) x_{l-1} \cdots x_0 \bullet \;=\; x_k \cdots (x_{l+1}+1) 0 (x_{l-1}+p-q) x_{l-2} \cdots x_0 \bullet \tag{9.4}$$

Since $x_l x_{l-1} \cdots x_0 = p x_{l-1} \cdots x_0 \prec p q^\omega$, we have $x_{l-1} \cdots x_0 \prec q^\omega$, and, consequently, $(x_{l-1}+p-q) x_{l-2} \cdots x_0 \prec p q^\omega$. Thus, the expression on the right-hand side of (9.4) is already the β-expansion of $x + \beta^l$, which is a contradiction with $x + \beta^l \notin \mathbb{Z}_\beta$.

(c) Let $x_l = q$. Since addition of 1 to the l^{th} coefficient x_l breaks the Parry condition, there exists $t \geq l$ such that $x_k \cdots x_0 = x_k \cdots x_{t+1} p q^{t-l} x_{l-1} \cdots x_0$. The β-representation of $x + \beta^l$, equal to $x_k \cdots x_{t+1} p q^{t-l-1} (q+1) x_{l-1} \cdots x_0 \bullet$, can be rewritten, using (9.2), as

$$x_k \cdots (x_{t+1}+1) 0^{t-l+1} (x_{l-1}+p-q) x_{l-2} \cdots x_0 \bullet$$

which is already the β-expansion of $x + \beta^l$. Thus, we arrive again at a contradiction with $x + \beta^l \notin \mathbb{Z}_\beta$. $\square$

Proposition 9.1.3. *Let $x, y \in \mathbb{Z}_\beta$, $x \geq y \geq 0$, and let all coefficients in the β-expansion of y be $\leq q$. Then the β-fractional part of $x + y$ is either 0 or $\frac{p-q}{\beta}$.*

Proof. We proceed by induction on the positive elements of $\mathbb{Z}_\beta$. Let $x_k \dots x_0 \bullet$ be the β-expansion of x.

For $y \in \{1, \dots, q\}$, it follows from Lemma 9.1.2 that either $x + i \in \mathbb{Z}_\beta$ for all $i \leq q$ or one can find the minimal $i \in \{1, \dots, q\}$ such that $\langle x+i \rangle_\beta = x_k \cdots (x_{s+1}+1)0^{s+1} \bullet (p-q)$. In the latter case, it is clear that also $x + j$, where $j \in \{i+1, \dots, q\}$, has the fractional part $\frac{p-q}{\beta}$.

Let $y \geq q+1$, $\langle y \rangle_\beta = y_l y_{l-1} \cdots y_0 \bullet$, where $y_l \geq 1$ and $y_i \leq q$ for all $i \in \{0, \dots, l\}$. If $x + \beta^l \in \mathbb{Z}_\beta$, then $x + y = \tilde{x} + \tilde{y}$, where $\tilde{x} = x + \beta^l$ and $\tilde{y} = y - \beta^l$, and the statement follows by applying the induction hypothesis on $\tilde{y} = y - \beta^l < y$. If $x + \beta^l \notin \mathbb{Z}_\beta$, then using Lemma 9.1.2, we obtain

$$x+y = x+\beta^l+(y-\beta^l) = x_k \cdots (x_{s+1}+1)0^{s-l}(y_l-1)(x_{l-1}+y_{l-1}-q)\cdots(x_0+y_0-q-1) \bullet (p-q) \tag{9.5}$$

Moreover, $y_l - 1 \leq q-1$ and $(x_{l-1}+y_{l-1}-q)\cdots(x_0+y_0-q-1) \preceq x_{l-1}\cdots x_0$. Consequently, the right-hand side of (9.5) is already the β-expansion of $x+y$. □

It is known that if $d_\beta(1)$ is infinite, then the set $Fin(\beta)$ is not closed under subtraction of positive elements. In our case, we have for instance: $\beta - 1 = (p-1) \bullet q^\omega$.

Lemma 9.1.4. *Let $x \geq y \geq 0$, $x, y \in \mathbb{Z}_\beta$, then $x - y \in \mathbb{Z}_\beta$ or $x - y \notin Fin(\beta)$.*

Proof. To prove this statement by contradiction, assume that the β-expansion of $x-y$ is finite, but $x-y$ is not a β-integer, i.e., $fp_\beta(x-y) \geq 1$. Observation 9.1.1 implies that $fp_\beta(x) = fp_\beta(x-y+y) \geq fp_\beta(x-y) \geq 1$, which is a contradiction with $x \in \mathbb{Z}_\beta$. □

Theorem 9.1.5. *Let β be a non-simple Parry number with the Rényi expansion of unity $d_\beta(1) = pq^\omega$, $p-1 > q \geq 1$. Then $L_\oplus(\beta) \leq \lceil \frac{p}{q} \rceil$.*

Proof. Let $x, y \in \mathbb{Z}_\beta$ and $x, y \geq 0$. If $x - y \in Fin(\beta)$, then necessarily $fp_\beta(x-y) = 0$, as we have mentioned in Lemma 9.1.4. Consequently, it suffices to consider the addition $x + y$. Without loss of generality, we can limit our considerations to the case $x \geq y$. Clearly, y can be written as

$$y = y^{(1)} + y^{(2)} + \cdots + y^{(s)},$$

where $s \leq \lceil \frac{p}{q} \rceil$ and the coefficients of $y^{(i)}$ are $\leq q$ for all $i = 1, \dots, s$. According to Proposition 9.1.3, if we add to a number of $Fin(\beta)$ a β-integer with coefficients $\leq q$, the length of the fractional part increases at most by 1. This proves the statement. □

As an immediate consequence of the previous proof, we have the following corollary.

Corollary 9.1.6. *Let $x, y \in \mathbb{Z}_\beta$ and $x, y \geq 0$. Then there exists $\varepsilon \in \{0, 1, \dots, \lceil \frac{p}{q} \rceil\}$ such that*

$$x + y \in \mathbb{Z}_\beta + \varepsilon\, \frac{p-q}{\beta}.$$

9.2 Arithmetics of $\mathbb{Z}_\beta$ and the balance property of u_β

With the results on arithmetics of $\mathbb{Z}_\beta$ from the previous section in hand, we are able to illustrate how closely the arithmetical and combinatorial properties of $\mathbb{Z}_\beta$ are related. Particularly, we deduce an upper bound on the constant c such that u_β is c-balanced, which turns out to be very close to the optimal value of c given in Theorem 8.1.6.

Conversely, employing the optimal value of c from Theorem 8.1.6, we obtain a lower bound on $L_\oplus(\beta)$. In consequence, the characteristics $L_\oplus(\beta)$ are determined with accuracy of ± 1 for quadratic non-simple Parry numbers β.

9.2.1 Almost optimal balance bound on u_β

Proposition 9.2.1. *The infinite word u_β is $\lceil \frac{p}{q} \rceil$-balanced. Moreover, the number of letters 0 in any prefix of u_β is greater than or equal to the number of letters 0 in any other factor of u_β of the same length.*

Proof. Let w be a factor of u_β of length n and u be the prefix of u_β of the same length. Find β-integers x and y, $x < y$, such that the sequence of distances between neighboring β-integers in the segment of $\mathbb{Z}_\beta$ from x to y corresponds to the factor w. We recall that $\Delta_0 = 1$ and $\Delta_1 = \beta - p = 1 - \frac{p-q}{\beta}$. Clearly,

$$y = x + |w|_0 \Delta_0 + |w|_1 \Delta_1. \tag{9.6}$$

The prefix u corresponds to the β-integer

$$z = |u|_0 \Delta_0 + |u|_1 \Delta_1. \tag{9.7}$$

Corollary 9.1.6 implies that there exists $\hat{z} \in \mathbb{Z}_\beta$ such that

$$x + z = \hat{z} + \varepsilon \frac{p-q}{\beta} = \hat{z} + \varepsilon(\Delta_0 - \Delta_1), \text{ for some } \varepsilon \in \{0, 1, \ldots, \lceil \tfrac{p}{q} \rceil\}. \tag{9.8}$$

Since $y, \hat{z} \in \mathbb{Z}_\beta$, it is possible to express the distance between y and $\hat{z}$ as a combination of the lengths Δ_0 and Δ_1, i.e., there exist $L, M \in \mathbb{N}_0$ such that

$$\hat{z} - y = \pm(L\Delta_0 + M\Delta_1). \tag{9.9}$$

Using (9.6), (9.7), and (9.8), we get

$$\begin{aligned} \hat{z} - y = x + z - \varepsilon(\Delta_0 - \Delta_1) - x - |w|_0\Delta_0 - |w|_1\Delta_1 = \\ (|u|_0 - |w|_0 - \varepsilon)\Delta_0 + (|u|_1 - |w|_1 + \varepsilon)\Delta_1 = \\ (|u|_0 - |w|_0 - \varepsilon)\Delta_0 - (|u|_0 - |w|_0 - \varepsilon)\Delta_1 \end{aligned} \tag{9.10}$$

In the last equation, we have used the fact that the factors w and u have the same lengths, and, consequently, $|u|_0 + |u|_1 = |w|_0 + |w|_1$. As $\Delta_0 = 1$ and $\Delta_1 = 1 - \frac{p-q}{\beta}$ are linearly independent over $\mathbb{Q}$, the expression of $\hat{z} - y$ in (9.10) as their integer combination is unique. Since L, M are non-negative, from (9.9) and (9.10) it follows that $|u|_0 - |w|_0 - \varepsilon = 0$, i.e.,

$$|u|_0 = |w|_0 + \varepsilon,$$

where $\varepsilon \in \{0, 1, \ldots, \lceil \frac{p}{q} \rceil\}$, which proves both statements of the proposition. $\square$

Notice that the optimal constant c such that u_β is c-balanced, determined to be $c = \lceil \frac{p-1}{q} \rceil$ in Theorem 8.1.6, is smaller by 1 than the upper bound $\lceil \frac{p}{q} \rceil$ from Proposition 9.2.1 only in case when q divides $p - 1$, otherwise both upper bounds coincide. In addition, the proof of Proposition 9.2.1 is more elegant than the techniques used for proving Proposition 8.1.1.

9.2.2 Lower bound on $L_\oplus(\beta)$

For the derivation of a lower bound on $L_\oplus(\beta)$, we make use of the optimality of the balance bound $c = \lceil \frac{p-1}{q} \rceil$ from Theorem 8.1.6. We apply the fact that there exist a factor w and a prefix u of u_β of the same length such that $|u|_0 = |w|_0 + \lceil \frac{p-1}{q} \rceil$. Let x, y be β-integers, $x < y$, such that the distances between consecutive β-integers in the segment from x to y correspond to the word w. Furthermore, let $z \in \mathbb{Z}_\beta$ be the β-integer corresponding to the prefix u. Then

$$x + z = y + \left\lceil \frac{p-1}{q} \right\rceil (\Delta_0 - \Delta_1) = y + \left\lceil \frac{p-1}{q} \right\rceil \frac{p-q}{\beta}.$$

From Observation 9.1.1, it follows that

$$fp_\beta(x+z) = fp_\beta\left(y + \left\lceil \tfrac{p-1}{q} \right\rceil \tfrac{p-q}{\beta}\right) \geq fp_\beta\left(\left\lceil \tfrac{p-1}{q} \right\rceil \tfrac{p-q}{\beta}\right) \geq fp_\beta\left(\left\lfloor \tfrac{p-1}{q} \right\rfloor \tfrac{p-q}{\beta}\right). \tag{9.11}$$

Now, we verify that $fp_\beta\left(\lfloor \frac{p-1}{q} \rfloor \frac{p-q}{\beta}\right) = \lfloor \frac{p-1}{q} \rfloor$.

Lemma 9.2.2. *For $j = 1, \ldots, \lfloor \frac{p-1}{q} \rfloor$, the β-expansion of the number $j\frac{p-q}{\beta}$ is*

$$\left\langle j\tfrac{p-q}{\beta} \right\rangle_\beta = (j-1) \bullet a_j \cdots a_1\,,$$

where $a_1 := p - q$ and $a_i := (p-1) - iq$ for $i = 2, \ldots, \lfloor \frac{p-1}{q} \rfloor$.

Proof. The numbers a_i are defined so that $a_i \geq 0$ and $(j-1)a_j a_{j-1} \cdots a_1 \prec pq^\omega$. Thus, the expression $(j-1) \bullet a_j \cdots a_1$ is the β-expansion of a positive number. Now, we have to show that

$$j\frac{p-q}{\beta} = j - 1 + \frac{a_j}{\beta} + \frac{a_{j-1}}{\beta^2} + \cdots + \frac{a_1}{\beta^j}.$$

The validity for $j = 1$ is trivial. It is readily seen that if the equality holds for some $j < \lfloor \frac{p-1}{q} \rfloor$, then it holds also for $j + 1$. $\square$

Lemma 9.2.2 shows that $fp_\beta\left(\lfloor \frac{p-1}{q} \rfloor \frac{p-q}{\beta}\right) = \lfloor \frac{p-1}{q} \rfloor$. Applying (9.11), we see that $\lfloor \frac{p-1}{q} \rfloor$ is a lower bound on $L_\oplus(\beta)$. To sum up, we have derived the following theorem.

Theorem 9.2.3. *Let β be a non-simple Parry number with the Rényi expansion of unity $d_\beta(1) = pq^\omega$, $p - 1 > q \geq 1$. Then*

$$\left\lfloor \tfrac{p-1}{q} \right\rfloor \leq L_\oplus(\beta) \leq \left\lceil \tfrac{p}{q} \right\rceil.$$

Let us remark that the difference between the upper bound $\lceil \frac{p}{q} \rceil$ and the lower bound $\lfloor \frac{p-1}{q} \rfloor$ is always 1. Our computer experiments support the conjecture $L_\oplus(\beta) = \lfloor \frac{p-1}{q} \rfloor$.

Chapter 10

Asymptotic behavior of beta-integers for Parry numbers

Parry numbers (defined in Section 2.1.4) give rise to β-integers which realize only a finite number of distances between consecutive elements and are thus in a certain sense closest to ordinary integers. We will illustrate affinity of $\mathbb{N}_0$ and $\mathbb{Z}_\beta^+ = \{b_n \mid n \in \mathbb{N}_0\}$ for β being a Parry number by proving two properties:

1. We will show that $c_\beta := \lim_{n\to\infty} \frac{b_n}{n}$ exists and we will provide a simple formula for c_β.
2. For β being moreover a Pisot number such that its minimal and its Parry polynomial (defined in Section 2.1.4) coincide, we will prove that $(b_n - c_\beta n)_{n\in\mathbb{N}_0}$ is a bounded sequence.

Let us mention that exact formulae for β-integers b_n, and, hence, both of the previous asymptotic characteristics are known for β being a quadratic unit.

Proposition 10.0.4 ([59]). *If β is a quadratic simple Parry unit, then*

$$\mathbb{Z}_\beta^+ = \left\{ b_n = c_\beta n + \frac{1}{\beta}\frac{1-\beta}{1+\beta} + \frac{\beta-1}{\beta}\left\{\frac{n+1}{1+\beta}\right\},\ n\in\mathbb{N}_0 \right\},\ \textit{where}\quad c_\beta = \frac{1+\beta^2}{\beta(1+\beta)}. \tag{10.1}$$

If β is a quadratic non-simple Parry unit, then

$$\mathbb{Z}_\beta^+ = \left\{ b_n = c_\beta n + \frac{1}{\beta}\left\{\frac{n}{\beta}\right\},\ n\in\mathbb{N}_0 \right\},\ \textit{where}\quad c_\beta = 1 - \frac{1}{\beta^2}. \tag{10.2}$$

In order to derive some information about asymptotic properties of β-integers, let us recall the essential relation between a β-integer b_n and its coding by a prefix of the associated infinite word u_β (for the definition of u_β and the associated substitution see Section 2.3.1) revealed by Fabre [49].

Proposition 10.0.5. *Let u_β be the infinite word associated with a Parry number β, and let φ be the associated substitution of β, then, for every β-integer b_n, it holds*

$$\langle b_n\rangle_\beta = a_{k-1}\dots a_1a_0\bullet \quad\Longleftrightarrow\quad \varphi^{k-1}(0^{a_{k-1}})\dots\varphi(0^{a_1})0^{a_0}\ \textit{is a prefix of } u_\beta \textit{ of length } n.$$

Since every prefix of u_β codes a β-integer b_n, Proposition 10.0.5 implies the following corollary.

Corollary 10.0.6. *Let w be a prefix of u_β, then there exist $k \in \mathbb{N}$ and $a_0,\ a_1, \dots, a_{k-1} \in \mathbb{N}_0$ such that*

$$w = \varphi^{k-1}(0^{a_{k-1}}) \dots \varphi(0^{a_1})0^{a_0},$$

where $a_{k-1} \dots a_1 a_0 \bullet$ is the β-expansion of a β-integer.

Let us denote $B_i := |\varphi^i(0)|$. Then $(B_i)_{i\in\mathbb{N}_0}$ is a canonical numeration system associated with the Parry number β (defined and called β-numeration system by Bertrand [19] and studied by Fabre [49]). For details on numeration systems consult [84]. Lemma 10.0.5 implies that the greedy representation of an integer n in this system is given by

$$n = \sum_{i=0}^{k-1} a_i B_i \quad \text{if} \quad b_n = \sum_{i=0}^{k-1} a_i \beta^i.$$

Applying (2.19), the sequence $(B_i)_{i=0}^{\infty}$ may be expressed employing the substitution matrix M of φ defined in (2.18) in the following way

$$B_i = \begin{pmatrix} 1, & 0, & \dots, & 0 \end{pmatrix} M^i \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}. \tag{10.3}$$

10.1 Simple Parry numbers

Let β be a simple Parry number (for the definition see Section 2.3.1). Then the Rényi expansion of unity is of the form $d_\beta(1) = t_1 t_2 \dots t_m$ and β is the largest root of the Parry polynomial $p(x) = x^m - (t_1 x^{m-1} + t_2 x^{m-2} + \dots + t_{m-1}x + t_m)$. Let us recall that $p(x)$ may be reducible.

Our first aim is to confirm existence and to provide a simple formula for the constant c_β such that $b_n \sim c_\beta n$. For any root γ of the Parry polynomial $p(x)$, it is easy to verify that $(\gamma^{m-1},\ \gamma^{m-2}, \dots, \gamma,\ 1)$ is a left eigenvector of the substitution matrix M associated with γ. (Notice that the Parry polynomial and the characteristic polynomial coincide in this case.) On the other hand, according to Section 2.2.13 (Perron-Frobenius theorem), the unique positive left eigenvector $(\rho_0, \rho_1, \dots, \rho_{m-1})$ of M associated with β, fulfilling $\sum_{i=0}^{m-1} \rho_i = 1$, satisfies that ρ_i is the frequency of letter i in u_β. Combining the two previous facts, we obtain for the letter frequencies the following formula:

$$\rho_i = \frac{\beta^{m-1-i}}{\sum_{i=0}^{m-1} \beta^i}. \tag{10.4}$$

Let $(\Delta_0,\ \Delta_1, \dots, \Delta_{m-1})$ be the right eigenvector of M associated with β such that $\Delta_0 = 1$, then it is easy to verify that Δ_i is the distance between consecutive β-integers which is coded by letter i in the infinite word u_β (see the formula for distances in (2.8)). For our purposes, the following easily derivable formula for distances will be useful:

$$\Delta_i = \beta^i - \sum_{j=1}^{i} t_j \beta^{i-j}, \quad i \in \{0, 1, \dots, m-1\}. \tag{10.5}$$

Theorem 10.1.1. *Let $p(x)$ be the Parry polynomial of a simple Parry number β. Then*

$$c_\beta := \lim_{n\to\infty} \frac{b_n}{n} = \frac{\beta - 1}{\beta^m - 1} p'(\beta).$$

Proof. Let us denote by u the prefix of u_β of length n, then

$$b_n = |u|_0\Delta_0 + |u|_1\Delta_1 + \cdots + |u|_{m-1}\Delta_{m-1}.$$

Since frequencies of letters exist, $\lim_{n\to\infty}\frac{b_n}{n}$ exists and obeys the following formula

$$\lim_{n\to\infty}\frac{b_n}{n} = \rho_0\Delta_0 + \rho_1\Delta_1 + \cdots + \rho_{m-1}\Delta_{m-1}.$$

Applying (10.4) and (10.5), we obtain

$$\begin{aligned}
\lim_{n\to\infty}\tfrac{b_n}{n} &= \tfrac{1}{\sum_{i=0}^{m-1}\beta^i}\left(\sum_{i=0}^{m-1}\beta^{m-1-i}(\beta^i - \sum_{j=1}^{i} t_j\beta^{i-j})\right)\\
&= \tfrac{1}{\sum_{i=0}^{m-1}\beta^i}\left(m\beta^{m-1} - \sum_{j=1}^{m-1} t_j \sum_{i=j}^{m-1}\beta^{m-1-j}\right)\\
&= \tfrac{1}{\sum_{i=0}^{m-1}\beta^i}\left(m\beta^{m-1} - \sum_{j=1}^{m-1} t_j (m-j)\beta^{m-1-j}\right)\\
&= \tfrac{p'(\beta)}{\sum_{i=0}^{m-1}\beta^i} = \tfrac{\beta-1}{\beta^m-1}p'(\beta).
\end{aligned}$$

□

Corollary 10.1.2. *Let the roots $\beta=\beta_1,\beta_2,\ldots,\beta_m$ of the Parry polynomial $p(x)$ of a simple Parry number β be mutually different. Then*

$$\lim_{n\to\infty}\frac{b_n}{n} = \frac{\beta-1}{\beta^m-1}\prod_{k=2}^{m}(\beta-\beta_k).$$

Proof. $p(x)=\prod_{i=1}^m(x-\beta_i)$, $p'(x)=\sum_{k=1}^m\prod_{i=1,i\neq k}^m(x-\beta_i)$, thus $p'(\beta)=\prod_{i=2}^m(\beta-\beta_i)$. □

Remark 10.1.3. *If $p(x)$ is an irreducible polynomial, then β is an algebraic integer of order m and $\beta_2,\ldots,\beta_m$ are algebraic conjugates of β, and hence mutually different.*

Secondly, we will study the asymptotic behavior of the sequence $(b_n - c_\beta n)_{n\in\mathbb{N}_0}$. We know already that the limit $\lim_{n\to\infty}\frac{b_n}{n}$ exists. Therefore, the limit of any subsequence exists and takes the same value. In particular,

$$\lim_{n\to\infty}\frac{b_n}{n} = \lim_{n\to\infty}\frac{b_{B_n}}{B_n} = \lim_{n\to\infty}\frac{\beta^n}{B_n}.$$

Under the assumption that all roots of $p(x)$ are mutually different, we will find a useful expression for B_n. Since M is diagonalizable, there is a transition matrix, say P, satisfying

$$PMP^{-1} = \begin{pmatrix} \beta_1 & 0 & 0 & \ldots & 0\\ 0 & \beta_2 & 0 & \ldots & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & 0 & \ldots & \beta_m \end{pmatrix}.$$

Using (10.3), we may write

$$B_n = (1,\ 0,\ldots,0)P^{-1}\begin{pmatrix} \beta_1^n & 0 & 0 & \ldots & 0\\ 0 & \beta_2^n & 0 & \ldots & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & 0 & \ldots & \beta_m^n \end{pmatrix} P \begin{pmatrix} 1\\ 1\\ \vdots\\ 1\end{pmatrix}. \tag{10.6}$$

It follows from the Perron-Frobenius theorem that $\beta > |\beta_i|$, hence, the formula (10.6) leads to the following expression

$$\frac{1}{c_\beta} = \lim_{n\to\infty}\frac{B_n}{\beta^n} = (1,\ 0,\dots,0)P^{-1}\begin{pmatrix} 1 & 0 & 0 & \dots & 0\\ 0 & 0 & 0 & \dots & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & 0 & \dots & 0\end{pmatrix} P \begin{pmatrix}1\\1\\ \vdots\\1\end{pmatrix}. \tag{10.7}$$

Now, let us turn our attention to the difference $b_n - c_\beta n$.

Let $\langle b_n\rangle_\beta = a_{k-1}\dots a_0\bullet$, thus $b_n = \sum_{i=0}^{k-1} a_i\beta^i$ and $n = \sum_{i=0}^{k-1} a_i B_i$. Employing (10.6) and (10.7), we obtain

$$\frac{1}{c_\beta}b_n - n = \sum_{i=0}^{k-1} a_i (1,\ 0,\dots,0)P^{-1}\left(\begin{pmatrix} \beta_1^i & 0 & 0 & \dots & 0\\ 0 & 0 & 0 & \dots & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & 0 & \dots & 0\end{pmatrix} - \begin{pmatrix} \beta_1^i & 0 & 0 & \dots & 0\\ 0 & \beta_2^i & 0 & \dots & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & 0 & \dots & \beta_m^i\end{pmatrix}\right) P \begin{pmatrix}1\\1\\ \vdots\\1\end{pmatrix} =$$

$$= (1,\ 0,\dots,0)P^{-1}\begin{pmatrix} 0 & 0 & 0 & \dots & 0\\ 0 & -z_2 & 0 & \dots & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & 0 & \dots & -z_m\end{pmatrix} P \begin{pmatrix}1\\1\\ \vdots\\1\end{pmatrix}, \tag{10.8}$$

where $z_j = \sum_{i=0}^{k-1} a_i\beta_j^i$. If we assume that β is a Pisot number, i.e., $|\beta_j| < 1$ for $j = 2,3,\dots,m$, and since the coefficients of β-expansion satisfy $a_i \in \{0,\dots,\lfloor\beta\rfloor\}$, it follows

$$|z_j| \le \sum_{i=0}^{k-1}|a_i||\beta_j^i| \le \frac{\beta}{1-|\beta_j|}. \tag{10.9}$$

Remark 10.1.4. *Suppose that the Parry polynomial $p(x)$ of a Parry number β is reducible, say $p(x) = q(x)\Delta r(x)$, where $q(x)$ is the minimal polynomial of β, and $r(x)$ is a polynomial of degree at least 1. Then the product of the roots of $r(x)$ is an integer and therefore either all roots of $r(x)$ lie on the unit circle or at least one among the roots of $r(x)$ is in modulus larger than 1. It implies that the set of z_j is bounded for all j if and only if β is a Pisot number and its Parry polynomial is the minimal polynomial of β.*

According to Remark 10.1.4 and as P does not depend on n, we have shown the following theorem.

Theorem 10.1.5. *Let β be a simple Parry number. If β is moreover a Pisot number and the Parry polynomial of β is its minimal polynomial, then $(b_n - c_\beta\, n)_{n\in\mathbb{N}}$ is a bounded sequence.*

Now, the transition matrix P can be chosen as follows

$$P = \begin{pmatrix} \beta^{m-1} & \beta^{m-2} & \dots & \beta & 1\\ \beta_2^{m-1} & \beta_2^{m-2} & \dots & \beta_2 & 1\\ \vdots & \vdots & \ddots & \vdots & \vdots\\ \beta_m^{m-1} & \beta_m^{m-2} & \dots & \beta_m & 1\end{pmatrix}, \text{then}\quad P\begin{pmatrix}1\\1\\ \vdots\\1\end{pmatrix} = \begin{pmatrix}\frac{1-\beta^m}{1-\beta}\\ \frac{1-\beta_2^m}{1-\beta_2}\\ \vdots\\ \frac{1-\beta_m^m}{1-\beta_m}\end{pmatrix}. \tag{10.10}$$

In order to have, for every $n \in \mathbb{N}_0$, an explicit formula for $\frac{1}{c_\beta}b_n - n$, it remains to determine $(1,\ 0,\dots,0)P^{-1}$, i.e., the first row of P^{-1}. Since $P^{-1} = \frac{1}{\det P}P^{adj}$, where $(P^{adj})_{1j} =$

$(-1)^{1+j}\det P(j,1)$ and $P(j,1)$ is obtained from P erasing the j-th row and the 1-st column, applying Vandermonde's result, we get

$$(P^{-1})_{1j} = \frac{(-1)^{1+j}\prod_{i<k,\ i,k\neq j}(\beta_i-\beta_k)}{\prod_{i<k}(\beta_i-\beta_k)} = \frac{1}{\prod_{k\neq j}(\beta_j-\beta_k)} = \frac{1}{p'(\beta_j)}. \tag{10.11}$$

Notice that since $p(x)$ does not have multiple roots, $p'(\beta_j)\neq 0$. It follows from formulae (10.8), (10.10), and (10.11) that

$$\frac{1}{c_\beta}b_n - n = \sum_{j=2}^{m}\frac{-z_j}{p'(\beta_j)}\frac{1-\beta_j^m}{1-\beta_j}. \tag{10.12}$$

In consequence, using the estimate (10.9), we may deduce an upper bound on $|b_n - c_\beta\, n|$

$$|b_n - c_\beta\, n| \leq \quad 2c_\beta\beta\sum_{j=2}^{m}\frac{1}{(1-|\beta_j|)^2}\frac{1}{|p'(\beta_j)|}\,. \tag{10.13}$$

Example 10.1.6. *Let us illustrate previous results for the simplest simple Parry number - the Fibonacci number $\beta=\tau$. Its Rényi expansion of unity is $d_\tau(1)=11$ and its Parry polynomial $p(x)=x^2-x-1$. The substitution matrix for the Fibonacci substitution $\varphi: 0\to 01,\ 1\to 0$ is $M=\begin{pmatrix}1 & 1\\ 1 & 0\end{pmatrix}$, consequently, $(B_n)_{n\in\mathbb{N}_0}$ satisfies $B_n=f_n$ for all $n\in\mathbb{N}_0$, where $(f_n)_{n\in\mathbb{N}_0}$ is the Fibonacci sequence given by*

$$f_{n+1}=f_n+f_{n-1},\ \ f_0=1,\ \ f_1=2.$$

Applying Theorem 10.1.1, we get

$$c_\tau = \frac{\tau-1}{\tau^2-1}p'(\tau) = \frac{p'(\tau)}{\tau+1} = \frac{2\tau-1}{\tau+1} = \frac{\tau^2+1}{\tau(\tau+1)},$$

which is in correspondence with Proposition 10.0.4.

Let us denote the second root of $p(x)$ (the Galois conjugate of τ) by τ', $\tau'=\frac{1-\sqrt{5}}{2}=1/\tau$. If $\langle b_n\rangle_\beta = a_{k-1}\ldots a_1a_0\bullet$, then $a_i\in\{0,1\}$, and, using (10.8), (10.10), and (10.11),

$$b_n - c_\tau\, n = c_\tau\left(\tfrac{1}{2\tau-1},\tfrac{1}{2\tau'-1}\right)\begin{pmatrix}0 & 0\\ 0 & -z_2\end{pmatrix}\begin{pmatrix}1+\tau\\ 1+\tau'\end{pmatrix} = \frac{1-\tau}{\tau(\tau+1)}\sum_{i=0}^{k-1}a_i(\tau')^i.$$

Since $\tau'=\frac{1-\sqrt{5}}{2}$, i.e., $|\tau'|<1$, the sequence $|b_n-c_\tau\, n|_{n\in\mathbb{N}}$ is bounded and we may easily determine an upper bound (taking into account that $\tau'<0$)

$$\frac{1-\tau}{\tau^3} \leq \frac{\tau-1}{\tau(\tau+1)}\sum_{i=1}^{\infty}(\tau')^{2i-1} \leq\ c_\tau\, n - b_n\ \leq \frac{\tau-1}{\tau(\tau+1)}\sum_{i=0}^{\infty}(\tau')^{2i} = \frac{1}{\tau^3},$$

thus, comparing the upper and lower bound, we deduce

$$|b_n - c_\tau\, n| \leq \frac{1}{\tau^3},$$

which is again in correspondence with Proposition 10.0.4, where we have replaced the fractional part $\left\{\frac{n+1}{1+\beta}\right\}$ with 1 in order to get an upper bound on $|b_n-c_\tau\, n|$.

10.2 Non-simple Parry numbers

Let β be a non-simple Parry number (for the definition see Section 2.3.1). Then the Rényi expansion of unity is of the form $d_\beta(1) = t_1 t_2 \dots t_m (t_{m+1} \dots t_{m+p})^\omega$ with m, p chosen to be minimal and β is the largest root of the Parry polynomial $p(x) = (x^p - 1)\left(x^m - t_1 x^{m-1} - \dots - t_m\right) - t_{m+1}x^{p-1} - \dots - t_{m+p-1}x - t_{m+p}$. Let us recall that $p(x)$ may be reducible.

Similarly as in the case of simple Parry numbers, our first goal is to derive a simple formula for the constant c_β such that $b_n \sim c_\beta n$. For any root γ of the Parry polynomial $p(x)$, the vector

$$\big(\underbrace{\gamma^{m-1}(\gamma^p - 1),\ \gamma^{m-2}(\gamma^p - 1), \dots, (\gamma^p - 1)}_{m \text{ components}}, \underbrace{\gamma^{p-1}, \dots, \gamma,\ 1}_{p \text{ components}}\big)$$

is a left eigenvector of the substitution matrix M associated with γ. (Notice that the Parry polynomial and the characteristic polynomial coincide also in this case.) On the other hand, according to Section 2.2.13 (Perron-Frobenius theorem), the unique positive left eigenvector $(\rho_0, \rho_1, \dots, \rho_{m+p-1})$ of M associated with β such that $\sum_{i=0}^{m+p-1} \rho_i = 1$ satisfies that ρ_i is the frequency of letter i in u_β. Combining the two previous facts, we obtain for the letter frequencies the following formula:

$$\rho_i = \frac{\varrho_i}{\sum_{i=0}^{m-1} \beta^i(\beta^p - 1) + \sum_{i=0}^{p-1} \beta^i} = \frac{\varrho_i(\beta - 1)}{\beta^m(\beta^p - 1)}, \tag{10.14}$$

where

$$\begin{aligned} \varrho_i &= \beta^{m-1-i}(\beta^p - 1) && \text{for } 0 \le i \le m-1, \\ \varrho_i &= \beta^{m+p-1-i} && \text{for } m \le i \le m+p-1. \end{aligned}$$

Let $(\Delta_0,\ \Delta_1, \dots, \Delta_{m+p-1})$ be the right eigenvector of M associated with β such that $\Delta_0 = 1$, then it is easy to verify that Δ_i is the distance between consecutive β-integers which is coded by letter i in the infinite word u_β (see the formula for distances in (2.8)). Similarly as for simple Parry numbers, also for non-simple Parry numbers, the following formula for distances holds and will be useful:

$$\Delta_i = \beta^i - \sum_{j=1}^{i} t_j \beta^{i-j}, \quad i \in \{0, 1, \dots, m+p-1\}. \tag{10.15}$$

Theorem 10.2.1. *Let $p(x)$ be the Parry polynomial of the non-simple Parry number β. Then*

$$c_\beta := \lim_{n\to\infty} \frac{b_n}{n} = \frac{\beta - 1}{\beta^m(\beta^p - 1)} p'(\beta).$$

Proof. Analogously as for simple Parry numbers, $\lim_{n\to\infty} \frac{b_n}{n}$ exists and we have

$$\lim_{n\to\infty} \frac{b_n}{n} = \rho_0\Delta_0 + \rho_1\Delta_1 + \dots + \rho_{m+p-1}\Delta_{m+p-1}.$$

Applying (10.14) and (10.15), we obtain $\lim_{n\to\infty} \dfrac{b_n}{n} = \dfrac{\beta - 1}{\beta^m(\beta^p - 1)}(A + B)$, where

$$A = \sum_{i=0}^{m-1} \beta^{m-1-i}(\beta^p - 1)\big(\beta^i - \sum_{j=1}^{i} t_j \beta^{i-j}\big) \quad \text{and} \quad B = \sum_{i=m}^{m+p-1} \beta^{m+p-1-i}\big(\beta^i - \sum_{j=1}^{i} t_j \beta^{i-j}\big).$$

It is then straightforward to prove that

$$A = (\beta^p - 1)\big(m\beta^{m-1} - \textstyle\sum_{j=1}^{m-1} t_j(m-j)\beta^{m-j-1}\big),$$

$$B = p\beta^{m+p-1} + p\textstyle\sum_{j=1}^{m-1} t_j\beta^{m+p-1-j} + \sum_{j=1}^{p-1}(p-j)t_{m+j}\beta^{p-j-1},$$

$$A + B = p'(\beta).$$

$\square$

Remark 10.2.2. *If we consider the infinite Rényi expansion of unity $d^*_\beta(1)$ instead of the "classical" Rényi expansion of unity $d_\beta(1)$, we have in the simple case $d^*_\beta(1) = (t_1 \dots t_{m-1}(t_m - 1))^\omega$, thus the length l of the preperiod is 0 and the length L of the period is m, and in the non-simple case, $d^*_\beta(1) = d_\beta(1) = t_1t_2 \dots t_m(t_{m+1} \dots t_{m+p})^\omega$, hence the length l of the preperiod is m and the length L of the period is p. With this notation, the formulae for c_β from Theorems 10.1.1 and 10.2.1 may be rewritten, for both simple and non-simple Parry numbers, in a unique way as*

$$c_\beta = \frac{\beta - 1}{\beta^l(\beta^L - 1)} p'(\beta).$$

Corollary 10.2.3. *Let the roots $\beta = \beta_1, \beta_2, \dots, \beta_{m+p}$ of the Parry polynomial $p(x)$ of a non-simple Parry number β be mutually different. Then,*

$$\lim_{n\to\infty} \frac{b_n}{n} = \frac{\beta - 1}{\beta^m(\beta^p - 1)} \prod_{k=2}^{m+p} (\beta - \beta_k).$$

Proof. An analogy of the proof of Corollary 10.1.2. $\square$

Remark 10.2.4. *If $p(x)$ is an irreducible polynomial, then β is an algebraic integer of order $m+p$ and $\beta_2, \dots, \beta_{m+p}$ are algebraic conjugates of β, and hence mutually different.*

Secondly, in an analogous way as in the simple Parry case, we will investigate the asymptotic behavior of the sequence $(b_n - c_\beta n)_{n\in\mathbb{N}_0}$. As we know already that the limit $\lim_{n\to\infty} \frac{b_n}{n}$ exists, we may rewrite it in terms of the subsequence (B_n),

$$\lim_{n\to\infty} \frac{b_n}{n} = \lim_{n\to\infty} \frac{b_{B_n}}{B_n} = \lim_{n\to\infty} \frac{\beta^n}{B_n}.$$

Under the assumption that all roots of $p(x)$ are mutually different, we will express B_n in an easier form. As M is diagonalizable, there is a transition matrix, say P, satisfying

$$PMP^{-1} = \begin{pmatrix} \beta_1 & 0 & 0 & \dots & 0 \\ 0 & \beta_2 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & \beta_{m+p} \end{pmatrix}.$$

Using (10.3), we may write

$$B_n = (1,\ 0, \dots, 0)P^{-1} \begin{pmatrix} \beta_1^n & 0 & 0 & \dots & 0 \\ 0 & \beta_2^n & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & \beta_{m+p}^n \end{pmatrix} P \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}. \tag{10.16}$$

It follows from the Perron-Frobenius theorem that $\beta > |\beta_i|$, hence, the formula (10.16) results in the following expression

$$\frac{1}{c_\beta} = \lim_{n\to\infty} \frac{B_n}{\beta^n} = (1,\ 0,\ldots,0)P^{-1} \begin{pmatrix} 1 & 0 & 0 & \ldots & 0 \\ 0 & 0 & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \ldots & 0 \end{pmatrix} P \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}. \tag{10.17}$$

Now, let us focus our attention on the difference $b_n - c_\beta n$.

Let $\langle b_n\rangle_\beta = a_{k-1}\ldots a_0\bullet$, thus $b_n = \sum_{i=0}^{k-1} a_i\beta^i$ and $n = \sum_{i=0}^{k-1} a_i B_i$. Employing (10.16) and (10.17), we obtain

$$\frac{1}{c_\beta}b_n - n = \sum_{i=0}^{k-1} a_i (1,\ 0,\ldots,0)P^{-1}\left(\begin{pmatrix} \beta_1^i & 0 & 0 & \ldots & 0 \\ 0 & 0 & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \ldots & 0 \end{pmatrix} - \begin{pmatrix} \beta_1^i & 0 & 0 & \ldots & 0 \\ 0 & \beta_2^i & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \ldots & \beta_{m+p}^i \end{pmatrix}\right) P \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} =$$

$$= (1,\ 0,\ldots,0)P^{-1} \begin{pmatrix} 0 & 0 & 0 & \ldots & 0 \\ 0 & -z_2 & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \ldots & -z_{m+p} \end{pmatrix} P \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}, \tag{10.18}$$

where $z_j = \sum_{i=0}^{k-1} a_i\beta_j^i$. If β is a Pisot number, i.e., $|\beta_j| < 1$ for $j = 2, 3, \ldots, m+p$, and since the coefficients of β-expansion satisfy $a_i \in \{0,\ldots,\lfloor\beta\rfloor\}$, we have

$$|z_j| \le \sum_{i=0}^{k-1} |a_i||\beta_j^i| \le \frac{\beta}{1-|\beta_j|}. \tag{10.19}$$

According to Remark 10.1.4 and since P does not depend on n, we have shown the following theorem.

Theorem 10.2.5. *Let β be a non-simple Parry number. If β is moreover a Pisot number and the Parry polynomial of β is its minimal polynomial, then $(b_n - c_\beta\, n)_{n\in\mathbb{N}}$ is a bounded sequence.*

The transition matrix P is in this case equal to

$$P = \begin{pmatrix} \beta^{m-1}(\beta^p-1) & \beta^{m-2}(\beta^p-1) & \ldots & (\beta^p-1) & \beta^{p-1} & \ldots & \beta & 1 \\ \beta_2^{m-1}(\beta_2^p-1) & \beta_2^{m-2}(\beta_2^p-1) & \ldots & (\beta_2^p-1) & \beta_2^{p-1} & \ldots & \beta_2 & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots & & & \\ \beta_{m+p}^{m-1}(\beta_{m+p}^p-1) & \beta_{m+p}^{m-2}(\beta_{m+p}^p-1) & \ldots & (\beta_{m+p}^p-1) & \beta_{m+p}^{p-1} & \ldots & \beta_{m+p} & 1 \end{pmatrix}.$$

Hence,

$$P \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{\beta^m(1-\beta^p)}{1-\beta} \\ \frac{\beta_2^m(1-\beta_2^p)}{1-\beta_2} \\ \vdots \\ \frac{\beta_{m+p}^m(1-\beta_{m+p}^p)}{1-\beta_{m+p}} \end{pmatrix}. \tag{10.20}$$

In order to have, for all $n \in \mathbb{N}$, an explicit formula for $\frac{1}{c_\beta}b_n - n$, it remains to determine $(1,\ 0,\ldots,0)P^{-1}$, i.e., the first row of P^{-1}. By contrast to the simple Parry case, the matrix

P is not in the Vandermonde's form. However, we notice that its determinant is equal to a Vandermonde determinant through a simple addition of columns. More precisely, we start with the addition of the last column to the m-th column, the last but one column to the $(m-1)$-st column and so forth. It is readily seen that this procedure leads after m steps to a Vandermonde matrix of order $m+p$ with the same determinant as P.

So $\det P = \prod_{i<k}(\beta_i - \beta_k)$. The expression of $(P^{-1})_{1j},\ j \in \{1, \ldots, m+p\}$, is then given by

$$(P^{-1})_{1j} = \frac{(-1)^{1+j}\prod_{i<k,\ i,k\neq j}(\beta_i - \beta_k)}{\prod_{i<k}(\beta_i - \beta_k)} = \frac{1}{\prod_{k\neq j}(\beta_j - \beta_k)} = \frac{1}{p'(\beta_j)}. \tag{10.21}$$

Notice that since $p(x)$ does not have multiple roots, $p'(\beta_j) \neq 0$.

We obtain applying expressions (10.18), (10.20), and (10.21)

$$\frac{1}{c_\beta} b_n - n = \sum_{j=2}^{m+p} \frac{-z_j}{p'(\beta_j)} \frac{\beta_j^m (1-\beta_j^p)}{1-\beta_j}. \tag{10.22}$$

In consequence, we may deduce an upper bound on $|b_n - c_\beta\, n|$

$$|b_n - c_\beta\, n| \leq \quad 2c_\beta \beta \sum_{j=2}^{m} \frac{1}{(1-|\beta_j|)^2} \frac{1}{|p'(\beta_j)|}\,. \tag{10.23}$$

Example 10.2.6. *Let us illustrate the previous results for the simplest non-simple Parry number β with the Rényi expansion of unity $d_\beta(1) = 21^\omega$ and the Parry polynomial $p(x) = x^2 - 3x + 1$, i.e., $\beta = \tau^2 = \frac{3+\sqrt{5}}{2}$. The substitution matrix for the associated substitution $\varphi : 0 \to 001,\ 1 \to 01$ is the square of the Fibonacci substitution matrix, i.e., $M_\varphi = \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix}$. Consequently, $(B_n)_{n\in\mathbb{N}}$ is just a subsequence of the Fibonacci sequence $(f_n)_{n\in\mathbb{N}}$ (defined in Example 10.1.6) given by $B_n = f_{2n}$.*

Applying Theorem 10.2.1, we get

$$c_\beta = \frac{\beta - 1}{\beta(\beta-1)} p'(\beta) = \frac{p'(\beta)}{\beta} = \frac{2\beta - 3}{\beta} = 1 - \frac{1}{\beta^2},$$

which is in correspondence with Proposition 10.0.4.

Let us denote the second root of $p(x)$ by β', $\beta' = \frac{3-\sqrt{5}}{2}$. Let $\langle b_n \rangle_\beta = a_{k-1} \ldots a_1 a_0 \bullet$, then $a_i \in \{0, 1, 2\}$ and

$$b_n - c_\beta\, n = c_\beta \left(\tfrac{1}{2\beta-3}, \tfrac{-1}{2\beta'-3}\right) \begin{pmatrix} 0 & 0 \\ 0 & -z_2 \end{pmatrix} \begin{pmatrix} \beta \\ \beta' \end{pmatrix} = \frac{-1}{\beta^2} \sum_{i=0}^{k-1} a_i (\beta')^i.$$

Since $\beta' = \frac{3-\sqrt{5}}{2}$, i.e., $0 < \beta' < 1$, the sequence $(b_n - c_\beta\, n)_{n\in\mathbb{N}}$ is bounded and we may easily determine an upper bound (taking into account that coefficients in β-expansions satisfy the Parry condition)

$$|b_n - c_\beta\, n| \leq \frac{1}{\beta^2}\left(2 + \sum_{i=1}^{\infty} (\beta')^i\right) = \frac{1}{\beta^2}\left(2 + \frac{\beta'}{1-\beta'}\right) = \frac{1}{\beta^2}\left(2 + \frac{1}{\beta - 1}\right) = \frac{1}{\beta}\ ,$$

which is in correspondence with the estimate we get if we replace the fractional part $\left\{\frac{n}{\beta}\right\}$ with 1 in Proposition 10.0.4.

Chapter 11

Schrödinger operators with aperiodic potentials

Schrödinger equation, the fundamental equation of quantum mechanics, was proposed by the Austrian physicist Erwin Schrödinger in 1926. It is also often called the Schrödinger wave equation. It describes how the wavefunction of a quantum mechanical system evolves over time. It is of central importance in non-relativistic quantum mechanics, for both elementary particles, such as electrons, and systems of particles, such as atoms and molecules.

The one-dimensional form of the *Schrödinger equation*, for a single particle of mass m in the presence of potential V, reads:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial^2 x}\psi(x,t) + V(x)\psi(x,t) \equiv (H\psi)(x,t), \tag{11.1}$$

where H is a Hamiltonian operator, called the *Schrödinger operator*, a self-adjoint operator describing the total energy of the system. The Schrödinger equation defines the behavior of ψ, but does not interpret ψ. It was Max Born who introduced a successful interpretation of $|\psi|^2$ as the *probability distribution of the position* of a pointlike object and ψ as the *probability amplitude*.

The most interesting states of any quantum system are those states in which the system has a definite total energy, and it turns out that for these states, the wave function is a standing wave, analogous to the familiar standing waves on a string. For example, a single electron in an unexcited atom is described in quantum mechanics by a static spherically symmetric wave surrounding the nucleus.

When the time-dependent Schrödinger equation is applied to these standing waves, it reduces to a simpler equation called the *time-independent Schrödinger equation*:

$$(H\psi)(x) = -\frac{\hbar^2}{2m}\frac{d^2}{d^2 x}\psi(x) + V(x)\psi(x) = E\psi(x). \tag{11.2}$$

This time-independent equation lets us find the wave functions of the standing waves and the corresponding allowed energies. Possible energies E of the particle in question correspond to the eigenvalues, or, more precisely, to the spectral values (pure point spectrum plus absolutely continuous plus singular continuous spectrum) of the time-independent Schrödinger operator H.

The task to treat the Schrödinger equation, both time-dependent and time-independent, analytically or numerically turns out to be hard. In consequence, discrete approximations are of great importance.

One of the most popular discretization methods is the so-called *tight-binding approximation*. In the tight binding model, it is assumed that the full Hamiltonian H of the system may be approximated by the Hamiltonian H_{at} of an isolated atom centered at each atom. The atomic orbitals Ψ_n, which are eigenfunctions of the single atom Hamiltonian H_{at}, are supposed to be very small at distances exceeding the interatomic distance. This is what is meant by tight-binding. A solution Ψ to the time-independent single electron Schrödinger equation is then assumed to be a linear combination of the atomic orbitals Ψ_n. The search for the appropriate linear combination of the atomic orbitals leads to the study of the *discrete Schrödinger operator* H on $l^2(\mathbb{Z})$ defined by:

$$(H\psi)(n) := \psi(n+1) + \psi(n-1) + \omega_n \psi(n),$$

where $(\omega_n)_{n\in\mathbb{Z}}$ takes only a finite number of values. Notice that this operator is bounded, in contrast to the continuous Schrödinger operator.

The spectral type of the discrete Schrödinger operator H (consult Appendix A) has important consequences for the transport properties of the system: if H has an absolutely continuous spectrum, we expect a conductor, while if H has a pure point spectrum, we expect to have an insulator. The singular continuous spectrum was considered somewhat exotic and it is still much less understood than the other spectral types. However, for aperiodic potentials, a purely singular continuous spectrum occurs quite commonly and it is expected to give rise to interesting new transport phenomena.

In the sequel, we exclusively treat discrete Schrödinger operators, we call them Schrödinger operators for short.

11.1 Schrödinger operators modeling quasicrystals

Since the discovery of quasicrystals, besides searching for appropriate structural models, a lot of effort has been devoted to the study of Schrödinger operators with purely singular continuous spectra, describing the behavior of an electron in one-dimensional quasicrystalline potentials being intermediate between periodic (leading to absolutely continuous spectrum) and disordered (leading to pure point spectrum).

All investigated one-dimensional Schrödinger operators with potentials generated by primitive substitutions exhibit this so far unusual spectral type and it is conjectured that all such operators have purely singular continuous spectra. While the absence of absolutely continuous spectrum has been proved in full generality (Kotani's theory), the absence of pure point spectrum is not understood in similar generality. However, no counterexample is known, so we suppose that the case of our interest – Schrödinger operators with potentials generated by substitutions associated with Parry numbers – will manifest purely singular continuous spectrum.

Since Kotani's theory concerning the absence of absolutely continuous spectrum and the result of Lenz [81] describing the Lebesgue measure and the topology of the spectrum are valid for a larger class of Schrödinger operators than just for the operators with potentials generated by primitive substitutions, we present first a more general framework of ergodic families of Schrödinger operators. Afterwards, we summarize consequences for Schrödinger operators with potentials generated by primitive substitutions and we recall and apply several methods for excluding pure point spectrum – they are based on local symmetries in the potential, i.e., block repetition (Gordon-type arguments) and mirror symmetry (palindromic criteria by Hof *et al.*). Finally, we give a detailed description of a particular case of Schrödinger operators with potentials generated by substitutions associated with Parry numbers.

11.2 Ergodic families of Schrödinger operators

The concept of ergodic families of Schrödinger operators is required for the application of Kotani's theory concerning the absence of absolutely continuous spectrum and of an essential theorem saying that almost all Schrödinger operators belonging to the same ergodic family have the same spectrum and spectral type.

In order to define an ergodic family, we need to introduce some basics from ergodic theory. Let Ω be a compact metric space and let $T : \Omega \to \Omega$ be a homeomorphism. The pair (Ω, T) is called a *topological dynamical system*. Given some $\omega \in \Omega$, the set $\{T^n\omega \mid n \in \mathbb{Z}\}$ is called the *orbit* of ω. Denote by $\mathcal{B}(\Omega)$ the Borel σ-algebra on Ω. A Borel probability measure μ is said to be T-*invariant* if $\mu(T(B)) = \mu(B)$ for every $B \in \mathcal{B}(\Omega)$. A Borel set B is called T-*invariant* if $T(B) = B$. In the field of ergodic theory, the following notions are of particular importance. We call a T-invariant measure *ergodic* if every T-invariant set has measure zero or one. We say that a topological dynamical system (Ω, T) is

- *minimal* if the orbit of every $\omega \in \Omega$ is dense in Ω,
- *uniquely ergodic* if there exists a unique ergodic measure,
- *strictly ergodic* if it is both minimal and uniquely ergodic.

It is well known that if there exists a unique T-invariant measure μ, then μ is ergodic (see [109]).

Given a uniquely ergodic topological dynamical system (Ω, T) and a measurable function $g : \Omega \to \mathbb{R}$, one may associate with every $\omega \in \Omega$ a biinfinite sequence $V_\omega : \mathbb{Z} \to \mathbb{R}$ by $V_\omega(n) = g(T^n\omega)$. This sequence is regarded as the potential of a discrete Schrödinger operator H_ω on $l^2(\mathbb{Z})$ defined by

$$(H_\omega\psi)(n) := \psi(n+1) + \psi(n-1) + V_\omega(n)\psi(n). \tag{11.3}$$

The family $(H_\omega)_{\omega\in\Omega}$ is called an *ergodic family of Schrödinger operators*. Let us admit that ergodic families of Schrödinger operators may be defined also for topological dynamical systems which are not uniquely ergodic, it suffices to fix an ergodic measure. However, the restriction to topological dynamical systems with a unique T-invariant measure suppresses the dependence of ergodic families on the choice of measure and is sufficient for our further purposes.

The following essential theorem by Pastur [93] justifies the choice of this framework stating that the spectrum and the spectral type of Schrödinger operators in an ergodic family are μ-almost surely ω-independent.

Theorem 11.2.1. *Let $(H_\omega)_{\omega\in\Omega}$ be an ergodic family of Schrödinger operators. Then there exist sets $\Omega_0 \subset \Omega$, Σ, Σ_{pp}, Σ_{sc}, $\Sigma_{ac} \subset \mathbb{R}$ such that $\mu(\Omega_0) = 1$ and $\sigma(H_\omega) = \Sigma$, $\sigma_{pp}(H_\omega) = \Sigma_{pp}$, $\sigma_{sc}(H_\omega) = \Sigma_{sc}$, $\sigma_{ac}(H_\omega) = \Sigma_{ac}$ for every $\omega \in \Omega_0$.*

Absolutely continuous spectrum for almost all Schrödinger operators in an ergodic family may be excluded applying Kotani's theory.

Theorem 11.2.2 (Kotani)**.** *Let $(H_\omega)_{\omega\in\Omega}$ be an ergodic family of Schrödinger operators. If the potentials V_ω are aperiodic and take only finitely many values for all $\omega \in \Omega$, then $\Sigma_{ac} = \emptyset$ (keeping the notation from Theorem 11.2.1).*

11.3 Schrödinger operators associated with subshifts

Let us turn our attention to a particular dynamical system – subshift – which allows us, in the special case of minimal subshifts, to strengthen Theorem 11.2.1.

Let $\mathcal{A}$ be an alphabet. We define the *shift* $T : \mathcal{A}^{\mathbb{Z}} \to \mathcal{A}^{\mathbb{Z}}$ by $(T\omega)(n) = \omega_{n+1}$ for $\omega \in \mathcal{A}^{\mathbb{Z}}$. In this context, we recall that $\mathcal{A}^{\mathbb{Z}}$ is a compact metric space (the metric on $\mathcal{A}^{\mathbb{Z}}$ is defined analogously as the metric on $\mathcal{A}^{\mathbb{N}_0}$ given in (10.5); for a precise definition see [83]).

Let Ω be a closed and T-invariant subset of $\mathcal{A}^{\mathbb{Z}}$. Then (Ω, T) is a topological dynamical system, called *subshift*. We will consider subshifts generated as follows. Given an infinite word $u \in \mathcal{A}^{\mathbb{N}_0}$, we define Ω_u to be the set of all biinfinite words whose language is a subset of $\mathcal{L}(u)$, i.e.,

$$\Omega_u = \{\omega \in \mathcal{A}^{\mathbb{Z}} \mid \mathcal{L}(\omega) \subset \mathcal{L}(u)\}.$$

Clearly, Ω_u is closed and T-invariant. Moreover, unique ergodicity and minimality can be characterized in a combinatorial way (see [95]). The subshift (Ω_u, T) is

- uniquely ergodic if and only if frequencies ρ of factors of u exist,
- minimal if and only if u is uniformly recurrent.

In the uniquely ergodic case, the unique T-invariant measure fulfills

$$\mu(\{\omega \in \Omega_u \mid \omega_k \dots \omega_{k+|w|-1} = w\}) = \rho(w)$$

for every $w \in \mathcal{L}(u)$ and for every $k \in \mathbb{Z}$ (in other words, for every cylinder $[w]$ in Ω_u). As cylinders generate the Borel σ-algebra on Ω_u, μ is completely determined by factor frequencies of u.

In correspondence with (11.3), let us define Schrödinger operators with potentials generated by subshifts. Let $\mathcal{A} = \{0, 1, \dots, d\}$ and let u be an infinite word on $\mathcal{A}$ such that frequencies of its factors exist. We define then, for each $\omega = (\omega_n)_{n\in\mathbb{Z}} \in \Omega_u$, a discrete Schrödinger operator H_ω on $l^2(\mathbb{Z})$ by

$$(H_\omega\psi)(n) := \psi(n+1) + \psi(n-1) + \omega_n\psi(n). \tag{11.4}$$

The following strengthening (proved by Reed and Simon in [97] and by Last and Simon in [78]) of Theorem 11.2.1 holds for strictly ergodic subshifts (Ω_u, T).

Theorem 11.3.1. *Let u be a uniformly recurrent infinite word on $\mathcal{A} = \{0, 1, \dots, d\}$ such that frequencies of its factors exist, i.e., (Ω_u, T) is a strictly ergodic subshift. Then there exist sets Σ, $\Sigma_{ac} \subset \mathbb{R}$ such that the ergodic family $(H_\omega)_{\omega\in\Omega_u}$ of Schrödinger operators defined in* (11.4) *satisfies $\sigma(H_\omega) = \Sigma$ and $\sigma_{ac}(H_\omega) = \Sigma_{ac}$ for every $\omega \in \Omega_u$.*

Let us remark that strict ergodicity of a subshift does not imply constancy of its pure point spectrum σ_{pp} or singular continuous spectrum σ_{sc}. Combining Theorem 11.2.2 and Theorem 11.3.1, absolutely continuous spectrum may be excluded for operators with potentials generated by aperiodic minimal subshifts.

Corollary 11.3.2. *Let u be an aperiodic uniformly recurrent infinite word on $\mathcal{A} = \{0, 1, \dots, d\}$ such that frequencies of its factors exist and let $(H_\omega)_{\omega\in\Omega_u}$ be the ergodic family of Schrödinger operators defined in* (11.4)*. Then $\sigma_{ac}(H_\omega) = \emptyset$ for every $\omega \in \Omega_u$.*

In case of linearly recurrent words u, the Lebesgue measure and the topology of the spectrum have been revealed by Lenz [81].

Theorem 11.3.3. *Let u be an aperiodic linearly recurrent infinite word on $\mathcal{A} = \{0, 1, \ldots, d\}$ such that frequencies of its factors exist. Then Σ is a Cantor set of Lebesgue measure zero.*

Let us remark that the assumption of linear recurrence may be replaced by a weaker assumption of uniform positivity of weights, which requires existence of $C > 0$ such that

$$\liminf_{|v| \to \infty,\ v \in \mathcal{L}(u)} \frac{\#\{\text{occurrences of } w \text{ in } v\}}{|v|} |w| \geq C \quad \text{for every } w \in \mathcal{L}(u).$$

However, with respect to our particular interest in potentials generated by primitive substitutions, the restriction to the slightly rougher result provided in Theorem 11.3.3 is sufficient.

11.4 Schrödinger operators with potentials generated by primitive substitutions

Let us first explain why all results from Section 11.3 are valid also for Schrödinger operators with potentials generated by primitive substitutions, and, second, let us list some methods for excluding pure point spectrum.

Ergodic families of Schrödinger operators with potentials generated by primitive substitutions are of the form $(H_\omega)_{\omega \in \Omega_\varphi}$, where φ is a primitive substitution on $\mathcal{A} = \{0, 1, \ldots, d\}$ and $\Omega_\varphi := \Omega_u$ for any fixed point u of φ. This definition is correct since Proposition 2.2.8 says that all fixed points of a primitive substitution have the same language. (Ω_φ, T) is then called a *substitution dynamical system associated to φ*. In reference to Section 2.2.13, fixed points of primitive substitutions are linearly recurrent and frequencies of their factors exist, the following corollary concerning their spectra is deduced combining Theorem 11.3.1, Corollary 11.3.2, and Theorem 11.3.3.

Corollary 11.4.1. *Let φ be a primitive substitution on $\mathcal{A} = \{0, 1, \ldots, d\}$ with aperiodic fixed points and let $(H_\omega)_{\omega \in \Omega_\varphi}$ be the ergodic family of Schrödinger operators with potentials generated by φ. Then the following statements hold:*

- *There exists a Cantor set $\Sigma \subset \mathbb{R}$ of Lebesgue measure zero such that $\sigma(H_\omega) = \Sigma$ for every $\omega \in \Omega_\varphi$.*
- *Absolutely continuous spectrum is empty; that is, $\sigma(H_\omega) = \sigma_{pp}(H_\omega) \cup \sigma_{sc}(H_\omega)$ for every $\omega \in \Omega_\varphi$.*

As a consequence, when studying the spectral type of H_ω, we only need to distinguish between pure point spectrum and singular continuous spectrum. So far, no Schrödinger operators with potentials generated by a primitive substitution with other than purely singular continuous spectra are known. The next part of this section introduces several methods allowing to exclude pure point spectrum for such operators.

Define $\Omega_c := \{\omega \in \Omega_\varphi \mid \sigma_{pp}(H_\omega) = \emptyset\}$. The methods are usually discriminated according to the absence of eigenvalues they provide (see for instance a survey by Damanik [35]). We say that the absence of eigenvalues is:

- *uniform* if $\Omega_c = \Omega_\varphi$,
- *almost sure* if $\mu(\Omega_c) = 1$,
- *generic* if Ω_c is a dense G_δ, i.e., a countable intersection of open sets which is dense in Ω_φ.

The following implications are valid:

$$\text{uniform absence} \quad \Rightarrow \quad \text{almost sure absence} \quad \Rightarrow \quad \text{generic absence.}$$

All known methods for excluding eigenvalues are based either on translation symmetry - block repetition (Gordon type arguments), or based on mirror symmetry - palindromic structure (Hof *et al.* [70]).

Uniform absence of eigenvalues

To get a result on uniform absence of eigenvalues, it is in general necessary to consider each ω individually and to apply pointwise methods. The first method was proposed by Deylon and Petritis [42].

Theorem 11.4.2 (Three-block method)**.** *Assume that there exist $\omega \in \Omega_\varphi$ and a sequence $n_k \to \infty$ satisfying, for every k,*

$$\omega_{j-n_k} = \omega_j = \omega_{j+n_k}, \quad 1 \leq j \leq n_k,$$

then $\sigma_{pp}(H_\omega) = \emptyset$.

Nevertheless, it was shown by Damanik in [37] that the three-block Gordon argument cannot prove more than an almost sure statement in the sense that for every minimal aperiodic subshift Ω, there exists an element $\omega \in \Omega$ such that ω does not have the infinitely many three block structure needed for an application of Theorem 11.4.2.

To present a result of Jitomirskaya and Simon [73], we need to know that $\omega \in \mathcal{A}^\mathbb{Z}$ is called *strongly palindromic* if ω contains palindromes $w^{(i)}$ of length l_i centered at $k_i \to \infty$ such that l_i grows exponentially fast with respect to k_i, i.e., there exists $B > 0$ such that $B^{k_i}/l_i \to 0$.

Theorem 11.4.3. *If $\omega \in \Omega_\varphi$ is strongly palindromic, then $\sigma_{pp}(H_\omega) = \emptyset$.*

Almost sure absence of eigenvalues

Since Ω_c is T-invariant, $\mu(\Omega_c)$ is either 1 or 0 by ergodicity of μ. Hence, for a result on almost sure absence of eigenvalues, it suffices to bound $\mu(\Omega_c)$ by a positive number from below.

Let us denote by $\mathcal{L}(\varphi) := \mathcal{L}(u)$ for any fixed point u of a primitive substitution φ. This definition is correct since all fixed points of a primitive substitution have the same language. The *index* of a factor w in $\mathcal{L}(\varphi)$ is defined by

$$\operatorname{ind}(w) = \sup\{r \in \mathbb{Q} \mid w^r \in \mathcal{L}(\varphi)\}, \tag{11.5}$$

where w^r denotes the word $(xy)^m x$, where $m \in \mathbb{N}$, $w = xy$, and $r = m + |x|/|w|$. The following result is due to Damanik [37].

Theorem 11.4.4. *Let $\mathcal{L}(\varphi)$ contain a factor w with ind$(w) > 3$, then $\mu(\Omega_c) = 1$.*

Generic absence of eigenvalues

In order to establish a result on generic absence of eigenvalues, it is sufficient to exclude eigenvalues for just one $\omega \in \Omega_\varphi$, as claimed by Damanik [35].

Proposition 11.4.5. *If Ω_c is non-empty, then Ω_c is a dense G_δ.*

The first result is based on block repetition and it is a consequence of Theorem 11.4.2 and Proposition 11.4.5.

Corollary 11.4.6 (Three-block method)**.** *Assume that there exist $\omega \in \Omega_\varphi$ and a sequence $n_k \to \infty$ satisfying, for every k,*

$$\omega_{j-n_k} = \omega_j = \omega_{j+n_k}, \quad 1 \leq j \leq n_k,$$

then Ω_c is a dense G_δ.

The second result by Hof *et al.* [70] is based on mirror symmetry.

Theorem 11.4.7. *Let $\mathcal{L}(\varphi)$ contain infinitely many palindromes. Then Ω_c is a dense G_δ.*

11.5 Substitutions associated with Parry numbers

Substitutions associated with Parry numbers have been defined in Section 2.3.2. In both cases – for simple and non-simple Parry numbers – φ is a primitive substitution. In consequence, all results from Section 11.4 hold true, in particular, Corollary 11.4.1 remains valid. Since β-integers having only a finite number of distances between neighbors – which happens solely for Parry numbers β – are considered as appropriate models for one-dimensional quasicrystals, we tend to show that the spectra of Schrödinger operators with potentials generated by substitutions associated with Parry numbers are purely singular continuous.

Let us apply methods excluding pure point spectrum when possible.

Uniform absence of eigenvalues

The spectra of Schrödinger operators with potentials generated by Sturmian sequences are known to be purely singular continuous (proved by Damanik and Lenz [38]). According to Remark 2.3.4, the fixed points of substitutions φ associated with Parry numbers β are Sturmian words if and only if

- β is a simple Parry number with $d_\beta(1) = p1$, $p \in \mathbb{N}$, thus $\varphi(0) = 0^p1,\ \varphi(1) = 0$,
- β is a non-simple Parry number with $d_\beta(1) = p(p-1)^\omega$, thus $\varphi(0) = 0^p1,\ \varphi(1) = 0^{p-1}1$.

Almost sure absence of eigenvalues

For almost sure results, we need to study the index of factors in $\mathcal{L}(\varphi)$, defined by (11.5).

Lemma 11.5.1. *Let $t_1 \geq 2$ in the case of φ associated with simple Parry numbers or $t_1 \geq 3$ in the case of φ associated with non-simple Parry numbers, then $\mathcal{L}(\varphi)$ contains a factor of index > 3.*

Proof. If φ associated with a simple Parry number satisfies $t_1 \geq 2$, then either $t_1 + t_m \geq 4$ and 0000 is a factor of $\mathcal{L}(\varphi)$ with $\mathrm{ind}(0000) = 4$, or $t_1 = 2$ and $t_m = 1$ (since t_m is non-zero and $t_1 \geq t_m$ according to (2.6)), hence $t_1 + t_m = 3$ and $0001 \in \mathcal{L}(\varphi)$. Let $j := \min\{i \geq 1 \mid t_{i+1} > 0\}$. Such j exists since $t_m = 1$. It is readily seen that $\varphi^j(0)\varphi^j(0)\varphi^j(0)0^{t_{j+1}}$ is a factor of $\mathcal{L}(\varphi)$ with index > 3. The proof of the statement for the non-simple Parry case is analogous. ∎

Combining Lemma 11.5.1 with Theorem 11.4.4, we obtain the following corollary.

Corollary 11.5.2. *Let $t_1 \geq 2$ in the case of φ associated with simple Parry numbers or $t_1 \geq 3$ in the case of φ associated with non-simple Parry numbers, then $\mu(\Omega_c) = 1$.*

Generic absence of eigenvalues

In Section 4.2.6, it is shown that $\mathcal{L}(\varphi)$, for a substitution φ associated with a simple Parry number β, contains an infinite number of palindromes if and only if β is a confluent Parry number, i.e., the substitution is of the form

$$\varphi(0) = 0^t 1,\ \varphi(1) = 0^t 2, \ldots,\ \varphi(m-2) = 0^t(m-1),\ \varphi(m-1) = 0^s,$$

where $t \geq s \geq 1$.

Among non-simple Parry numbers, in reference to Section 4.3, there are infinitely many palindromes in $\mathcal{L}(\varphi)$ only for the quadratic case, i.e., if the substitution is of the form

$$\varphi(0) = 0^p 1, \quad \varphi(1) = 0^q 1, \quad p-1 \geq q \geq 1.$$

Combining this fact with Theorem 11.4.7, we deduce the following corollary.

Corollary 11.5.3. *Let φ be a substitution associated with a confluent simple Parry number β or a quadratic non-simple Parry number β, then Ω_c is a dense G_δ in Ω_φ.*

Let us conclude that the spectrum of the Schrödinger operator with potential generated by a substitution associated with a Parry number is purely singular continuous if the fixed point of the substitution is a Sturmian word. On one hand, we are able to say more, on the other hand, there are still many pending cases left. Let us take into account all possible parameters t_i corresponding to a Rényi expansion of unity, i.e., obeying the rule from (2.4). We summarize for which parameters t_i, the pure point spectrum is absent almost surely and generically, and, for which t_i, the problem is still open:

Simple Parry case

- If $t_1 \geq 2$, then the pure point spectrum is almost surely absent.
- If $t_1 = 1 = t_2 = \cdots = t_m$, then the pure point spectrum is generically absent. (In the quadratic case, the absence is even uniform.)
- If $t_1 = 1 = t_m$, and at least one $t_i = 0$, then we do not know.

Non-simple Parry case

- If $t_1 \geq 3$, then the pure point spectrum is almost surely absent.
- If $t_1 = 2$ and $t_2 = 1$, i.e., β is quadratic, then the pure point spectrum is uniformly absent.
- If $t_1 = 2$ and β is at least cubic, then we do not know.

Chapter 12

Diffraction on beta-integers

This closing chapter is devoted to a very important tool for the study of crystalline structure – diffraction of X-rays, electrons, or, neutrons by crystals. We have already pointed out its importance in the introduction. It was the electron diffraction that enabled in 1984 the discovery of quasicrystals. As the diffraction image inherits the symmetries of its atomic pattern, crystallographers observed that periodicity is not necessary for producing Bragg peaks on a diffraction image; periodicity is not equivalent with long range order.

In what follows, we prefer to leave the real word of 3-dimensional atomic structures and to pass instead to the mathematical diffraction on one-dimensional structures (basics summarized in Appendix B), in particular, to a theoretical one-dimensional model of quasicrystals: beta-integers. We tend to summarize briefly all known results that may be possibly applied in order to describe the diffraction spectrum of beta-integers. In addition, we suggest some directions of a further study of diffraction on beta-integers, using the asymptotic behavior of beta-integers deduced in Chapter 10.

12.1 Diffraction on finite and infinite sets

Let us sketch out why diffraction on infinite sets of atoms is described by the Fourier transform of the autocorrelation (defined in Appendix B and denoted ibidem by $\hat{\gamma}$). Consider, in the space, an assembly of N identical structureless atoms at positions $x_1, \ldots, x_N$ on a straight line. This assembly is usually modeled by a bounded measure $\mu_N = \sum_{j=1}^{N} \delta_{x_j}$. If this assembly is irradiated by X-rays, eventually another kind of radiation, then its intensity is given by

$$I_N(K) = \Big|\sum_{j=1}^{N} e^{-2\pi i \langle x_j, K\rangle}\Big|^2,$$

where $K = k' - k$ is the scattering vector and k and k' are the wavevectors of the incident and scattered plane wave, respectively. Note that $I_N = |\hat{\mu}_N|^2 = (\widehat{\mu_N * \tilde{\mu}_N})$. The convolution product $\mu_N * \tilde{\mu}_N$ is known as the "autocorrelation". (Note that the autocorrelation as defined in Appendix B is zero for any bounded measure!) The sequence (I_N) does not converge as $N \to \infty$, not vaguely to a measure and not even in the sense of distributions. In consequence, this notion has to be modified for infinite systems. One considers the sequence (I_N/N), the scattering power per atom. If the infinite system has a unique autocorrelation γ in the sense of Appendix B, then (I_N/N) converges vaguely to $\hat{\gamma}/\gamma(\{0\})$ as $N \to \infty$ (observe that $\gamma(\{0\})$ is the particle density).

Like any positive measure, $\hat{\gamma}$ can have a pure point part, an absolutely continuous part, and a singular continuous part. The pure point part (in addition to the point mass at 0, which is always present) is interpreted as a sign of order, the absolutely continuous part as a sign of disorder, and the singular continuous part as a kind of order between quasiperiodicity and randomness.

12.2 Pure point diffraction and dynamical spectra

Let us only briefly mention a possible reformulation of the problem of proving pure pointedness of a diffraction spectrum. Following the standard method of associating a dynamical system with an aperiodic structure (see for instance [103]), we may deduce some information on the diffraction spectrum of a structure knowing the dynamical spectrum of the associated system.

1. A key observation made by Dworkin [48] is that pure pointedness of a dynamical spectrum implies pure pointedness of the corresponding diffraction spectrum.
2. According to Section 2.2.13, one may associate with every primitive substitution a self-similar Delone set Λ. Then, if the dynamical spectrum of the associated dynamical system is pure point, then the diffraction spectrum of Λ is pure point as well.
3. Much attention is paid to the so-called *Pisot discrete spectrum conjecture* which claims that every Pisot type substitution gives rise to a dynamical system with pure point spectrum. Recently, the case of binary substitutions has been settled affirmatively by Hollander and Solomyak [72]. For more letters, it remains unanswered.

Since the notions of Pisot and Parry numbers coincide in the quadratic case, it is a straightforward consequence of the above listed known results that the diffraction spectrum of $\mathbb{Z}_\beta$ is pure point for every quadratic Parry number β.

12.3 Diffraction on one-dimensional cut and project sets

Cut-and-project sets have been defined in the introduction and their role of suitable models for quasicrystals have been highlighted. It was proved by Hof [68], through the dynamical systems approach, that regular C&P sets have pure point diffraction spectrum.

Let us mention how the diffraction measure of a one-dimensional C&P set Σ looks like. In reference to Section 2.4.4, there exist two distinct irrational parameters ϵ, η and a bounded interval Ω such that

$$\Sigma = \Sigma_{\epsilon,\eta}(\Omega) = \{a + b\eta \mid a, b \in \mathbb{Z},\ a + b\epsilon \in \Omega\}.$$

Applying Hof's result, we learn that the diffraction measure of $\mu = \sum_{x\in\Sigma} \delta_x$ is unique and is given by

$$\hat{\gamma}_\Sigma = \sum_{(a,b)\in\mathbb{Z}^2} |c_{(a,b)}|^2 \delta_{a+b\epsilon},$$

where

$$c_{(a,b)} = \frac{\text{dens}(\Sigma)}{\text{vol}(\Omega)} \int_\Omega e^{2\pi i(a+b\epsilon)y} dy.$$

The density of Σ is defined by $\text{dens}(\Sigma) = \lim_{R\to\infty} \frac{(-R,R)\cap\Sigma}{2R}$. Since the density of Σ is proportional to the volume of Ω, the expression $\frac{\text{dens}(\Sigma)}{\text{vol}(\Omega)}$ depends only on the choice of η, ϵ and is independent from the choice of Ω. This property is related to the uniform distribution of $\pi_2(\mathbb{Z}^2)$ in V_2. We see that the support of the diffraction measure is a dense set. Nevertheless, it holds for any positive constant α that the set of Bragg peaks with intensity greater than α, i.e., $\{a + b\epsilon \mid |c_{(a,b)}|^2 > \alpha\}$, is uniformly discrete.

12.4 Diffraction on beta-integers

Let us first treat such sets $\mathbb{Z}_\beta$ that are close to the C&P sets, i.e., whose non-negative part $\mathbb{Z}_\beta^+$ coincides with the non-negative part of a C&P set. Such numbers β have been determined by Gazeau, Masáková, and Pelantová in [61].

Proposition 12.4.1. *The non-negative part of the set $\mathbb{Z}_\beta$ coincides with the non-negative part of a C&P set $\Sigma_{\epsilon,\eta}(\Omega)$ if and only if β is a quadratic Pisot unit.*

Acording to Remark 2.3.4, there are two types of quadratic Pisot units among Parry numbers:

1. simple Parry numbers β with $d_\beta(1) = p1,\ p \geq 1$,
2. non-simple Parry numbers β with $d_\beta(1) = p(p-1)^\omega,\ p \geq 2$.

The characterization of $\mathbb{Z}_\beta^+$ and $\mathbb{Z}_\beta^-$ in terms of C&P sets from [61] reads,

$$\begin{array}{lll} \text{in the simple Parry case,} & \mathbb{Z}_\beta^+ = \Sigma_{\beta',\beta}(-1,\beta) \cap \mathbb{R}^+, & \mathbb{Z}_\beta^- = \Sigma_{\beta',\beta}(-\beta,1) \cap \mathbb{R}^-, \\ \text{in the non-simple Parry case,} & \mathbb{Z}_\beta^+ = \Sigma_{\beta',\beta}[0,\beta) \cap \mathbb{R}^+, & \mathbb{Z}_\beta^- = \Sigma_{\beta',\beta}(-\beta,0] \cap \mathbb{R}^-. \end{array}$$

Another important property of Pisot quadratic units β is that $\mathbb{Z}_\beta$ is a Meyer set. More precisely, it has been proved in [55] that

$$\begin{array}{ll} \text{in the simple Parry case,} & \mathbb{Z}_\beta - \mathbb{Z}_\beta \subset \mathbb{Z}_\beta + \{0, \pm(1-\frac{1}{\beta})\}, \\ \text{in the non-simple Parry case,} & \mathbb{Z}_\beta - \mathbb{Z}_\beta \subset \mathbb{Z}_\beta + \{0, \pm\frac{1}{\beta}\}. \end{array}$$

In analogy with Hof's results for C&P sets, together with the fact that $\mathbb{Z}_\beta$ is a Meyer set, we expect the diffraction spectrum of $\mathbb{Z}_\beta$ in the case of quadratic Pisot units β to be pure point. Our expectation is correct, as justified by the result on dynamical spectra cited in Section 12.2. Let us recall a method by Gazeau and Verger-Gaugry from [59] of determining the diffraction spectrum support and the values of intensity. This method works even for weighted Dirac combs supported by $\mathbb{Z}_\beta = \{b_n \mid n \in \mathbb{Z}\}$ for a quadratic Parry unit β.

We illustrate the method only for simple Parry units since the non-simple case is an analogy. Let us consider the Dirac comb $\mu = \sum_{n\in\mathbb{Z}} \delta_{b_n}$. According to Appendix B, μ is a translation bounded measure. In consequence, μ is a tempered measure and its Fourier transform

$$\widehat{\mu}(q) = \sum_{n\in\mathbb{Z}} e^{-2\pi i q b_n} \tag{12.1}$$

is a tempered distribution. With the help of Proposition 10.0.4, we can express the Fourier exponential in (12.1) for $n \geq 0$ as follows

$$e^{-2\pi i q b_n} = e^{-2\pi i q n c_\beta}\, e^{-2\pi i q \frac{1}{\beta}\left\{\frac{n}{\beta}\right\}}. \tag{12.2}$$

The function $x \to \{x\}$ is periodic of period 1, so is the piecewise continuous function $e^{-iq\alpha\{x\}}$. We expand (12.2) in Fourier series:

$$e^{-2\pi i q b_n} = e^{-2\pi i q n c_\beta} \sum_{m\in\mathbb{Z}} c_m(q)\, e^{2\pi i m\left\{\frac{n}{\beta}\right\}}, \tag{12.3}$$

where the coefficients may be easily calculated and the convergence is punctual in all non-integer points; in particular, it is punctual in all points $\left\{\frac{n}{\beta}\right\}$. Since

$$e^{2\pi i m\{x\}} = e^{2\pi i m x}\, e^{-2\pi i m\lfloor x\rfloor} = e^{2\pi i m x},$$

we get the following Fourier expansion:

$$e^{-2\pi i q b_n} = \sum_{m\in\mathbb{Z}} c_m(q)\, e^{-2\pi i n\left(qc_\beta - \frac{m}{\beta}\right)}. \tag{12.4}$$

Finally, implanting (12.4) in (12.1) and exchanging the order of summation, we obtain the following expression (to be understood in the weak sense):

$$\widehat{\mu}(q) = \sum_{m\in\mathbb{Z}} c_m(q) \sum_{n\in\mathbb{Z}} e^{-2\pi i n c_\beta\left(q - \frac{1}{c_\beta}\frac{m}{\beta}\right)}. \tag{12.5}$$

Finally, applying a well-known equality (in the distributional sense) mentioned in Example B.0.4 in Appendix B, we are led to the following formula for the Fourier transform of μ:

$$\widehat{\mu}(q) = \frac{1}{c_\beta} \sum_{m,n\in\mathbb{Z}} c_m(q)\delta(q - \tfrac{1}{c_\beta}\tfrac{m}{\beta} - \tfrac{n}{c_\beta}). \tag{12.6}$$

The right-hand side of the above equality is a translation bounded measure. Unfortunately, the equality is to be understood in the weak, not vague sense. At this moment, we are forced to leave a rigorous way, provided we want to continue the description of the diffraction spectrum. In accordance with a popular, but never proved, conjecture of Bombieri and Taylor [20], the right-hand side of (12.6) and the diffraction measure $\hat{\gamma}$ have the same support, and, moreover, $|\hat{\mu}(\{x\})|^2 = \hat{\gamma}(\{x\})$ for each point $x \in \mathbb{R}$. Knowing that the diffraction spectrum is pure point, this conjecture leads to its complete description.

To conclude, let us give some instructions for possible further investigation of the diffraction spectra of the set $\mathbb{Z}_\beta = \{b_n \mid n \in \mathbb{Z}\}$ for Parry numbers β in general. The above described method for the transformation of the Fourier transform of μ into a weighted Dirac comb, in the distributional sense, is based on a precise formula for the n-th β-integer in the case of Pisot quadratic units β. To be specific, it is important to have the following form $b_n = c_\beta n + \{\alpha(n)\}$. We have provided a precise formula for b_n in both simple (10.12) and non-simple (10.22) Parry case. The only problem, but probably very hard to solve, is the dependence of the formula for b_n on the β-expansion of b_n. We propose to start with some concrete examples of quadratic non-unit Parry numbers.

Chapter 13

Conclusion and open problems

This thesis embodies three main areas of interest – combinatorics, arithmetics, and application in physics of β-integers. We do not want to sum up again the most important results since it has been already done in details in the preface. We use this place instead as a list of open problems and perspectives of further research on β-integers, ordered in accordance with the three studied domains.

Combinatorics

The complexity of infinite words u_β associated with Parry numbers β has been determined so far only for confluent simple Parry numbers, simple Parry numbers with the Rényi expansion $d_\beta(1) = t_1 t_2 \dots t_m$ with $t_1 > \max\{t_2, \dots, t_{m-1}\}$, and quadratic non-simple Parry numbers. It is desirable to derive the complexity, or, at least, to describe special factors of infinite words u_β associated with Parry numbers β for more classes of Parry numbers. This task seems to be rather difficult and technical, but it is still possible to search for suitable upper and lower bounds on the complexity $\mathcal{C}(n)$, eventually only for large lengths n, of infinite words u_β associated with Parry numbers.

The palindromic complexity has been derived for infinite words u_β associated with confluent simple Parry numbers and with quadratic non-simple Parry numbers. These are the only classes of β for which the language $\mathcal{L}(u_\beta)$ is closed under reversal. It is a largely open problem to deduce the palindromic structure for the other Parry numbers; hence, for infinite words u_β containing only a finite number of distinct palindromes.

The equivalence of the notion of fullness and opulence has been proved for all infinite words with language closed under reversal. It would be interesting to show whether this result may be extended for all recurrent words.

We have characterized infinite words with m return words for every factor, in terms of complexity and bispecial factors, for $m = 3$. We have also pointed out that this characterization does not hold for $m \geq 4$. It is therefore challenging to find another characterization for $m \geq 4$ as elegant as the one we provided for $m = 3$.

Observing the evolution of reduced Rauzy graphs of infinite words u_β associated with quadratic non-simple Parry numbers, we have obtained the sets of their factor frequencies. It is possible to use an analogous method also for other infinite words u_β. However, it is not at all evident how to avoid technicalities.

The only Parry numbers β, for which an optimal balance bound on u_β has been found, are the quadratic ones. We have proposed a method which may be applied also for Parry numbers of higher degrees.

Arithmetics

We have highlighted close relation between the balance property and arithmetical properties of β-integers for quadratic non-simple Parry numbers β. It is our great wish to show that such proximity of combinatorics and arithmetics has much more general validity.

We have shown that the maximal number $L_\oplus(\beta)$ of β-fractional positions which may occur if two β integers are added, provided the sum has a finite β-expansion, is bounded from below and from above as follows

$$\left\lfloor \tfrac{p-1}{q} \right\rfloor \leq L_\oplus(\beta) \leq \left\lceil \tfrac{p}{q} \right\rceil .$$

We aim to confirm our conjecture that $L_\oplus(\beta) = \lfloor \frac{p-1}{q} \rfloor$. It would be convenient to deduce also a good upper and lower bound on $L_\otimes(\beta)$ for quadratic non-simple Parry numbers. More generally, good estimates on $L_\oplus(\beta)$ and $L_\otimes(\beta)$ are desirable for Parry numbers of higher degrees as well.

Application in physics

We studied the asymptotic behavior of β-integers for Parry numbers β. We have stated that the n-th β-integer b_n behaves asymptotically as $c_\beta n$ for all Parry numbers β and that the sequence $(b_n - c_\beta n)$ is bounded for Pisot numbers β having the same minimal and Parry polynomial. We conjecture that this implication may be reversed. Our further aim is to study the asymptotic behavior of β-integers also for non-Parry algebraic numbers β. Among non-Parry numbers, one may distinguish two cases:

• If the length of blocks of zero's in $d_\beta(1)$ is bounded, say by a length L, then the β-integers form a Delone set since the shortest distance between consecutive points is at least $\frac{1}{\beta^L}$ and the largest distance is 1.

• If $d_\beta(1)$ contains strings of zero's of unbounded length, then the set of distances between consecutive β-integers have 0 as its accumulation point, see Equation (2.8). It means that in this case, the β-integers do not form a Delone set.

The first question to be answered in both cases is whether the limit b_n/n does exist for some non-Parry numbers β. We think that the following two references will be very helpful in the advanced study of asymptotic behavior of β-integers: Schmidt [100] in case of Salem numbers β and Gazeau and Verger-Gaugry [60] in case of Perron numbers β.

We have indicated in our treatise on diffraction that the method revealing the diffraction spectra of β-integers for quadratic Parry units might be extended to general Parry numbers, using the results concerning their asymptotic behavior. Another widely open problem is to prove the Bombieri-Taylor conjecture for a larger class of measures μ. So far, a result of Hof claims that this conjecture holds under the hypothesis that $\hat{\mu}$ is a translation bounded measure. However, this problem is out of our sphere of activity. It concerns theory of distributions and measure theory.

We have dealt with one more possible application in physics – infinite words u_β associated with Parry numbers β as models of potentials of discrete Schrödinger operators. If a Schrödinger operator with aperiodic potential has a purely singular continuous spectrum, then its potential models a quasicrystalline material. So far, all examined Schrödinger operators with potentials generated by primitive substitutions have had this type of spectrum. Therefore, we tend to show for all Schrödinger operators with potentials generated by infinite words u_β associated with Parry numbers β that their spectrum is purely singular continuous. We have solved this problem only partially.

In an “idle land” state has remained an eventual application of the results of this thesis for random number generators and in non-standard wavelet analysis.

Appendix A

Glance at functional analysis

We will indeed only take a glance at a specific part of functional analysis. We assume that the reader is familiar with basic notions from functional analysis and measure theory. For details, proofs, and more general statements of theorems, [97] is recommended for consultation.

The main aim is to sketch out a decomposition of the spectrum of a linear bounded operator on a Hilbert space, interesting from the point of view of quantum mechanics, in particular, for the study of discrete Schrödinger operators.

Let $\mathcal{X}$ be a Banach space and $\mathcal{B}(\mathcal{X})$ the Banach algebra of bounded operators on $\mathcal{X}$. A complex number λ belongs to the *spectrum* $\sigma(T)$ of an operator $T \in \mathcal{B}(\mathcal{X})$, if $T - \lambda I$ has no bounded inverse. Spectrum $\sigma(T)$ is a compact non-empty subset of $\mathbb{C}$. Three mutually disjoint subsets of $\sigma(T)$ are usually distinguished according to the reason of non-inversibility of $T - \lambda I$: point spectrum $\sigma_p(T)$ consisting of eigenvalues of T, continuous spectrum $\sigma_c(T)$, and residual spectrum $\sigma_r(T)$.

If $\mathcal{H}$ is a complex Hilbert space, we may introduce the continuous functional calculus, which enables us, for a fixed self-adjoint operator $T \in \mathcal{B}(\mathcal{H})$, to associate with a vector $h \in \mathcal{H}$ the so-called spectral measure μ_h via the Riesz-Markov representation theorem. Then, applying a refined Lebesgue decomposition theorem, we decompose the spectral measure μ_h. Finally, having extended the continuous functional calculus to the Borel functional calculus, we may translate the measure decomposition to the searched spectral decomposition.

Self-adjoint operator

We recall that the *adjoint operator* T^* of an operator $T \in \mathcal{B}(\mathcal{H})$ is defined by

$$\langle x, T^* y\rangle := \langle Tx, y\rangle \quad \text{for all } x, y \in \mathcal{H},$$

where $\langle x, y\rangle$ denotes the scalar product of $x, y \in \mathcal{H}$. It is easy to verify that $\sigma_r(T) \subset \sigma_p(T^*) \subset \sigma_r(T) \cup \sigma_p(T)$. In particular, for a *self-adjoint* operator $T = T^*$, it holds $\sigma(T) \subset \mathbb{R}$ and $\sigma_r(T) = \emptyset$ and the norm of T is equal to the *spectral radius*

$$||T|| = \sup_{\lambda \in \sigma(T)} |\lambda|.$$

Continuous functional calculus

Two most important ingredients of the continuous functional calculus are:

1. If T is self-adjoint, then, for any polynomial p, the operator norm obeys

$$||p(T)|| = \sup_{\lambda \in \sigma(T)} |p(\lambda)|.$$

2. The Stone-Weierstrass theorem stating that the family of polynomials (with complex coefficients) is dense in $C(\sigma(T))$, the complex continuous functions on $\sigma(T)$.

When endowed with the supremum norm, $C(\sigma(T))$ is a Banach space. So the mapping $p \to p(T)$ is an isometric homomorphism from a dense subset of $C(\sigma(T))$ to the Banach space $\mathcal{B}(\mathcal{H})$. Extending the mapping by continuity gives a bounded linear operator, called the *continuous functional calculus*, defined, for every $f \in C(\sigma(T))$, by

$$f \to f(T) := \lim_{n\to\infty} p_n(T),$$

where $(p_n)_{n\in\mathbb{N}}$ is a sequence of polynomials such that $p_n \underset{n\to\infty}{\to} f$ uniformly.

Riesz-Markov representation theorem

For a fixed $h \in \mathcal{H}$ and a fixed self-adjoint operator $T \in \mathcal{B}(\mathcal{H})$, the functional $f \to \langle h, f(T)h\rangle$ is a positive linear functional on $C(\sigma(T))$. *Positivity* means that if $f(x) \geq 0$ for all $x \in \sigma(T)$, then $\langle h, f(T)h\rangle \geq 0$.

We recall the Riesz-Markov representation theorem restricted to real compact spaces.

Theorem A.0.2 (Riesz-Markov representation theorem)**.** *Let Y be a real compact space. For any positive linear functional ψ on $C(Y)$, there is a unique non-negative Borel regular measure μ on Y such that $\psi(f) = \int_Y f d\mu$ for all $f \in C(Y)$.*

Regularity of the measure μ means that for every Borel set E in Y, we have $\mu(E) = \inf\{\mu(U) \mid E \subset U \subset Y,\, U \text{ open}\}$, or, equivalently, $\mu(E) = \sup\{\mu(K) \mid K \subset E,\ K \text{ compact}\}$.

According to the Riesz-Markov representation theorem, there exists a unique non-negative Borel regular measure μ_h on $\sigma(T)$ such that

$$\int_{\sigma(T)} f d\mu_h = \langle h, f(T)h\rangle$$

for all $f \in C(\sigma(T))$. This measure is sometimes called the *spectral measure* associated with $h \in \mathcal{H}$.

Borel functional calculus

The spectral measures can be used to extend the continuous functional calculus to the Borel functional calculus, i.e., to define $g(T) \in \mathcal{B}(\mathcal{H})$ for every bounded Borel function g on $\mathbb{R}$. We may define, for every bounded Borel measurable function g,

$$\langle h, g(T)h\rangle := \int_{\sigma(T)} g d\mu_h.$$

Then, using the polarization identity for the scalar product on $\mathcal{H}$

$$\begin{aligned} 4\langle k, g(T)h\rangle &= \langle k+h, g(T)(k+h)\rangle - \langle k-h, g(T)(k-h)\rangle - \\ &\quad -i\langle k+ih, g(T)(k+ih)\rangle + i\langle k-ih, g(T)(k-ih)\rangle, \end{aligned}$$

we get the value of $\langle k, g(T)h\rangle$ for every $k \in \mathcal{H}$, which determines uniquely $g(T)h$.

Lebesgue decomposition theorem

Suppose μ is a non-negative Borel measure on $\mathbb{R}$. Denote by S the set of pure points of μ, i.e., $S = \{x \in \mathbb{R} \mid \mu(\{x\}) \neq 0\}$. Since μ is a Borel measure ($\mu(K) < \infty$ for any compact set $K \subset \mathbb{R}$), S is a countable set. Define $\mu_{pp}(E) := \mu(E \cap S) = \sum_{x \in E \cap S} \mu(\{x\})$ for every Borel set $E \subset \mathbb{R}$. Then, μ_{pp} is a non-negative Borel measure on $\mathbb{R}$. In addition, define $\mu_c := \mu - \mu_{pp}$. It is also a non-negative Borel measure with the property $\mu_c(\{x\}) = 0$ for all $x \in \mathbb{R}$ (it has no pure points). It implies that any non-negative Borel measure μ on $\mathbb{R}$ may be uniquely decomposed into a sum $\mu = \mu_{pp} + \mu_c$, where μ_c is a *continuous* measure, i.e., μ_c has no pure points, while μ_{pp} is a *pure point* (also called *discrete*) measure, i.e., $\mu_{pp}(E) = \sum_{x \in E} \mu_{pp}(\{x\})$ for every Borel set $E \subset \mathbb{R}$.

Consider the Lebesgue measure λ on $\mathbb{R}$. We say that μ is *absolutely continuous* with respect to the Lebesgue measure λ, we write $\mu \ll \lambda$, if $\mu(E) = 0$ whenever $\lambda(E) = 0$ for a Borel set $E \subset \mathbb{R}$. Whereas μ and λ are mutually *singular*, we write $\mu \perp \lambda$, if there exists a Borel set $E \subset \mathbb{R}$ such that $\mu(E) = 0 = \lambda(\mathbb{R} - E)$.

Let us recall a refinement of the Lebesgue decomposition theorem.

Theorem A.0.3 (Lebesgue decomposition theorem)**.** *Let μ be a non-negative Borel measure on $\mathbb{R}$ and λ the Lebesgue measure. Then the following statements hold:*

- *There exists a unique decomposition*

$$\mu = \mu_{ac} + \mu_s, \quad \mu_{ac} \ll \lambda, \quad \mu_s \perp \lambda.$$

- *The decomposition may be refined by*

$$\mu_s = \mu_{sc} + \mu_{pp},$$

  where μ_{sc} is continuous and μ_{pp} is pure point.

In the previous theorem, μ_{sc} is called *singular continuous* part of μ since it is the continuous part of the singular component of μ.

Let $h \in \mathcal{H}$ and μ_h be the corresponding spectral measure on $\sigma(T)$. Clearly, μ_h is a finite non-negative Borel measure, and, similarly, the restriction of the Lebesgue measure λ to $\sigma(T)$ is a finite non-negative Borel measure on $(\sigma(T), \mathcal{B}_{\sigma(T)})$. According to the Lebesgue decomposition theorem, μ_h can be decomposed as:

$$\mu_h = \mu_{ac} + \mu_{sc} + \mu_{pp},$$

where μ_{ac} is absolutely continuous with respect to the Lebesgue measure λ, μ_{sc} and μ_{pp} are singular with respect to λ, μ_{sc} is a continuous measure, and μ_{pp} is a pure point measure.

Orthogonal decomposition of Hilbert space

Choose any $h \in \mathcal{H}$ and a self-adjoint operator $T \in \mathcal{B}(\mathcal{H})$ and consider the associated spectral measure $\mu := \mu_h$. Let us recall that the *support* of a Borel measure μ on $\mathbb{R}$ is defined to be the set of all points x in $\mathbb{R}$ for which every open neighborhood of x has positive measure, i.e., supp $\mu := \{x \in \mathbb{R} \mid x \in N \text{ open in } \mathbb{R} \Rightarrow \mu(N) > 0\}$. Support of any measure is a closed, therefore a Borel set. Since measures $\mu_{ac}, \mu_{sc}, \mu_{pp}$ are mutually singular, they have mutually disjoint supports M_{ac}, M_{sc}, M_{pp}.

We define $\mathcal{H}_{ac} = \chi_{M_{ac}}(T)\mathcal{H}$, $\mathcal{H}_{sc} = \chi_{M_{sc}}(T)\mathcal{H}$, and $\mathcal{H}_{pp} = \chi_{M_{pp}}(T)\mathcal{H}$, where χ_E denotes the characteristic function of E. It is easy to see that $\mathcal{H}_{ac}$ consists of vectors whose spectral measure is absolutely continuous with respect to the Lebesgue measure. Similarly for $\mathcal{H}_{sc}$ and $\mathcal{H}_{pp}$. These spaces are linear and mutually orthogonal. Moreover $\chi_{M_{ac}}(T)+\chi_{M_{sc}}(T)+\chi_{M_{pp}}(T) = I$. We deduce that

$$\mathcal{H} = \mathcal{H}_{ac} \oplus \mathcal{H}_{sc} \oplus \mathcal{H}_{pp}.$$

Spectral decomposition with respect to spectral measure

Let us now study the spectra of restrictions of T to $\mathcal{H}_{ac}, \mathcal{H}_{sc}$, and $\mathcal{H}_{pp}$. They form the searched decomposition of spectrum $\sigma(T)$. The restrictions make sense since $\mathcal{H}_{ac}, \mathcal{H}_{sc}$, and $\mathcal{H}_{pp}$ are T-invariant. Spectrum of T restricted to

1. $\mathcal{H}_{ac}$ is called the *absolutely continuous spectrum* of T, $\sigma_{ac}(T)$,
2. $\mathcal{H}_{sc}$ is called the *singular continuous spectrum* of T, $\sigma_{sc}(T)$,
3. $\mathcal{H}_{pp}$ is called the *pure point spectrum* of T, $\sigma_{pp}(T)$.

The point spectrum of T fulfills $\overline{\sigma_p(T)} = \sigma_{pp}(T)$. In consequence, the spectrum of T is a union of the following form

$$\sigma(T) = \sigma_{ac}(T) \cup \sigma_{sc}(T) \cup \overline{\sigma_p(T)}.$$

Appendix B

Mathematical diffraction theory

The answer to the question which distributions of matter diffract is still incomplete, and many results are heuristic, short of rigorous mathematical explanation. Here, we prefer to focus on basic and rigorous mathematical theory of diffraction. This section is entirely inspired by Baake's lecture notes [8].

Mathematical diffraction theory is concerned about the spectral properties of the Fourier transform of the autocorrelation measure of translation bounded complex measures. Let us therefore first introduce and discuss the notions involved. We will restrict ourselves to one-dimensional sets since we consider exclusively one-dimensional models of quasicrystals.

Translation bounded measures

Let $C_c(\mathbb{R})$ be the space of complex-valued continuous functions with compact support. A complex measure μ on $\mathbb{R}$ is a linear functional on $C_c(\mathbb{R})$ with the additional condition that for every compact set $K \subset \mathbb{R}$, there is a constant a_K such that

$$|\mu(f)| \leq a_K ||f||_\infty$$

for every $f \in C_c(\mathbb{R})$ with support in K, here $||f||_\infty = \sup_{x \in K} |f(x)|$ is the supremum norm of f. The term "complex measure" for such a linear functional is adequate: the Riesz-Markov representation theorem A.0.2 claims that complex measures as defined above are in a one-to-one correspondence with regular complex Borel measures. In particular, we write $\mu(A)$ (measure of a set) and $\mu(f)$ (measure of a function) for simplicity. A measure μ is called *positive* if $\mu(f) \geq 0$ for all $f \geq 0$. For every measure μ, there is a smallest positive measure, denoted by $|\mu|$, such that $|\mu(f)| \leq |\mu|(f)$ for all non-negative $f \in C_c(\mathbb{R})$, and $|\mu|$ is called the *total variation* (or *absolute value*) of μ. For our purposes, it is convenient to work with a subset of complex measures. A measure μ is said to be *translation bounded* if for every compact $K \subset \mathbb{R}$ there is a constant $b_K > 0$ such that

$$\sup_{x \in \mathbb{R}} |\mu|(x + K) \leq b_K.$$

For instance, if Λ is a uniformly discrete set, the weighted Dirac comb

$$\mu_\Lambda = \sum_{x \in \Lambda} w(x) \delta_x, \tag{B.1}$$

where δ_x is the Dirac measure at point x, is clearly translation bounded if the coefficients $w(x)$ satisfy $\sup_{x \in \Lambda} |w(x)| < \infty$.

Autocorrelation

If f and g are in $C_c(\mathbb{R})$, one can define their *convolution* by

$$(f * g)(x) := \int_{\mathbb{R}} f(x-y)g(y)dy,$$

which can be extended to the case of one function bounded and the other one integrable. Recall that the convolution of two measures μ and ν is again a measure, given by

$$(\mu * \nu)(f) := \int_{\mathbb{R}\times\mathbb{R}} f(x+y)d\mu(x)d\nu(y),$$

which is well defined if at least one of the two measures has compact support, or is a finite measure, while the other is translation bounded.

For $R > 0$, let $I_R = [-R, R]$ and denote μ_R the restriction of a measure μ to the interval I_R. Denote by $\tilde{\mu}$ the measure associated with a measure μ by $\tilde{\mu}(f) = \overline{\mu(\tilde{f})}$ for every $f \in C_c(\mathbb{R})$, where $\tilde{f}(x) = \overline{f(-x)}$ for all $x \in \mathbb{R}$. Since μ_R has compact support,

$$\gamma_R := \frac{\mu_R * \tilde{\mu}_R}{2R}$$

is well defined. Let us define vague convergence. We say that a measure γ is a vague limit of γ_R if for every $f \in C_c(\mathbb{R})$, we have $\gamma(f) = \lim_{R\to\infty} \gamma_R(f)$. Every vague limit point of γ_R, as $R \to \infty$, is called an *autocorrelation* of μ. If the limit of γ_R exists, the unique autocorrelation is called the *natural autocorrelation* of μ and is denoted γ_μ. If the natural autocorrelation of a translation bounded measure exists, it is known to be also translation bounded. Let us mention that adding or removing finitely many points from Λ, or points of density 0, does not change γ_μ, if it exists. Let us focus on the weighted Dirac comb μ defined in (B.1) with Λ being a discrete set of finite local complexity (thus a uniformly discrete set). Let us assume for the moment that its natural autocorrelation γ_μ exists and is unique (this is not always true, as shown by a counterexample constructed by Lagarias and Pleasants in [77]). A simple calculation shows that $\tilde{\mu} = \sum_{x\in\Lambda} \overline{w(x)}\delta_{-x}$. Since $\delta_x * \delta_y = \delta_{x+y}$, we get

$$\gamma_\mu = \sum_{z\in\Lambda-\Lambda} \eta(z)\delta_z, \tag{B.2}$$

where the autocorrelation coefficient $\eta(z)$, for $z \in \Lambda - \Lambda$, is given by the limit

$$\eta(z) = \lim_{R\to\infty} \frac{1}{2R} \sum_{\substack{x \in \Lambda \cap I_R, \\ x - z \in \Lambda}} w(x)\overline{w(x-z)}.$$

Conversely, if the above limit exists for all $z \in \Lambda$, the natural autocorrelation exists, too, because $\Lambda - \Lambda$ is discrete and closed by assumption, and (B.2) thus uniquely defines a translation bounded measure of positive type. This is one of the advantages of using sets of finite local complexity.

Fourier transform and distributions

The Fourier transform will enable us to tie the previous with the theory of tempered distributions. Let $\mathcal{S}(\mathbb{R})$ be the space of Schwartz functions, i.e., rapidly decreasing C^∞-functions. This space certainly contains all C^∞-functions with compact support, but also functions such as $p(x)\exp(-x^2)$, where p is an arbitrary polynomial. By the Fourier transform of a Schwartz function ψ, we mean

$$(\mathcal{F}\psi)(x) = \hat{\psi}(x) := \int_{\mathbb{R}} e^{2\pi ixy}\psi(y)dy,$$

which is again a Schwartz function. The Fourier transform $\mathcal{F}$ is a linear bijection from $\mathcal{S}(\mathbb{R})$ onto itself, and is bi-continuous. The Fourier transform of convolution takes a simple form $(\widehat{\psi_1 * \psi_2}) = \hat{\psi}_1 \cdot \hat{\psi}_2$.

A *tempered distribution* is a continuous linear functional on the Schwartz space. According to the definition of Schwartz space, it is obvious that every tempered distribution is also a "classical" distribution, i.e., a continuous linear functional on C^∞-functions with compact support. The definition of the Fourier transform of a tempered distribution T is given by

$$\hat{T}(\psi) := T(\hat{\psi}) \quad \text{for all } \psi \in \mathcal{S}(\mathbb{R}).$$

The weak convergence of tempered distributions $T_n \to T$ implies the weak convergence of their Fourier transforms $\hat{T}_n \to \hat{T}$. By weak convergence, we mean $\lim_{n\to\infty} T_n(\psi) = T(\psi)$ for all $\psi \in \mathcal{S}(\mathbb{R})$.

Example B.0.4. *The Fourier transform of the Dirac measure δ_x at x is given for all $\psi \in \mathcal{S}(\mathbb{R})$ by*

$$\hat{\delta}_x(\psi) = \int_{\mathbb{R}} e^{-2\pi ixy}\psi(y)dy,$$

which rewritten in the distributional sense reads $\hat{\delta}_x(y) = e^{-2\pi ixy}$.

The so-called Dirac comb $\delta_\Gamma = \sum_{x\in\Gamma}\delta_x$, where Γ is a lattice, i.e., $\Gamma = \{\alpha n \mid n \in \mathbb{Z}\}$ for some $\alpha > 0$, obeys the Poisson summation formula for distributions

$$\hat{\delta}_\Gamma = \tfrac{1}{\alpha}\delta_{\Gamma^*},$$

where Γ^* is the reciprocal lattice, i.e., $\Gamma^* = \{\frac{n}{\alpha} \mid n \in \mathbb{Z}\}$. From the previous two equalities, we deduce the following equality, to be understood in the distributional sense

$$\sum_{k\in\Gamma} e^{-2\pi ixk} = \tfrac{1}{\alpha}\delta_{\Gamma^*}(x).$$

Measures and distributions

Measures are defined as linear functionals on continuous functions of compact support, while tempered distributions as linear functionals on the Schwartz space.

Measures need not be tempered distributions. In the case that a measure is a tempered distribution as well, we call it a *tempered measure*. Every translation bounded measure is tempered, so this does not cause any problem in our study.

Conversely, a tempered distribution need not define a measure. If we start with a tempered measure μ, then its Fourier transform need not be a measure. However, if μ is of *positive type* (also called *positive definite*) in the sense that $\mu(\psi * \tilde{\psi}) \geq 0$ for all $\psi \in \mathcal{S}(\mathbb{R})$, then $\hat{\mu}$ is a positive measure by the Bochner-Schwartz theorem. Every autocorrelation γ is, by construction, a measure of positive type, so that $\hat{\gamma}$ is a positive measure. We will call $\hat{\gamma}$ the *diffraction measure*. The observed intensity pattern is represented by this positive measure $\hat{\gamma}$ that tells us which amount of intensity is present in a given volume.

Decomposition of measures

Taking the Lebesgue measure as a reference, the Lebesgue decomposition theorem A.0.3 allows us to decompose the positive measure $\hat{\gamma}$ uniquely into three parts,

$$\hat{\gamma} = \hat{\gamma}_{pp} + \hat{\gamma}_{sc} + \hat{\gamma}_{ac},$$

where the most interesting part is the most countable set $\hat{\gamma}_{pp}$, called the *Bragg part of the spectrum*. If the spectrum of $\hat{\gamma}_{\mu}$ consists only of Bragg peaks, then μ corresponds to a crystalline structure. The absolutely continuous part $\hat{\gamma}_{ac}$ is usually called *diffuse scattering* in crystallography, and, logically, describes the diffuse background of the diffraction image. The term “singular continuous” does not appear in the standard crystallographic literature.

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